

Nonequilibrium Statistical Mechanics: Stochastic thermodynamics and heat conduction in low dimensional systems

A Thesis

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by

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Certificate

This is to certify that this dissertation entitled Nonequilibrium Statistical Mechanics: Stochastic thermodynamics and heat conduction in low dimensional systems towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research, Pune represents study carried out by Sambit Ratha at IISER Pune under the supervision of Prof. Deepak Dhar, Department of Physics, IISER Pune during the academic year 2018-2019.



Professor Deepak Dhar



Sambit Ratha

Declaration

I hereby declare that the matter embodied in the report entitled Nonequilibrium Statistical Mechanics: Stochastic thermodynamics and heat conduction in low dimensional systems are the results of the work carried out by me at the Department of Physics, Indian Institute of Science Education and Research, Pune, under the supervision of Prof. Deepak Dhar and the same has not been submitted elsewhere for any other degree.



Professor Deepak Dhar



Sambit Ratha

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Sambit Ratha
Pune, 2019

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Abstract

I review the main results of stochastic thermodynamics, for systems under external driving or in a nonequilibrium steady state. These include *Crook's identity*, *Jarzynski relation* and *Gallovati-Cohen fluctuation theorem*. These give the ratio of probability of entropy production for a trajectory of the system to that of the time-reversed trajectory, and therefore can be thought of as a natural generalization of the second law of thermodynamics. After outlining the derivations of these results, various sources of entropy productions are illustrated for the exclusion process. Though the theorems are valid under very general conditions, their applicability is restricted as the quantities appearing are not always directly measurable. However, one recovers near-equilibrium results as limiting cases.

The second part of the thesis is a review of calculations of thermal conductivity for some low dimensional models. The first is a chain of identical harmonic oscillators, with nearest-neighbour interactions, coupled at its ends to stochastic reservoirs at different temperatures. The system is found to have infinite thermal conductivity in the thermodynamic limit. A more realistic model, the harmonic chain with mass disorder is considered next, and the dependence of thermal conductivity on system size L is found to be \sqrt{L} . Lastly the disordered Lorentz gas is shown to have finite thermal conductivity.

1 Introduction

Equilibrium statistical mechanics provides us the methods to identify and describe the behaviour of macroscopic degrees of freedom of a system in thermal equilibrium in terms of the microscopic ones, and its success can not be overstated. It is well-established for systems that are sufficiently large and relax at time scales sufficiently fast compared to observation times. In this thesis, I have tried to explore problems that are not addressed by the methods of equilibrium statistical mechanics, in particular stochastic thermodynamics and heat transport in low dimensional systems. The following subsections are summaries of well established results, which will be elaborated upon in the rest of the thesis.

In this thesis, my focus is exclusively on classical systems. Throughout, the Boltzmann constant is taken to be 1. Therefore entropy is a dimensionless quantity and temperature has units of energy.

1.1 Stochastic thermodynamics

Stochastic thermodynamics is a broad framework which emerged as an attempt to extend the success of equilibrium statistical mechanics for system far from equilibrium. Where as in equilibrium, the probability of observing a micro-state is given by a distribution over suitable ensemble, no such formulae valid in general are known if a parameter of the system is externally driven, or if the system is brought in contact with multiple reservoirs. The micro-state of the system now undergoes stochastic evolution. The specification of the driving protocol or baths prescribes a path (time evolution of microstate) ensemble. Physical quantities such as work, heat, entropy change etc., being functionals of the trajectory followed by the system, are also random variables.

Consider a system in contact with heat bath under time dependent forcing. To discuss *irreversibility*, one can define a conjugate *time-reversed* trajectory corresponding to each trajectory. Although the probability of observing a trajectory is not known, it has been proven, under some assumptions, that the ratio of probabilities of observing a trajectory to that of observing the conjugate trajectory is given by the exponential of the entropy produced in the trajectory. Section 2.1 elaborates on this result due to Crooks [1], detailing definitions and assumptions involved, along with a short proof. This leads to a relation between the equilibrium free energy and the nonequilibrium average $\langle \exp(-\beta W) \rangle$, W, β denoting the work and inverse temperature. This was one of the earliest exact result valid arbitrarily far from equilibrium [2]. As reliable measurements of $\langle \exp(-\beta W) \rangle$ for

large systems are not feasible, the full scope of this result is not yet explored.

If the physical quantity under consideration is a time-integral over contributions throughout the trajectory (e.g. currents), its probability, over a long-run of the process, depends exponentially on the time-span, with a rate called the *rate function* [3]. Thus after a long run of the process the problem of finding moments of currents, and describing transport properties of the system, reduces to the task of evaluating the rate function. Though this is a formidable task in general, for the observable *entropy flow* a certain symmetry property of this function is known. Section 2.3 deals with the formulation of this result. It will be shown that the ratio of probability of a value of entropy production, to the probability of the negative of that value, is exponential of the value of entropy production [4], similar to the statement of Crook's identity.

Although these so called *fluctuation theorems* are derived in considerable generality (in fact, the only major assumption is that the micro-states evolve as a Markov process), the interpretation of entropy production can be rather obscure. Section 2.4 is on an example in which the entropy production has a clear meaning. Finally, a proof of the well-known *Kubo-Green* expression of conductivity is presented in Section 2.5. This demonstrates that, when nonequilibrium effects can be treated perturbatively, the results given here encapsulate linear response.

1.2 Heat conduction

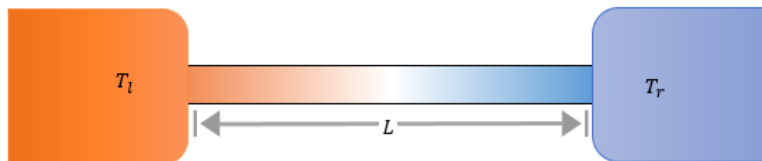


Figure 1: Schematic diagram of a heat conductor in steady state

Systems not in equilibrium are characterized by the presence of non-vanishing currents, arising due to inhomogeneities of corresponding physical quantity. In general, there is no statistical mechanical procedure for predicting the probability distributions of these currents, and one often aims for a phenomenological description by postulating a linear response to the gradients that cause the flow. For instance, consider an isotropic system in contact with multiple heat baths at different temperatures at its boundaries, then assuming there is a clear separation

of microscopic and macroscopic scales of length and time, the local heat current density \mathbf{j} (heat flow per unit area per unit time) at point \mathbf{r} , at time t , is related to the local temperature T , by the well known phenomenological expression,

$$\mathbf{j}(\mathbf{r}, t) = -\kappa(T(\mathbf{r})) \nabla T(\mathbf{r}, t), \quad (1.2.1)$$

proposed by Joseph Fourier in the early 19th century. Here the phenomenological constant κ is the conductivity of the material at the local temperature T . In such a formulation, *local thermal equilibrium* is assumed i.e. the distribution of micro-states in a volume of size small compared to the system size yet macroscopic when compared to microscopic length scales, and over times much smaller compared to macroscopic observation times yet much larger than microscopic time scales, is an equilibrium distribution with the local temperature. This means the variations of thermodynamic quantities across these "mesoscopic" regions is small compared to the equilibrium fluctuations of these quantities in the region [18]. Though often taken as granted, the task of establishing its validity is quite non-trivial, and there are simple counter-examples where it is not valid [8]. Given (1.2.1), one can use local conservation of energy¹ to write the evolution of the temperature as

$$\frac{\partial T(\mathbf{r}, t)}{\partial t} = \frac{1}{c_V(T)} \nabla(\kappa(T) \nabla T(\mathbf{r}, t)), \quad (1.2.2)$$

with $c_V(T)$ the specific heat per unit volume.

A large number of attempts to derive (1.2.1) from the underlying microscopic dynamics of the system have been made [7][9][10]. One of the earliest kinetic justification for it runs as follows. Consider a system with a temperature gradient only in the x -direction. Local thermal equilibrium means a collision at (\mathbf{r}, t) results in an energy drawn from equilibrium (canonical) distribution of temperature $T(\mathbf{r}, t)$. Let the average energy density be given by $u(T(\mathbf{r}, t))$. The energy flux into an infinitesimal region to the right of a point at \mathbf{r} is the average energy carried by the particle times the x -component of the velocity of the particle, v_x . The average energy of the particle is its equilibrium value at last encountered collision, which, on an average, is at a distance of *mean free path*, λ away from \mathbf{r} . Similarly, the average energy leaving the region is $u(T(\mathbf{r}))v_x$. Both fluxes must be finally averaged over all incoming directions, $\hat{\mathbf{v}}$. Thus, the average current is

$$\mathbf{j}(\mathbf{r}, t) \sim \langle v_x u(T(\mathbf{r} - \lambda \hat{\mathbf{v}})) \rangle - \langle v_x u(T(\mathbf{r})) \rangle \sim c_V v \lambda \frac{\partial T(\mathbf{r})}{\partial x}.$$

¹assuming there is no other transport mechanism at play except conduction

The conductivity depends on temperature via its dependence on the specific heat, root mean square velocity v and mean free path of the carriers on temperature. For an ideal gas this goes as \sqrt{T} .

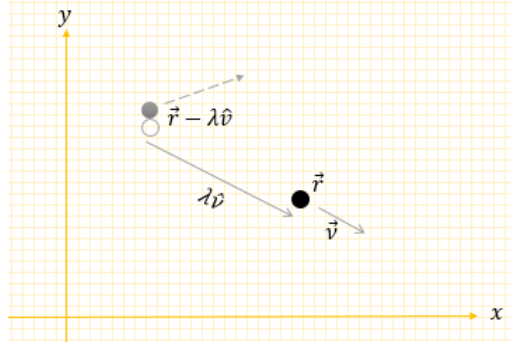


Figure 2: Random flight of a particle. The particle considered (in Black) underwent a collision (random event) with another (in Grey) to reach position \vec{r} with velocity \vec{v} .

This argument underscores that in essence, Fourier's law can be derived if we assume the dynamics of the heat carriers (*phonons* for an insulating solid, molecules for a fluid) to be a *Markovian* random walk: with correlations extending only as far back as the last collision. This assumption is not fully justified, and is in fact not always true, and the resulting transport is not always diffusive.

Let us assume that an one dimensional system has reached a nonequilibrium steady state between baths at temperatures $T, T + \Delta T$ at its two ends i.e. the current density j is independent of space and time. Then we have a precise definition of thermal conductivity at temperature T , for system length L as

$$\kappa(T) = \lim_{L \rightarrow \infty} \lim_{\Delta T \rightarrow 0} \frac{jL}{\Delta T}. \quad (1.2.3)$$

If this limit (in this order) does not exist, then the system does not obey Fourier's law. This means the current does not scale as L^{-1} for arbitrarily small temperature differences. The anomalous exponent α , defined as the scaling $\kappa \sim L^\alpha$, is non-zero.

Another expression for thermal conductivity, in the thermodynamic limit, with small temperature gradients (characteristic of linear response results) is the *Kubo*—

Green formula [17], given by

$$\kappa(T) = \frac{1}{2T^2} \lim_{t \rightarrow \infty} \lim_{L \rightarrow \infty} \int_0^t dt' \int_0^L dx \langle \hat{j}(x, t') \hat{j}(0, 0) \rangle_{eq} \quad (1.2.4)$$

The right hand side is an average over equilibrium distribution at T of the current density \hat{j} expressed as a function of microscopic degrees of freedom, for instance all phase space variables of constituent particles. In terms of the space-integrated current $\hat{q}(t) = \int_{-\infty}^{\infty} dx \hat{j}(x, t)$,

$$\kappa(T) = \frac{1}{2T^2} \int_0^{\infty} dt' \lim_{L \rightarrow \infty} \frac{1}{L} \langle \hat{q}(t') \hat{q}(0) \rangle_{eq}.$$

Note that the order of thermodynamic and long time limits is the same as in (1.2.4). Anomalous heat transport can now be seen as the result of *long-time tails*, or power-law decay of equilibrium current fluctuations.

Before proceeding, a few remarks on the derivation of the Kubo-green formula. [7] [10] have derivations which usually begin by assuming Fourier's law to be valid, or model temperature gradients as a perturbation to the Hamiltonian of the system, thereafter proceeding with standard techniques of linear response. I will present a derivation using the steady-state fluctuation theorem in Section 2.5. Local thermal equilibrium is assumed in all the derivations, however the derivation presented here has the advantage of having only one more assumption: the coupling to heat bath is Markovian, which is rather plausible.

In light of the above general discussion, it is seen that the thermal conductivity is divergent for many one or two dimensional models, and even in higher dimensions the necessary and sufficient conditions for its validity are not fully known. I reviewed three models, the first of which is the *Rieder-Lieb-Lebowitz* [11] model. This is simply a collection of nearest-neighbour coupled harmonic oscillators, with baths modelled by a Gaussian white-noise force acting on the ends (*Langevin* dynamics). As the energy of each normal mode is conserved, and the modes extend over the full length of system, the current does not decay with length, and conductivity is divergent with $\alpha = 1$, which will be demonstrated in Section 3.1, with exact solution for the steady state phase space distribution. The temperature across the bulk of the system is constant at the mean of bath temperatures. A similar model is the one-dimensional fluid of identical hard spheres that undergo elastic collisions among each other, and collisions with the walls lead to reflection with a random velocity drawn from *Maxwellian* distribution. This model has the same anomalous exponent, again due to absence of scattering of heat carriers.

To model more realistic solids, disorder is introduced in the above model [12]. The masses are taken to randomly distributed. As all the normal modes may be *localized* [19] in two or lower dimensions, only the low frequency modes, extending over lengths of the order of system size, contribute to heat flow. Section 3.2 begins with an estimation of localization lengths of modes, then proceeding to evaluate currents. If the end particles of the system are pinned via springs, the anomalous exponent is found to be $\alpha = -1/2$, the system behaves as an insulator. In the limit of weak-noise, the temperature profile is also known, and is found to vary between the bath temperatures. This model also has a continuum (elastic string) analogue [14], which can be considered with free boundary conditions. The disorder is here is equivalent to a random "refractive index" for the longitudinal waves. The energy current can be related to the *transmission coefficients* for the system, which can be readily estimated. It is found to decay as \sqrt{L} , or $\alpha = 1/2$.

Finally, I will consider the disordered two dimensional *Lorentz gas* with the baths being Maxwellian [16]. The system consists of a box of non-interacting particles with fixed hard sphere scatterers. The particles move freely between scatterers, and undergo elastic collisions. It will be shown that there is no local thermal equilibrium, for any configuration of scatterers. The disorder is introduced over scatterer configurations. For this system, in the limiting case of high density scatterers with their radius tending to zero, such that the mean free path of gas particles is kept constant, the current density is found to be inversely proportional to L , validating Fourier's law.

1.3 Entropy, entropy production, entropy flow

Let us conclude this chapter with the most widely used definition of entropy and its time evolution for a Markov chain. The quantities defined below will be useful in the next chapter.

Consider a Markov chain, ranging over discrete configurations (denoted by C, C' etc.) and continuous time t . The dynamics is given by the transition matrix $w(C, C')$, the (time-independent) rate of transition from C' to C . If $p(C, t)$ denotes the probability of being in state C at time t , the rate equation is

$$\dot{p}(C, t) = \sum_{C'} w(C, C') p(C', t). \quad (1.3.1)$$

The *Gibbs-Shannon entropy* will be a frequently encountered quantity in the thesis, and it is worthwhile to explore its time evolution. It is defined by

$$S(t) = - \sum_C p(C,t) \ln p(C,t) \quad (1.3.2)$$

Its time derivative

$$\begin{aligned} \dot{S}(t) &= - \sum_C \dot{p}(C,t) [1 + \ln p(C,t)] = - \sum_C \dot{p}(C,t) \ln p(C,t) \\ &= - \sum_{C,C'} w(C,C') p(C') \ln p(C) \\ &= - \sum_{C,C'} w(C,C') p(C') \ln \frac{p(C)w(C',C)}{p(C')w(C,C')} + \sum_{C,C'} w(C,C') p(C') \ln \frac{w(C',C)}{p(C')w(C,C')}. \end{aligned}$$

Symmetrizing the first term by interchanging C, C'

$$\Sigma(t) = \frac{1}{2} \sum_{C,C'} [w(C',C)p(C) - w(C,C')p(C')] \ln \frac{p(C)w(C',C)}{p(C')w(C,C')} \geq 0 \quad (1.3.3)$$

which can be called *entropy production*. Analogous term is seen in Boltzmann's *H-theorem*, which indeed concerns relaxation to equilibrium and irreversibility (but for a deterministically evolving system). The second term

$$\begin{aligned} \sum_{C,C'} w(C,C') p(C') \ln \frac{w(C',C)}{p(C')w(C,C')} &= - \sum_{C,C'} w(C,C') p(C') \ln p(C') \\ &\quad + \sum_{C,C'} w(C,C') p(C') \ln \frac{w(C',C)}{w(C,C')} \end{aligned}$$

of which the first vanishes as it contains a column-sum of rate matrix. The remaining term

$$J_S(t) = \sum_C p(C,t) \sum_{C'} w(C',C) \ln \frac{w(C',C)}{w(C,C')} \quad (1.3.4)$$

can be called *entropy flow*, and is of the form of average of the inner summation. It can be interpreted as follows:

$$\ln \frac{w(C',C)}{w(C,C')}$$

is the entropy transfer for $C \rightarrow C'$ transition, as a measure of how likely is the backward transition compared to the forward, in a logarithmic scale. The inner sum weighs them over the rate of the forward transition, the outer sum over initial probabilities.

Together,

$$\dot{S}(t) = \Sigma(t) - J_S(t) \quad (1.3.5)$$

There is however some arbitrariness in the above identifications, as any positive term with a dependence on p similar to (1.3.4) can be added to both terms². Such choices are made depending on system under consideration. In steady state,

$$\dot{S}(t) = 0, \quad \Sigma(t) = J_S(t).$$

²linear positive functional of the distribution p , to be precise.

2 Stochastic Thermodynamics

2.1 Fluctuation theorems in the canonical ensemble

Let us consider a system described by micro-states $\{1, 2, \dots\}$, and their respective energies $\{E_1(\lambda), E_2(\lambda) \dots\}$, parametrised by a *work-parameter* λ . This could, for instance be the position of a piston for a volume of gas, the parameters appearing in potential for a trapped particle, the length of a macromolecule that is being stretched, applied magnetic field on a spin system or the voltage applied to an electrical circuit. We will consider processes in which this parameter is externally varied with time according to prescribed protocol. The system is in contact with a heat reservoir at inverse temperature β .

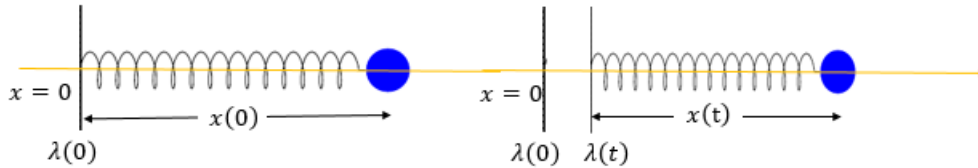


Figure 3: An example of a driven process. The position of left end λ of the spring-mass system is an example of a work parameter. The whole system is immersed in a heat bath.

The dynamics of the system is given by a discrete-time Markov process $X(t)$ ³. Also the energy levels of the system vary with time, via the change of the work-parameter. We denote the probability of the system being in state j at time t by $P_j(t)$, and probability of the transition event⁴ from initial $(i, \lambda(t))$ to final $(j, \lambda(t+1))$ as $P\{i, \lambda(t) \rightarrow j, \lambda(t+1)\}$. The Gibbs distribution

$$\rho_j(\lambda, \beta) = \frac{e^{-\beta E_j(\lambda)}}{\sum_i e^{-\beta E_j(\lambda)}} \quad (2.1.1)$$

is assumed to be the invariant distribution of the process, and the transition rates obey detailed balance with respect to this distribution,

$$\rho_i(\lambda, \beta) P\{i \xrightarrow{\lambda} j\} = \rho_j(\lambda, \beta) P\{j \xrightarrow{\lambda} i\}. \quad (2.1.2)$$

³ t should be thought of as a multiple of some small time, say τ , over which state of system undergoes an appreciable change

⁴this is a probability conditioned on the initial state

Further bits of notation for the *equilibrium partition function* and *free energy* are $Z(\lambda, \beta) = \sum_i e^{-\beta E_j(\lambda)}$ and $F(\lambda, \beta) = \frac{-1}{\beta} \log Z(\lambda, \beta)$. For a transition $(i, \lambda(t)) \rightarrow (j, \lambda(t+1))$, the heat exchanged (into the system) and work done (on the system) are defined to be

$$\Delta Q = E_j(t+1) - E_i(t+1), \quad \Delta W = E_i(t+1) - E_i(t) \quad (2.1.3)$$

i.e. heat exchanges are due to transitions between energy levels, where as work done are due to changes in energy of a fixed state, and their sum can be verified to be the total energy change of system $E_j(t+1) - E_i(t)$ in the transition. These definitions can be extended to realizations of a process by summing over all the transitions involved.

Consider a realization of a process, over time span $0, 1, \dots, T$,

$$[\mathbf{x}] = (x_0, \lambda_0) \rightarrow (x_1, \lambda_1) \rightarrow (x_2, \lambda_2) \rightarrow \dots \rightarrow (x_{T-1}, \lambda_{T-1}) \rightarrow (x_T, \lambda_T)$$

from an ensemble of realizations in which the protocol for changing the work-parameter is fixed to be $\lambda_0 \rightarrow \lambda_1 \rightarrow \lambda_2 \rightarrow \dots \rightarrow \lambda_{T-1} \rightarrow \lambda_T$. Then the realization can be equivalently described as

$$[\mathbf{x}] = x_0 \xrightarrow{\lambda_1} x_1 \xrightarrow{\lambda_2} x_2 \dots x_{T-1} \xrightarrow{\lambda_T} x_T$$

so that each transition takes place at fixed value of work parameter and only heat is exchanged⁵. We can define the time-reversed realization of this, for the time-reversed protocol of changing the work parameter, to be

$$[\bar{\mathbf{x}}] = x_T \xrightarrow{\lambda_T} x_{T-1} \xrightarrow{\lambda_{T-1}} x_{T-2} \dots x_1 \xrightarrow{\lambda_1} x_0$$

Now, consider the ratio of probabilities of observing the forward realization (with fixed initial state) to the backward realization (with fixed final state), in their respective ensembles. Due to Markov property

$$\frac{P\{[\mathbf{x}]|x_0\}}{P\{[\bar{\mathbf{x}}]|x_T\}} = \frac{P\{x_0 \xrightarrow{\lambda_1} x_1\} P\{x_1 \xrightarrow{\lambda_2} x_2\} \dots P\{x_{T-1} \xrightarrow{\lambda_T} x_T\}}{P\{x_T \xrightarrow{\lambda_T} x_{T-1}\} P\{x_{T-1} \xrightarrow{\lambda_{T-1}} x_{T-2}\} \dots P\{x_1 \xrightarrow{\lambda_1} x_0\}} \quad (2.1.4)$$

⁵the works are done when the system is in the same state and can be given step label of half integers i.e. $\Delta W_{n+\frac{1}{2}}$ is the work done in n th step

and the detailed balance condition (2.1.2),

$$\frac{P\{\mathbf{x}|x_0\}}{P\{\bar{\mathbf{x}}|x_T\}} = \prod_{n=0}^{T-1} \frac{\rho_{x_{n+1}}(\lambda_{n+1})}{\rho_{x_n}(\lambda_{n+1})} = \prod_{n=0}^{T-1} \exp[-\beta\{E_{x_{n+1}}(\lambda_{n+1}) - E_{x_n}(\lambda_{n+1})\}] = e^{-\beta\mathcal{Q}[\mathbf{x}]} \quad (2.1.5)$$

where $\mathcal{Q}[\mathbf{x}]$ is the total heat exchanged in course of the forward process. This identity is due to Crooks [1], from which many results follow as corollaries.

For a functional of the realizations \mathcal{F} , the average includes an average over the Gibbs distributed initial conditions as well

$$\langle \mathcal{F} \rangle_{fwd} = \sum_{x_0} \sum_{[\mathbf{x}]} \mathcal{F}[\mathbf{x}] P\{\mathbf{x}|x_0\} \rho_{x_0}(\lambda_0, \beta)$$

This is an average over forward realizations of a process. The average over backward realizations is

$$\langle \mathcal{F} \rangle_{bkwd} = \sum_{x_T} \sum_{[\bar{\mathbf{x}}]} \mathcal{F}[\bar{\mathbf{x}}] P\{\bar{\mathbf{x}}|x_0\} \rho_{x_T}(\lambda_T, \beta)$$

Using the ratio

$$\frac{P\{\mathbf{x}|x_0\} \rho_{x_0}(\lambda_0, \beta)}{P\{\bar{\mathbf{x}}|x_0\} \rho_{x_T}(\lambda_T, \beta)} = e^{-\beta\mathcal{Q}[\mathbf{x}]} \frac{e^{-\beta E_{x_0}(\lambda_0)}}{e^{-\beta E_{x_T}(\lambda_T)}} e^{-\beta\Delta F} = e^{\beta(\mathcal{W}[\mathbf{x}] - \Delta F)} \quad (2.1.6)$$

and defining the time-reversal conjugate of the functional as $\tilde{\mathcal{F}}[\mathbf{x}] = \mathcal{F}[\bar{\mathbf{x}}]$, it follows

$$\langle \mathcal{F} \rangle_{fwd} = \langle \tilde{\mathcal{F}} e^{-\beta\mathcal{W}_e} \rangle_{bkwd}, \quad (2.1.7)$$

where $\mathcal{W}_e[\mathbf{x}]$, referred to as the *excess* or *dissipative work*, is the difference of work expenditure of the given process and a process between the same thermodynamic states carried out reversibly.

$$\mathcal{W}_e[\mathbf{x}] = \mathcal{W}[\mathbf{x}] - (F(\lambda_T, \beta) - F(\lambda_0, \beta)) = \mathcal{W}[\mathbf{x}] - \Delta F \quad (2.1.8)$$

$\beta\Delta E - \beta\Delta F$ is the (total) entropy change of the system, of which $\beta\mathcal{Q}$ is accounted for as inflow from the bath. Thus $\mathcal{W}_e[\mathbf{x}] = \beta\Delta E - \beta\Delta F - \beta\mathcal{Q}$ is the *entropy produced* in the system, due relaxations at time scales much smaller compared to changes in the work parameter.

Substituting delta function of the excess work, and the dissipative work being odd under time reversal,

$$\mathcal{F}[\mathbf{x}] = \delta(\beta\mathcal{W}_e - \Sigma), \quad \tilde{\mathcal{F}}[\mathbf{x}] = \delta(\beta\mathcal{W}_e + \Sigma),$$

one obtains

$$\frac{P_{\text{fwd}}(\Sigma)}{P_{\text{bkwd}}(-\Sigma)} = e^{\Sigma}. \quad (2.1.9)$$

This expression, in terms of entropy production, is perhaps the most frequently found form of the fluctuation theorem. It is a quantification of the exponentially low probability of observing negative entropy productions, sometimes misleadingly called "Second law violation".

In terms of work done, it follows that the ratio of probabilities of observing a value of work \mathcal{W} in a process, to that of observing the value $-\mathcal{W}$ in the reversed process, is again $e^{\beta(\mathcal{W}-\Delta F)}$. The two probabilities are same for a reversible process, their common value being ΔF .

Lastly, $\mathcal{F} = 1$, results in the famous Jarzynski⁶ relation.

$$\langle e^{-\beta\mathcal{W}} \rangle = e^{-\beta\Delta F} \quad (2.1.10)$$

The second law of thermodynamics, as in $W \geq \Delta F$, is an immediate consequence of Jensen's inequality, with W as the average work. The Jarzynski relation is sometimes used in reverse, to estimate free energy from nonequilibrium work measurements or simulations.

2.2 Jarzynski's Equality in absence of heat bath

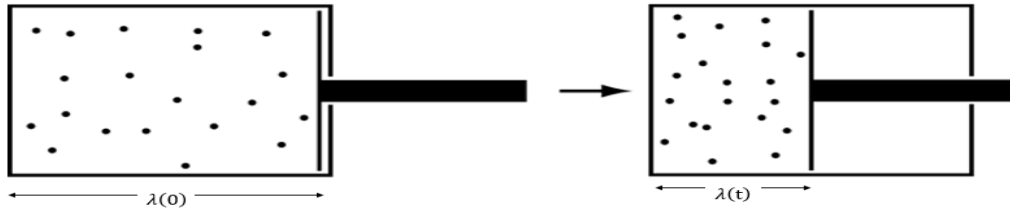


Figure 4: Compression or expansion of a box of gas as the position of piston λ is changed. The system is initially prepared at inverse temperature β , then isolated by adiabatic walls.

Consider a system, initially in thermal equilibrium at inverse temperature β , under going Hamiltonian evolution with (time-dependent) Hamiltonian $H(x, \lambda(t))$,

⁶His original derivation in [2] of the result was for a system undergoing Hamiltonian evolution, to be discussed in the next section

where x is the phase space variable (microstate) of the system and λ is the work parameter as in the previous section, changed over time interval $(0, T)$. The work functional is now just a function of initial micro-state (the final state carrying the implicit dependence on initial state) as

$$\mathcal{W} = H(x(T), \lambda(T)) - H(x(0), \lambda(0))$$

Then $\langle e^{-\beta\mathcal{W}} \rangle$ can be evaluated as the average over initial states distributed according to Gibbs distribution $\rho(x, \lambda(0))$,

$$\langle e^{-\beta\mathcal{W}} \rangle = \int dx \rho(x, \lambda(0)) e^{-\beta\mathcal{W}(x(0))}.$$

Simplifying,

$$\begin{aligned} \langle e^{-\beta\mathcal{W}} \rangle &= \int dx \rho(x, \lambda(0)) e^{-\beta\mathcal{W}(x(0))} = \int dx \frac{e^{-\beta H(x, \lambda(0))}}{\int dy e^{-\beta H(y, \lambda(0))}} e^{-\beta H(x(T), \lambda(T))} e^{\beta H(x, \lambda(0))} \\ &= \frac{\int dx e^{-\beta H(x(T), \lambda(T))}}{\int dy e^{-\beta H(y, \lambda(0))}} \end{aligned}$$

where x, y are both the fiducial integration variables running over the initial micro-states. Now using Liouville's theorem to change integration variable in numerator from x to $x(T)$, one obtains a ratio of partition functions at initial and final value of λ , resulting in (2.1.10).

As the derivation demonstrates, the temperature appearing in the relation is the initial temperature in which system was in equilibrium. The final temperature is a valid notion only after the system is allowed to equilibrate at time T , with λ held constant. Also this indicates possible extensions to thermodynamic cycles (heat engines) between multiple heat baths, as well as other thermodynamic ensembles.

2.3 Fluctuation theorems for nonequilibrium Steady States

Consider a Markov chain, ranging over discrete configurations (denoted by C, C' etc.) and discrete time (t in $0, 1, 2, \dots$), and an associated observable (often called "current") of the form

$$J_T[\mathbf{C}_t] = \sum_{t=1}^{T-1} j_1(C_{t+1}, C_t), \quad (2.3.1)$$

when the process has had the trajectory $[C_0 \rightarrow C_1 \rightarrow C_2 \rightarrow \dots \rightarrow C_{T-1} \rightarrow C_T]$, with j_1 an time-independent function of subsequent states. The dynamics is given

by the transition matrix $M(C, C')$, the probability of transition from C' to C , and $p(C, t)$ denotes the probability of being in state C at time t . In general, the transition probabilities do not satisfy detailed balance. After a long time, the system reaches a unique steady state⁷, characterised by invariant p_*

$$\sum_{C'} M(C, C') p_*(C') = p_*(C). \quad (2.3.2)$$

The quantity of interest is the probability distribution of the current. Since for physical systems the number of configurations increases exponentially with system size, finding it by direct solution for p_* is, in general, not feasible. However, for large times the probability distribution for current $P(J_T)$ is expected to have a large deviation form [3],

$$P(j_T) \approx \exp(-T\varepsilon(j_T)) \quad (2.3.3)$$

for the scaled variable $j_T = J_T/T$. More precisely this means

$$\lim_{T \rightarrow \infty} \frac{1}{T} \ln P(j_T) = -\varepsilon(j), \quad \lim_{T \rightarrow \infty} \frac{J_T}{T} = j$$

To fully exploit this simplification, we need to know the explicit form of the *rate function* ε , which has been done only for a few examples. Motivated by the discussion in Section (1.3), let us consider the function

$$a_1(C, C') = \ln \frac{M(C, C')}{M(C', C)}.$$

The resulting current A_T , for now called the *action* functional, is related to the logarithm of ratio of probabilities of a realization and its time reversal conjugate. A symmetry property of the resulting rate function is valid independent of the system under consideration, which I will prove in this section.

The joint probability distribution for action and configuration evolves as

$$P(C, T; A_T | C_0) = \sum_{C'} M(C, C') P(C', T; A_T - a_1(C, C') | C_0). \quad (2.3.4)$$

The generating function, or Laplace transform with respect to the action

$$G(C, T; \kappa | C_0) = \int dA_T e^{-\kappa A_T} P(C, T; A_T | C_0)$$

⁷we assume the system is *ergodic* and the steady state is unique

evolves as

$$G(C, T; \kappa | C_0) = \sum_{C'} M(C, C') e^{-\kappa a(C, C')} G(C', t; \kappa | C_0). \quad (2.3.5)$$

Defining the *tilted* matrix

$$M_\kappa(C, C') = M(C, C') e^{-\kappa a(C, C')}, \quad (2.3.6)$$

results in a linear recursion relation for G . All of (2.3.4)-(2.3.6) is valid for any current and leads to

$$G(C, T; \kappa | C_0) = M_\kappa^T(C, C_0) \quad (2.3.7)$$

The specific form of a_1 results in the following property of the tilted matrix,

$$\begin{aligned} M_\kappa(C, C') &= M(C, C') e^{-\kappa a_1(C, C')} = M(C, C') \frac{M(C', C)^\kappa}{M(C, C')^\kappa} \\ &= M(C, C')^{1-\kappa} M(C', C)^\kappa, \end{aligned}$$

i.e.

$$M_\kappa(C, C') = M_{1-\kappa}(C', C). \quad (2.3.8)$$

The generating function evolves via a linear recursion relation, with the positive M_κ as the transfer matrix. According to Perron-Frobenius theorem, such matrices have a positive largest eigenvalue⁸, which can be denoted as $e^{-\phi(\kappa)}$. This means, by (2.3.8)

$$\phi(\kappa) = \phi(1 - \kappa). \quad (2.3.9)$$

Now for large T , using (2.3.3)

$$\begin{aligned} G(C, T; \kappa | C_0) &= \int dA_T e^{-\kappa A_T} P(C, T; A_T | C_0) \\ e^{-T\phi(\kappa)} &\approx \int dA e^{-\kappa T a} e^{-T\varepsilon(a)} \end{aligned}$$

Steepest descent for the integral means

$$\phi(\kappa) = \min_a \kappa a + \varepsilon(a), \quad \varepsilon(a) = \max_\kappa \phi(\kappa) - \kappa a \quad (2.3.10)$$

⁸additionally, the corresponding eigenspace is one dimensional, and has an eigenvector with all entries positive

and (2.3.9) leads to

$$\begin{aligned}\varepsilon(a) &= \max_{\kappa} \phi(\kappa) - \kappa a = \max_{\kappa} \phi(1 - \kappa) - \kappa a = \max_{\kappa'} \phi(\kappa') - (1 - \kappa')a \\ &= -a + \max_{\kappa} \phi(\kappa) - \kappa(-a),\end{aligned}$$

i.e.

$$\varepsilon(a) - \varepsilon(-a) = -a. \quad (2.3.11)$$

For the probability distribution of current (2.3.3), we obtain (for large T)

$$P(-a) \approx P(a)e^{-Ta} \quad (2.3.12)$$

This goes under the name of steady-state fluctuation theorem [4] or the Gallovati-Cohen⁹ fluctuation theorem. It is somewhat peculiar to see entropy flow, rather than entropy production, appearing in such a theorem. However they are equal in the steady state, and the interpretation as a quantification of irreversibility essentially carries over.

Instead of the above defined action

$$\begin{aligned}A_T[\mathbf{C}_t] &= \sum_{t=1}^{T-1} a_1(C_{t+1}, C_t) = \sum_{t=1}^{T-1} \ln \frac{M(C_{t+1}, C_t)}{M(C_t, C_{t+1})} \\ &= \ln \frac{P[\mathbf{C}_t]}{P[\bar{\mathbf{C}}_t]} + \ln \frac{p_*(C_T)}{p_*(C_0)},\end{aligned}$$

consider the related quantity

$$\Omega_T[\mathbf{C}_t] = A_T[\mathbf{C}_t] - \ln \frac{p_*(C_T)}{p_*(C_0)},$$

Which is simply the ratio of probabilities of a realization and its time-reversal conjugate. The corresponding generating function satisfies

$$\sum_{[\mathbf{C}_t]} \exp(-\kappa \Omega_T[\mathbf{C}_t]) P[\mathbf{C}_t] = \sum_{[\mathbf{C}_t]} P[\mathbf{C}_t]^{1-\kappa} P[\bar{\mathbf{C}}_t]^\kappa = \sum_{[\mathbf{C}_t]} \exp(-(1-\kappa) \Omega_T[\mathbf{C}_t]) P[\mathbf{C}_t] \quad (2.3.13)$$

means the symmetry relation holds, for all T . This result is referred to as *transient* fluctuation theorem. However, for small T , this does not lead to any obvious relation between probabilities of observables¹⁰. I am not aware of any physical application of this equation.

⁹originally observed in simulations of deterministically thermostated systems [5]

¹⁰in contrast to the Legendre transform pair (2.3.10)

2.4 Application to Exclusion Processes

In this section, I will demonstrate the meaning of the action functional for a simple example. First, consider a ring of L sites, each of which can be occupied by at most one particle. c_x denotes the occupation number of site x . The configurations of the system is then given by $C = (c_1, c_2, \dots, c_L)$. The dynamics (in continuous time) is governed by rates $r_{x,x+1}(C)$ of the sites x and its nearest neighbour $x+1$ exchanging their occupancy. Also, $C^{x,x+1}$ denotes a configuration differing from C only by exchange of occupation at site x and $x+1$, all other sites being same¹¹.

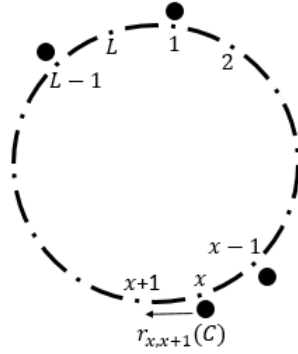


Figure 5: The exclusion process on a ring of length L

If the system is in equilibrium, the steady state distribution, is of the form $p_{eq}(C) \sim e^{-H_0(C)}$, where H_0 is the Hamiltonian of the system, with no assumptions about it's form. The rates satisfy detailed balance

$$r_{x,x+1}(C)e^{-H_0(C)} = r_{x,x+1}(C^{x,x+1})e^{-H_0(C^{x,x+1})}.$$

It is easy to see that, A_T is just the difference $H(C_0) - H(C_T)$, and the scaled action a vanishes. Somewhat more general is a situation in which the jumps are biased, so that after a long time a unique nonequilibrium steady state is achieved. However, if the driving force is a constant f , a *local detailed balance* or *local equilibrium* is assumed for the rates,

$$r_{x,x+1}(C)e^{-H_0(C)} = r_{x,x+1}(C^{x,x+1})e^{-H_0(C^{x,x+1}) + (c_x - c_{x+1})f}.$$

¹¹in terms of earlier notation $w(C^{x,x+1}, C) = r_{x,x+1}(C)$

The modified Hamiltonian is $H(C) = H_0 - f \sum_x x c_x$. However, the steady state is not of the form $e^{-H(C)}$, and there is no detailed balance unless $f = 0$.

Then,

$$a_1(C^{x,x+1}, C) = H_0(C) - H_0(C^{x,x+1}) + (c_x - c_{x+1})f$$

Noting that $c_x - c_{x+1}$ is 1 if a particle jumps from x to $x+1$ and -1 if vice-versa, the action is, ignoring boundary terms $H_0(C_0) - H_0(C_T)$,

$$A_T = f \sum_{\text{jumps}}^T \sum_x j_{x,x+1}$$

where $j_{x,x+1}$ is local current across the bond, which summed over sites x gives total current upto time T . This relation between action and current holds only in local equilibrium regime, otherwise the force f has no direct relation to the transition rates or the quantity a_1 . The fluctuation theorem here is a statement about the probability of a value of current to the probability of the negative of that value, for large times.

Next, instead of a ring, consider the system connected to two different reservoirs at either end. $N(C)$ will denote the number of particles in configuration C , C^x the configuration different from C only at a boundary site $x \in \{1, L\}$, $r_x(C)$ the rate of such transition, i.e of inserting or removing particles from system at the boundaries, leaving others unchanged.

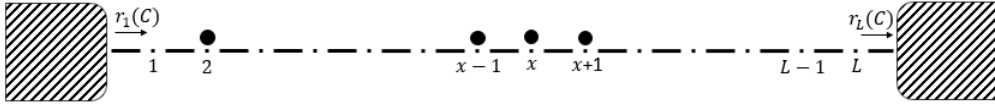


Figure 6: The exclusion process driven by reservoirs of different chemical potentials at boundaries

Detailed balance in the bulk means, for $x, x+1 \neq 1, L$

$$r_{x,x+1}(C)e^{-H_0(C)} = r_{x,x+1}(C^{x,x+1})e^{-H_0(C^{x,x+1})},$$

and local detailed balance at boundary means

$$r_x(C)e^{-H_0(C)} = r_x(C^x)e^{-H_0(C^x)}e^{\mu_x(1-2c_x)},$$

μ_1, μ_L being the chemical potentials of the respective reservoirs. A nonequilibrium steady state will be obtained only if the chemical potentials are unequal. Then,

$$a_1(C', C) = \begin{cases} H_0(C) - H_0(C^{x,x+1}) & \text{jump in the bulk} \\ H_0(C) - H_0(C^1) + \mu_1(N(C^1) - N(C)) & \text{jump at the left bath} \\ H_0(C) - H_0(C^L) + \mu_L(N(C^L) - N(C)) & \text{jump at the right bath} \end{cases}$$

and with currents j_1 out of the left bath and j_L into the right bath,

$$A_T = \sum_{jumps} [\mu_1 j_1 - \mu_L j_L].$$

Again, boundary terms $H_0(C_0) - H_0(C_T)$ are ignored. In the steady state, the rate of particles entering equals those exiting and

$$A_T = (\mu_1 - \mu_L) \sum_{jumps} j_1.$$

2.5 Application to heat conduction

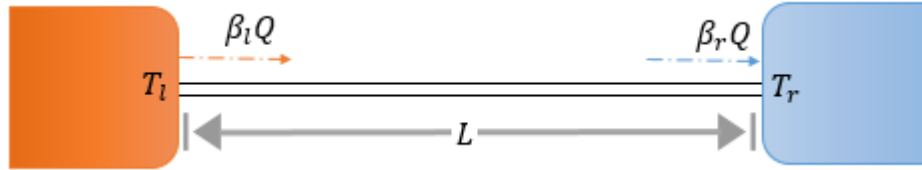


Figure 7: One-dimensional rod of length L between heat baths at differing temperatures

The system under consideration in this section is a one dimensional solid rod connecting two reservoirs at inverse temperatures $\beta_r > \beta_l$, with $\Delta\beta = \beta_r - \beta_l$. Let $j(t)$ be the heat current at time t , and $Q(t) = \int_0^t dt' j(t')$ the total heat flow upto time t . A steady state is assumed to be reached, when heat input at the left end equals heat output at right, and the corresponding entropy exchanged are $-\beta_l Q, \beta_r Q$ respectively. This means the entropy produced till time t is

$$Q(t)(\beta_r - \beta_l) \tag{2.5.1}$$

This, also is the action functional once the steady state is reached. Assuming the coupling to heat baths is sufficiently weak so that dynamics remains Markovian, for the scaled variable $j = Q/t$, in the long time limit, the steady state fluctuation theorem implies,

$$\varepsilon(j, \Delta\beta) - \varepsilon(-j, \Delta\beta) = \Delta\beta j, \quad (2.5.2)$$

where $\varepsilon(j, \Delta\beta)$ is the large deviation function for the scaled current (instead of the entropy production itself). Accounting for the factor $\Delta\beta$, the generating function $G(t, \lambda) = \langle \exp(-\lambda Q) \rangle$ satisfies

$$\begin{aligned} G(t, \lambda, \Delta\beta) &\approx e^{-t\phi(\lambda, \Delta\beta)} \\ \phi(\lambda, \Delta\beta) &= \phi(\Delta\beta - \lambda, \Delta\beta) \end{aligned} \quad (2.5.3)$$

As G was the cumulant generating function, $\phi(\lambda)$ has a power series expansion

$$-t\phi(\lambda, \Delta\beta) = \sum_{n=1}^{\infty} \frac{(-\lambda)^n}{n!} \langle Q^n \rangle_c$$

where the cumulants depend on the temperature difference. For small temperature difference and λ , expansion upto second order is

$$\begin{aligned} \phi(\lambda, \Delta\beta) &= \phi'(0, \Delta\beta)\lambda + \phi''(0, \Delta\beta)\frac{\lambda^2}{2} \\ \phi(\Delta\beta - \lambda, \Delta\beta) &= \phi'(0, \Delta\beta)(\Delta\beta - \lambda) + \phi''(0, \Delta\beta)\frac{(\Delta\beta - \lambda)^2}{2}. \end{aligned}$$

where $'$ is the derivative with respect to the first argument. Equating the coefficients of λ

$$2\phi'(0, \Delta\beta) = -\phi''(0, \Delta\beta)\Delta\beta$$

Expanding the left hand side with respect to $\Delta\beta$ again, and ignoring second order terms

$$2\phi'(0, \Delta\beta) = -\phi''(0, 0)\Delta\beta.$$

In terms of current correlations, the right side is the nonequilibrium steady state average $-2\langle Q \rangle/t$, where as the left side is the equilibrium (no temperature gradient) correlation $-\Delta\beta\langle Q^2 \rangle_{eq}/t$, which can be expressed as

$$\langle Q^2 \rangle_{eq} = \int_0^t dt_1 dt_2 \langle j(t_1)j(t_2) \rangle_{eq} = t \int_0^t dt' \langle j(0)j(t') \rangle_{eq},$$

using the time-translation invariance of equilibrium correlations.

Combining and expressing in terms of reservoir temperature T and difference ΔT , we get the *Kubo-Green* formula for conductivity

$$\kappa(T) = \lim_{\Delta T \rightarrow 0} \frac{jL}{\Delta T} = \frac{1}{2T^2} \int_0^\infty dt' \int_0^\infty dx \langle j(x, t') j(0, 0) \rangle_{eq}. \quad (2.5.4)$$

In fact many of the *linear response* results, which relate nonequilibrium averages (or transport coefficients) to equilibrium correlations, can be obtained from symmetry properties of large deviations. Heat conduction, however, is peculiar in the sense that temperature gradients can not be introduced as perturbations to the system's Hamiltonian (unlike an electric field, say). Many alternate derivations of the Kubo-Green formula for thermal conductivity either rely on such pseudo-perturbations [10], or tacitly assume diffusive heat flow [7].

2.6 Conclusion

The entropy produced till time t , denoted by Σ_t , in the steady state, in a variety of systems under going Markov evolution, was found to obey

$$\frac{\text{Prob}(\Sigma_t)}{\text{Prob}(-\Sigma_t)} \asymp e^{\Sigma_t}.$$

It means trajectories leading to overall decrease in entropy are exponentially unlikely. However for small systems, where the values of entropy production (compared to 1 in the units of our choice) are small, such trajectories can be observed and form the basis a large body of experimental work [6].

The identification and interpretation of entropy production varies. In some contexts it can be related to work, which leads to a nonequilibrium extension of the second law of thermodynamics, in the form of Jarzynski relation. For the exclusion process on a ring the entropy production is proportional to the bulk driving force times total particle current, provided a form of local detailed balance relates the force to the transition rates. In case of boundary driven exclusion process, it is difference of chemical potentials of the two reservoirs times the current. For a conductor between a hot and a cold reservoir, assuming steady state and local thermal equilibrium, a similar identification with difference of inverse temperatures times current can be made.

3 Heat conduction in low-dimensional systems

3.1 The harmonic chain

Consider N oscillators, with harmonic nearest neighbour interactions of equal natural frequency ω , the first and last of which are coupled to *Langevin* baths at temperatures T_l and T_r respectively, with the same dissipation constant γ . The mass of every oscillator is the same and is taken to be unity.

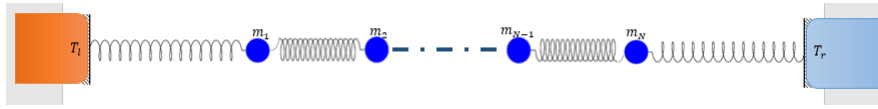


Figure 8: A chain of harmonic oscillators, between heat baths of different temperatures.

For co-ordinates q_n denoting displacement about equilibrium position of n th oscillator, and the corresponding momenta p_n , the equations of motion are,

$$\begin{aligned} \dot{q}_n &= p_n & n = 1, 2, \dots, N \\ \dot{p}_n &= -\omega^2 \sum_{m=1}^N G_{nm} q_m & n = 2, 3, \dots, N-1 \\ \dot{p}_n &= -\omega^2 \sum_{m=1}^N G_{nm} q_m - \gamma p_n + R_n \eta(t) & n = 1, N \end{aligned}$$

where $\eta(t)$ is the Gaussian white noise of unit strength satisfying $\langle \eta(t) \eta(t') \rangle = \delta(t - t')$ and $R_1^2 = 2\gamma T_l$, $R_N^2 = 2\gamma T_r$, by the *Einstein fluctuation-dissipation relation*. The tridiagonal $N \times N$ matrix \mathbf{G} is given by, 2's along the diagonal and -1 's along both the first semi-diagonals, with all other entries zero. Similarly, let

$$\Gamma = \text{diag}[\gamma, 0, \dots, 0, \gamma] \quad R = \text{diag}[R_1, 0, \dots, 0, R_N].$$

Then the equations can be cast in a matrix form, for columns $\mathbf{q} = (q_1, q_2, \dots, q_N)$, $\mathbf{p} = (p_1, p_2, \dots, p_N)$,

$$\begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} \mathbf{0}_N & \mathbb{I}_N \\ -\omega^2 \mathbf{G} & -\Gamma \end{pmatrix} \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} + \begin{pmatrix} \mathbf{0}_N & \mathbf{0}_N \\ \mathbf{0}_N & \mathbf{R} \end{pmatrix} \eta(t).$$

One can solve this linear matrix-differential equation by use of integrating factor, but even without explicitly doing so it can be seen that the solution is a linear combination of Gaussian driving terms $\eta(t)$. Thus the solution is a family (parametrised by t) of Gaussian random variables. Without directly dealing with exponentiation of large matrices, an alternate solution exploits this fact.

This set of Langevin equations are equivalent to a *Fokker-Planck* equation, for phase space density $\rho(\mathbf{x}, t)$, $\mathbf{x} = (\mathbf{q}, \mathbf{p})$,

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} = \nabla(\mathbf{A}\mathbf{x}\rho(\mathbf{x}, t)) + \frac{1}{2}\nabla(\mathbf{B}\nabla\rho(\mathbf{x}, t))$$

Where ∇ is the phase space gradient $(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \dots, \frac{\partial}{\partial q_n}, \frac{\partial}{\partial p_1}, \frac{\partial}{\partial p_2}, \dots, \frac{\partial}{\partial p_n})$ and

$$\mathbf{A} = \begin{pmatrix} \mathbf{0}_N & -\mathbb{I}_N \\ \omega^2 \mathbf{G} & \Gamma \end{pmatrix} \quad \mathbf{B} = \begin{pmatrix} \mathbf{0}_N & \mathbf{0}_N \\ \mathbf{0}_N & \mathbf{R}^2 \end{pmatrix}.$$

Since the general solution to this equation is a multivariate Gaussian, we take the steady-state solution to be of the form

$$\rho(\mathbf{x}) = \frac{1}{(2\pi)^N \det(S)} \exp[-\frac{1}{2}\langle \mathbf{x}, S^{-1}\mathbf{x} \rangle].$$

The correlations are given by the matrix

$$S(T_r, T_l) = \begin{pmatrix} S_{qq} & S_{qp} \\ S_{pq} & S_{pp} \end{pmatrix}.$$

It is useful to express the bath temperatures by their average $T = (T_l + T_r)/2$ and (half of) relative difference $\theta = (T_l - T_r)/2T$. Also, define dimensionless relative strength of couplings $\nu = \frac{\omega^2}{\gamma^2}$. Substituting the Gaussian in the Fokker-Planck equation and solving for elements of \mathbf{S} , which is algebraically non-trivial, but was accomplished by Rieder, Lieb, and Lebowitz [11], by virtuoso use of linear algebra, yields the correlations in terms of Chebyshev polynomials. The result is conveniently expressed after subtracting the equilibrium correlations $S(\theta = 0, T)$, which is the Gibbs distribution at temperature T ,

$$\rho_0(\mathbf{q}, \mathbf{p}) \sim \exp[-\frac{\langle \mathbf{p}, \mathbf{p} \rangle}{2T}] \exp[-\omega^2 \frac{\langle \mathbf{q}, \mathbf{G}\mathbf{q} \rangle}{2T}].$$

This means that the position-momenta correlations vanish and

$$S_{qq}^{-1}(0) = \omega^2 \frac{\mathbf{G}}{T} \quad S_{pp}^{-1}(0) = \frac{\mathbb{I}_N}{T}$$

Let

$$X = \frac{\omega^2}{\theta T} [S_{qq}(\theta) - S_{qq}(0)] \quad Y = \frac{1}{T\theta} [S_{pp}(\theta) - S_{pp}(0)]$$

$$Z = \frac{\gamma}{\theta T} S_{qp}(\theta).$$

The result by Rieder, Lieb, Lebowitz is

$$Z = \begin{pmatrix} 0 & \varphi_1 & \dots & \varphi_{N-1} \\ -\varphi_1 & 0 & \varphi_1 & \dots \\ \vdots & \ddots & \ddots & \ddots \\ -\varphi_{N-1} & \dots & -\varphi_1 & 0 \end{pmatrix} \quad X = \begin{pmatrix} \varphi_1 & \dots & \varphi_{N-1} & 0 \\ \varphi_2 & \dots & 0 & -\varphi_{N-1} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & -\varphi_{N-1} & \dots & -\varphi_1 \end{pmatrix}$$

$$Y = \nu X + \text{diag}[1, 0, \dots, 0, 1],$$

where

$$\cosh \alpha = 1 + \frac{\nu}{2} \quad \varphi_l = \frac{\sinh(N-l)\alpha}{\sinh N\alpha}.$$

For large N ,

$$\varphi_l = e^{-l\alpha} \quad e^{-\alpha} = \frac{\nu}{2} + 1 - \sqrt{4\nu + \nu^2}.$$

The *local temperature* near n th site is given by $(S_{pp})_{nn}$, the local kinetic energy, which in the limit of large N turns out to be,

$$T_n = \begin{cases} T[1 + \theta(1 - \nu\varphi_1)] & n = 1 \\ T[1 - \theta\nu\varphi_1^{2n-1}] & 1 < n \leq N/2 \\ T[1 + \theta\nu\varphi_1^{2(N-n)-1}] & N/2 < n < N \\ T[1 + \theta(1 - \nu\varphi_1)] & n = N \end{cases}$$

which is plotted below, for coupling parameters $\nu = 0.05, 0.2, 1.0$ (solid, dotted and dashed lines, respectively). It is almost constant in the bulk, even for as few as 16 oscillators, due to exponential dependence on distance from the nearest end. Another peculiar feature is that the minimum (maximum) temperature is obtained closer to the bath with a higher (lower) temperature. The deviations at these points from the bulk temperature increases with increasing coupling strength.

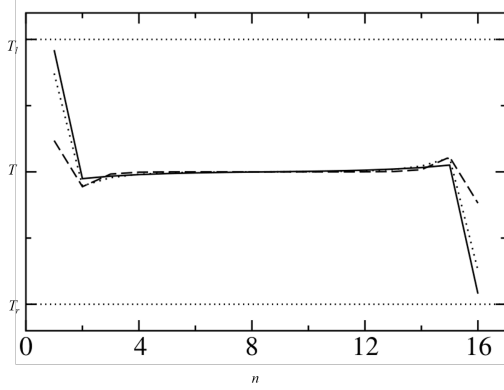


Figure 9: Steady state temperature profile of harmonic solid, from [10]

Defining the energy at site l as sum kinetic energy and half of the potential energies of interaction with both neighbouring sites, the energy current from l to $l + 1$ in steady state is

$$\langle j_{l+1,l} \rangle = \omega^2 \langle p_{l+1} q_l - p_{l+1} q_{l+1} \rangle = \frac{\theta T}{\gamma} Z_{l,l+1} = \frac{T_r - T_l}{\gamma} \varphi_1.$$

It is proportional to the temperature difference, not the gradient, in stark violation of Fourier's law. Equivalently, the conductivity κ is proportional to N , and diverges in the large N limit considered. This happens for the following reason: as all the springs and masses are identical, any disturbance (say, a pulse or a normal mode oscillation) arising due to driving at one end propagates to the other end without changing its amplitude and velocity, and carries all of its initial energy to the other end at a fixed rate. This means the current density does not decay with length, and hence the infinite conductivity.

3.2 Mass disordered solids

If the masses in the system in Section 3.1 are allowed to be random, many essential aspects of the problem are changed. A novel phenomena called *localization* comes into play [19], meaning that a normal mode has displacement profile q_n centred around some n_0 , decaying exponentially with increasing distance from it. Borrowing notations from Section 3.1, but including the masses m_n of n th oscillator, taken to be independent and identically distributed random variables, and

setting the natural frequency to unity, the normal mode of frequency ω satisfies,

$$-m_n \omega^2 u_n = u_{n-1} + u_{n+1} - 2u_n, \quad (3.2.1)$$

where u_n denotes displacement of n th oscillator, for $n \neq 1, N$. This is equivalent to a linear recursion

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} = \begin{pmatrix} 2 - m_n \omega^2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix} \quad (3.2.2)$$

The transfer matrix here is a random matrix. *Furstenberg's theorem* [13] states that, the norm¹² of a product of random matrices acting on any nonzero vector, $M_n M_{n-1} \dots M_1 \mathbf{v}$, has exponential n dependence as $n \rightarrow \infty$ with probability 1, provided

- i. They all have unit determinant.
- ii. The smallest closed matrix subgroup containing all the matrices which have non-zero probability of appearing, say G , is not bounded as a subset of all 2×2 matrices.
- iii. No subgroup of G having finitely many cosets is left invariant under action of itself.

These hypotheses hold if there are atleast two different masses [12]. Thus there exists $\xi > 0$, such that

$$E \left[\ln \left| \frac{u_N}{u_{N-1}} \right| \right] = \xi^{-1}.$$

Here and henceforth, E denotes average over the realizations of the random masses.

To estimate ξ , let $z_n = \frac{u_n}{u_{n-1}}$, then (3.2.1) means,

$$z_{n+1} = 2 - m_n \omega^2 - \frac{1}{z_n}. \quad (3.2.3)$$

The masses, m_n are independently drawn from a distribution $\mu(m)$, with mean \bar{m} , variance σ_m^2 . To find $\xi^{-1} = \lim_{n \rightarrow \infty} n^{-1} E[\ln |z_n|]$, first change variables to

$$z = \frac{\cos(\theta + \alpha)}{\cos \theta}, \quad \cos \alpha = 1 - \frac{\omega^2 \bar{m}}{2}. \quad (3.2.4)$$

¹²sum of squares of components

then

$$\begin{aligned}
\frac{\cos(\theta_{n+1} + \alpha)}{\cos \theta_{n+1}} &= \cos \alpha - \sin \alpha \tan \theta_{n+1} = 2 - m_n \omega^2 - \frac{\cos \theta_n}{\cos(\theta_n + \alpha)}, \\
\tan \theta_{n+1} &= \frac{\cos \alpha}{\sin \alpha} + \frac{1}{\sin \alpha} \frac{\cos \theta_n}{\cos(\theta_n + \alpha)} - \frac{2 - m_n \omega^2}{\sin \alpha} \\
&= \frac{\cos \alpha}{\sin \alpha} + \frac{1}{\sin \alpha} \frac{\cos \theta_n}{\cos(\theta_n + \alpha)} + \frac{(m_n - \bar{m}) \omega^2}{\sin \alpha} + \frac{\omega^2 \bar{m} - 2}{\sin \alpha} \\
&= \frac{1}{\sin \alpha} \frac{\cos \theta_n}{\cos(\theta_n + \alpha)} - \frac{\cos \alpha}{\sin \alpha} + \frac{(m_n - \bar{m}) \omega^2}{\sin \alpha} \\
&= \frac{1}{\sin \alpha} \frac{\cos(\theta_n + \alpha) \cos \alpha + (\sin \theta_n + \alpha) \sin \alpha}{\cos(\theta_n + \alpha)} - \frac{\cos \alpha}{\sin \alpha} + \frac{(m_n - \bar{m}) \omega^2}{\sin \alpha}
\end{aligned}$$

Thus the recursion relation is given by,

$$\tan \theta_{n+1} = \tan(\theta_n + \alpha) + \frac{(m_n - \bar{m}) \omega^2}{\sin \alpha}. \quad (3.2.5)$$

Let the inverse of this relation be of the form $\theta_n = h(\theta_{n+1}, m_n, \omega)$. For large n , the disorder averaged distribution $f(\theta, \omega)$ is expected to remain invariant. This means

$$f(\theta, \omega) = \int dm \mu(m) f(h(\theta, m), \omega) \frac{dh(\theta, m, \omega)}{d\theta} \quad (3.2.6)$$

and

$$\xi^{-1} = \int d\theta f(\theta, \omega) \ln \left| \frac{\cos(\theta + \alpha)}{\cos \theta} \right|.$$

Using expansion of h in powers of ω to determine coefficients of the expansion of f in ω , the inverse correlation length, in leading order for $\omega \rightarrow 0$ is found to be

$$\xi^{-1} = \frac{\sigma_m^2}{8\bar{m}} \omega^2. \quad (3.2.7)$$

As only extended modes i.e modes with ξ of the order of system size, contribute to energy transport, this turns out to be an important quantity. This means a normal mode of frequency ω is extended ($\xi \sim N$) if $\omega \lesssim N^{-1/2}$. Now for small frequencies the number of modes is almost uniformly distributed in wave number k , with a density proportional to N^{-1} . Thus, the number of extended modes is of the order \sqrt{N} .

Now by method similar to the one outlined in Section 3.1, (changing $q_n \rightarrow q_n\sqrt{m_n}$, $p_n = p_n/\sqrt{m_n}$), in the weak-noise limit $\gamma \rightarrow 0$, the temperature profile is found to be

$$T_n = \sum_{k=1}^N u_n(k)^2 \frac{T_l u_1(k)^2 + T_r u_N(k)^2}{u_1(k)^2 + u_N(k)^2}, \quad (3.2.8)$$

with $u_n(k)$ the n th component of normal mode k . This is not a closed form solution, since analytic expressions for normal modes is not known. In fact, it is known from numerical experiments that the temperature profile does not converge to an average in the thermodynamic limit $N \rightarrow \infty$, or temperature realizations (over disorders) are not self-averaging [10].

In steady state, energy current is just the work done on first particle by the bath,

$$j(L) = \frac{\gamma}{m_1} (T_r - T_l) = \gamma (T_l - T_r) \sum_{k=1}^N \frac{u_1(k)^2 u_N(k)^2}{u_1(k)^2 + u_N(k)^2}. \quad (3.2.9)$$

Assuming the low frequency extended modes are given by their ordered counterpart

$$u_n(k) = \sqrt{\frac{2\bar{m}}{N+1}} \sin\left(\frac{nk\pi}{N+1}\right),$$

it can be seen that each amplitude is of the order $k/N^{\frac{3}{2}}$, the sum being upto \sqrt{N} of these modes. Thus size dependence of current density is $N^{-3/2}$, the conductivity $N^{-1/2}$ and the system is an thermal insulator.

Let us consider the continuum analogue [14], longitudinal oscillations $u(x, t)$ of a string of length L , free to move at both ends. The wave equation for monochromatic $u(x)e^{-i\omega t}$, can be written assuming a space-dependent propagation speed $c(x)$

$$\frac{d^2 u(x)}{dx^2} + \frac{\omega^2}{c^2(x)} u(x) = 0, \quad (3.2.10)$$

the wavenumber $k = \omega/c$, with c being the propagation speed in absence of disorder. The mechanical analogue of refractive index, $n(x) = c/c(x)$, is the quantity that relates directly to mass disorder, via mass density $m(x)$, $c(x) \sim 1/\sqrt{m(x)}$ and $n^2(x) \sim m(x)$. Subtracting off the value in absence of disorder, let

$$y(x) = n^2(x) - 1.$$

This is a random field¹³, and if E denotes an average over disorder, $E[y] = 0$. The

¹³defined over all real x , though only $[0, L]$ part is relevant

field will be assumed to be Markovian, with range $[-1/2, +1/2]$ (corresponding to the range masses of discrete system being some $[m - \delta, m + \delta]$).

If a wave of incident amplitude is incident from right at $x = 0$,

$$u(x) = e^{ikx} + R(k, L)e^{-ikx}, \quad u(x) = T(k, L)e^{ikx} \quad (3.2.11)$$

are the waves to right of $x = 0$, and left of $x = L$, where $R(k, L), T(k, L)$ are the reflection and transmission coefficients. The boundary conditions are continuity of $u(x), u'(x)$ at both ends.

Defining

$$\phi(k, x) = \frac{1}{2} e^{-ikx} [u(x) + \frac{1}{ik} u'(x)] \quad \psi(k, x) = \frac{1}{2} e^{ikx} [u(x) - \frac{1}{ik} u'(x)],$$

the second order wave equation is now a coupled pair of linear first order ordinary differential equations,

$$\frac{d}{dx} \begin{pmatrix} \phi(k, x) \\ \psi(k, x) \end{pmatrix} = \frac{1}{2} ik y(x) \begin{pmatrix} 1 & e^{-2ikx} \\ -e^{2ikx} & -1 \end{pmatrix} \begin{pmatrix} \phi(k, x) \\ \psi(k, x) \end{pmatrix} \quad (3.2.12)$$

with

$$\begin{aligned} \phi(k, 0) &= 0, & \phi(k, L) &= T(k, L), \\ \psi(k, L) &= 0, & \psi(k, 0) &= R(k, L). \end{aligned}$$

The choice of white noise Langevin bath at temperature T_l to left is tantamount to assuming equal number of waves of any frequency are incident, and the fluctuation-dissipation theorem means this number is proportional to T_l . There is no loss of generality in assuming no waves are incident from right of $x = L$, thus The right bath can be assumed to have temperature zero.

The energy transmitted for each k is proportional to square of amplitude of transmitted wave, and thus the energy current is their sum over all k , weighted by the number of incident waves of each k . Averaging this over disorder,

$$j(L) = cT_l \int dk E[|T(k, L)|^2].$$

As the localization length for a mode with wave number k is of the order k^{-2} for small k , the suitable scaling limit is taken holding the number of extended modes constant $k \rightarrow k/\sqrt{L}, L \rightarrow \infty$. Thus

$$j(L) \sim \lim_{L \rightarrow \infty} \int_0^\infty \frac{dk}{\sqrt{L}} E[|T(k/\sqrt{L}, L)|^2] \quad (3.2.13)$$

Now from (3.2.3), a bound can be obtained via large-deviation properties¹⁴ of the Markov field y .

$$E[|T(k, L)|^2] \leq A \exp(-g(k)L),$$

with a positive function g , constant A , with the leading order dependence of $g(k)$ as k^2 . Then

$$\lim_{L \rightarrow \infty} \int_0^\infty dk E[|T(k/\sqrt{L}, L)|^2] < \infty \quad (3.2.14)$$

. Thus $j(L) \sim L^{-1/2}$ and Fourier's law is not valid. Also, the size dependence continues to remain the same for any other choice of frequency spectrum $\mathcal{S}(\omega)$ of baths, as long as

$$\lim_{L \rightarrow \infty} \int_0^\infty dk \mathcal{S}(\omega) E[|T(k/\sqrt{L}, L)|^2] < \infty.$$

The size dependence of conductivity is

$$\kappa(L) \sim \sqrt{L}.$$

3.3 The disordered Lorentz gas

Consider a rectangular box in the plane, bounded by lines $x = 0$, $x = L$, $y = -B$, $y = B$. Inside the box there are circular scatterers of radius a , centred at $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_j, \dots$, which may overlap over each other. The gas consists of non-interacting point particles of unit mass, evolving according to Newton's Laws in the interior i.e undergoing elastic collisions with scatterers as well as the top and bottom walls. Their interactions with left and right walls are prescribed as follows: on reaching $x = 0$, $x = L$ the particle is reflected with a speed drawn from distribution $\rho_l(v)$, $\rho_r(v)$ respectively, independent of its incoming velocity or position of impact. A particular case would be the distributions being *Maxwellians*, and it would model heat baths that interacts so strongly with the gas particles as to thermalize it instantly.

The scattering centres are randomly distributed. Assuming translation invariance (let the scatterers be all over the plane, though only the box is relevant to the problem), locations of the scattering centres is a *Poisson point process*. A configuration in which all scatterers are only in a horizontal strip would mean infinite thermal conductivity due to free flow of gas between reservoirs, and such distributions with long range correlations are automatically excluded. For the rest of the

¹⁴This is the continuum analogue of Fustenberg's theorem [15]

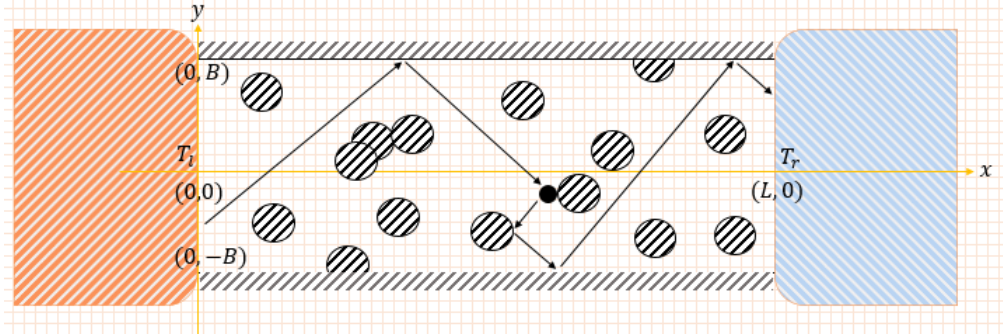


Figure 10: The Lorentz gas

discussion, let us assume the limit of large B . Then averaging over this disorder can be interpreted as average over a large number horizontal strips of height small compared to B but large enough to have no correlations across.

Let R denote a realization of the disorder. For a fixed R , the particle undergoes deterministic evolution in the bulk and near the insulating boundaries, while at the conducting boundaries the state (position and momentum) of a particle at the next instant is independent of initial momentum, the position dependence being deterministic. The process overall is Markovian.

The steady state number density $n(x,y)$ is uniform, and can be taken to be unity. If the trajectories are assumed to originate or terminate at the conducting walls, steady state distribution must be a constant along each trajectory $(\mathbf{q}_t, \mathbf{v}_t)^{(R)}$, a consequence of *Liouville's theorem*. Given position \mathbf{q} , velocity \mathbf{v} , let $p_l^{(R)}(\mathbf{q}, \mathbf{v})$ denote the probability of the trajectory passing through this point having originated at the left wall, and $p_r^{(R)}(\mathbf{q}, \mathbf{v})$ the similar probability for the right wall. These probabilities depend only on the direction \hat{v} . Then the steady state¹⁵ is

$$f^{(R)}(\mathbf{q}, \mathbf{v}) \sim p_l^{(R)}(\mathbf{q}, \hat{v})\rho_l(v) + p_r^{(R)}(\mathbf{q}, \hat{v})\rho_r(v) \quad (3.3.1)$$

Note that even for Maxwellian baths, the steady state distribution is not a Maxwellian. Hence there is no local thermal equilibrium.

A new process can be defined such that the probability of a phase space trajectory is the probability of the trajectory for a fixed R , averaged over all realizations

¹⁵Not unique, due to presence of trajectories that never reach either of the conducting walls. However, the measure of scatterer configurations $\{R\}$ for which such trajectories exist, in the limit considered, goes to zero.

of R , referred to as the *disordered Lorentz process*. This is not a Markov process, as the state of the system at next instant is determined by the probability of encountering a scatterer (disorder), and this in turn can be related to earlier collision with the same scatterer. At this point it is useful to introduce the following notations: a quantity (including probabilities) $F^{(R)}$ denotes its value for a fixed realization R , $F^{(a)}$ its value when averaged over the disorder.

The steady state of the Lorentz process is (3.3.1) averaged over disorder,

$$f^{(a)}(\mathbf{q}, \mathbf{v}) = \frac{1}{\mathcal{N}_a} [p_l^{(a)}(\mathbf{q}, \hat{v}) \rho_l(v) + p_r^{(a)}(\mathbf{q}, \hat{v}) \rho_r(v)].$$

Now consider the following limiting procedure :

$$a \rightarrow 0, \quad c \rightarrow \infty, \quad \text{such that} \quad \frac{1}{2ac} \rightarrow \lambda \quad (3.3.2)$$

i.e large density of small scatterers with the mean free path held constant, called the *Boltzmann-Grad limit*. The gas particles now move freely between collisions (as without the limit), with probability of a collision after a free flight of length r proportional to $\exp(-r/\lambda) dr$, independent of earlier history. Due to small size of scatterers, probability of re-collision with a scatterer is zero. The outcome of collision is a change in direction of the particle, according to a distribution that can be obtained by calculating scattering cross section. Collisions with boundaries are as described earlier. This process is evidently Markovian.

In this limit, the absorption probabilities can be shown [16] to be

$$p_l(\mathbf{q}, \hat{v}) = 1 - \frac{x}{L}, \quad p_r(\mathbf{q}, \hat{v}) = \frac{x}{L}. \quad (3.3.3)$$

The average heat current (x -component) can be expressed as

$$j(\mathbf{q}) = \int d^2\mathbf{v} v_x \frac{v^2}{2} f(\mathbf{q}, \mathbf{v}).$$

Using the estimate (3.3.3), and assuming Maxwellian distributions with temperatures T_l, T_r for the baths,

$$j(\mathbf{q}) = \frac{8}{3} \sqrt{\frac{2}{\pi}} \frac{\sqrt{T_l T_r}}{\sqrt{T_l} + \sqrt{T_r}} \lambda \frac{T_r - T_l}{L}. \quad (3.3.4)$$

This is the validation of Fourier's law of heat conduction, as far as scaling is concerned. Also temperature dependence of the conductivity is \sqrt{T} , the same as in an ideal gas.

3.4 Conclusion

The thermal conductivity of an one-dimensional electrically insulating solid, may not be independent of the length of the solid. Measurements of conductance have large sample to sample fluctuations. This means there is no linear relation relating the heat current density to the temperature gradient.

For a perfectly harmonic solid, the conductivity (κ) is proportional to the size (N) of the solid. The exponent α , defined for size dependence of conductivity, $\kappa \sim N^\alpha$, is the 1. This can be attributed to the lack of sufficient interaction between modes of vibration and indicates the role anharmonicity and disorder can play for transport properties of a system.

For a harmonic solid with disordered masses, the collective vibrations of the constituents experience localization in one and two dimensional systems. For low-frequency modes, the inverse localization length is proportional to square of the frequency. Among these low frequency modes, only those extending over the entire system contribute to energy transport. Accounting for these, α actually depends on the frequency distribution of fluctuations due to the bath, as well boundary conditions for the solid. The interactions with the baths being via white noise, if the ends of the solid are fixed, then $\alpha = -1/2$, and if they are free, $\alpha = 1/2$. The former is an insulator.

For a gas of non-interacting particles in a region with randomly distributed hard sphere scatterers, in the limit of point scatterers with infinite average density such that the mean free path of the particles is fixed, the current scales as required by Fourier's law. But there is no unique definition of local temperature, as there is no local thermal equilibrium (with or without the limit considered). This is mainly due to the fact that scatterings do not change the energies of the particles.

Many possible alterations to these models can be considered. For instance, one may include anharmonicity in the oscillator chains. For an anharmonic solid, as *crystal momentum* is conserved in all interactions, and a low energy collision can not involve higher momenta. Therefore, momentum is conserved at low temperatures, and any mode with initially non-vanishing crystal momentum never decays. Such modes lead to infinite thermal conductivity at low temperatures. At higher temperatures, it is expected that in presence of both anharmonicity and disorder, the conductivity will be finite in three dimensions. For lower dimensions however, the same cannot be said.

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