Thermal Transport in Quantum Chains

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Motivation

The Larger Context

- Understanding Irreversibilty
- Understanding basic laws of transport
- Anomalous transport in low dimensions

How does the macroscopic irreversible behavior arise from the underlying molecular dynamics, which is reversible?
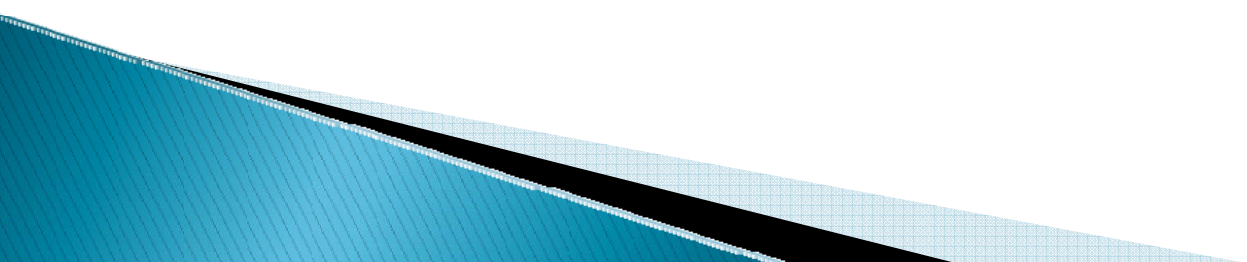
Understanding Transport

How does the system approach equilibrium?

  A non-equilibrium system typically undergoes a fast relaxation to a state of **Local Equilibrium**. The irreversible phenomena from this stage is described in terms of phenomenological laws.
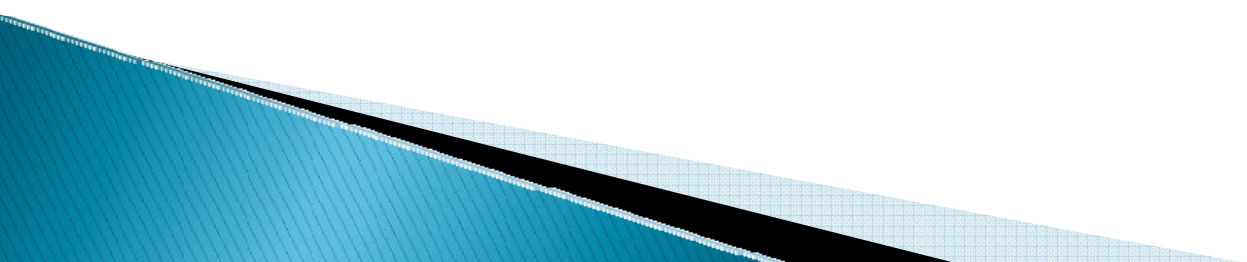
1. Ohm's law

$$J_{Charge} = - \sigma \, \mathbf{grad} \, V(r)$$

2. Fourier's Law

$$J_{heat} = - \kappa \, \mathbf{grad} \, T(r)$$

3. Fick's law

$$J_{matter} = - D \, \mathbf{grad} \, C(r)$$

Understanding Transport

The notion of **Local Equilibrium** is that, each small region of space is in thermodynamic equilibrium, with local values of thermodynamic parameters like pressure, temperature density etc.

Then the state of the system can be described in terms of few thermodynamic variables which vary slowly in space and time.

Do we understand the requirements on dynamics which will establish states of local equilibrium?
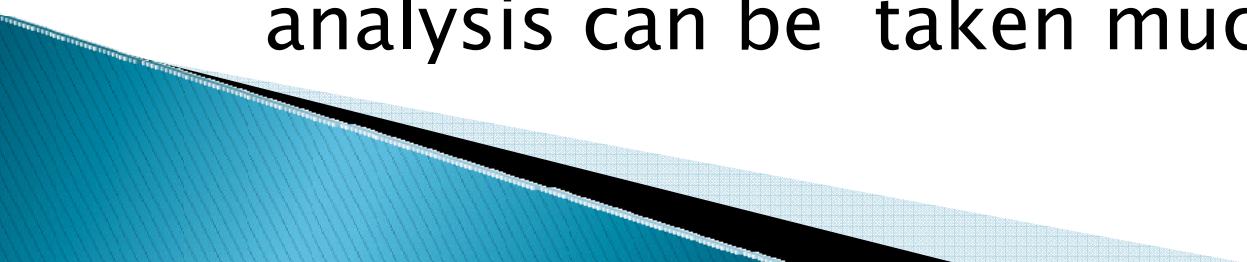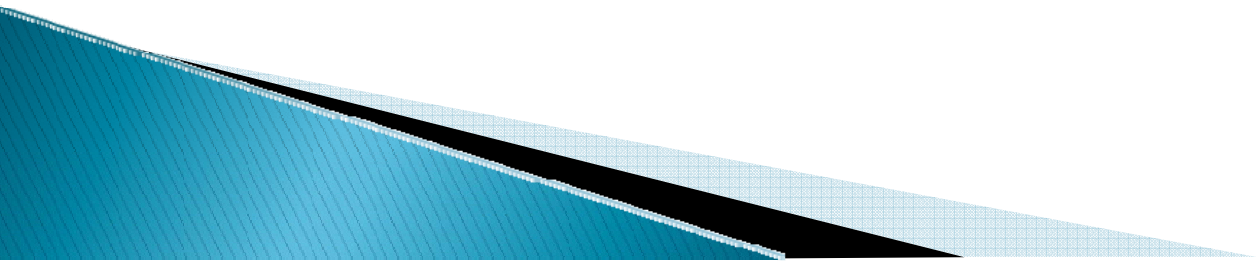
Understanding Transport

Boltzmann and Maxwell made the beginning by developing the kinetic theory and the Boltzmann Transport Equation for distribution functions and introducing the notions of mean free time and Molecular Chaos.

These questions remain unanswered, and are being pursued from several points of view.

One-dimensional models have proved very useful to analyze transport problems, as in many cases theoretical and numerical analysis can be taken much farther.

Transport in Low Dimensions

Transport in low dimensions exhibits anomalous behavior.
We consider the Fourier law.

$$J = -\kappa\ \mathbf{grad}\ T(r)$$

$$d\varepsilon/dt + \mathbf{div}\ J(r) = 0$$

$$\varepsilon(r,t) = C\ T(\mathbf{r}, t) \qquad C = \text{specific heat}$$

$$d\varepsilon/dt = \kappa/C\ \mathbf{grad}^2\ \varepsilon(\mathbf{r}, t)$$

$$\varepsilon(\mathbf{q},t) = \exp[-\kappa\ t/(C\ q^2)]\ \varepsilon(\mathbf{q},0)$$

$$= \exp(-t/\tau_q)\ \varepsilon(\mathbf{q},0) \qquad \tau_q = C/\kappa q^2$$

Thus the life time of an energy fluctuation of wavevector $\mathbf{q}$ diverges as $\mathbf{q}$ goes to 0.

Long wavelength fluctuations decay very slowly, and this has implications on equilibration in low dimensions.

Divergence of Thermal Conductivity in Low Dimensions

Due to energy conservation equilibration can take long time.

$$\kappa = \Sigma_q \, C_q \, v_q^2 \, \tau_q \qquad \text{phonon modes}$$
$$= \int k_B \, v^2 \, / q^2 \, d\mathbf{q}$$

Integral diverges in dimension $d \leq 2$.

Thus in low dimension the heat conduction processes cannot be described by the Fourier law.

One-Dimensional Models

Fermi-Pasta-Ulam (1955) studied the model

$$H = \Sigma_i [1/2 \, m \, u_i^2 + K/2 \, (u_i - u_{i+1})^2 +$$
$$g/3 \, (u_i - u_{i+1})^3 + v/4 \, (u_i - u_{i+1})^4 \,]$$

to understand the process of thermal equilibration.

This model has now been extensively used to study thermal conduction numerically. Thermal conduction is studied by putting two end atoms of the chain in contact with heat baths at different temperatures.

An extensive survey of the results is available in: S. Lepri, A. Livi and A. Politi, Phys. Rep. 377, 1 (2003).

The key result is: the conductivity κ diverges with system length.

Numerical Studies of Heat Conduction

For quartic potential
$$\kappa \propto L^{\alpha} \quad \text{with } \alpha \approx 0.38 \text{ to } 0.42$$

In earlier studies the value of α was found to be in this range for a large variation of parameters, a recent study by Mai et al (PRL 98, 184301, 2006) on longer chains claim a value of 1/3.

Studies on other systems give exponent α as: Toda lattice 0.4, Hard sphere gas 0.33, FPU chain with cubic nonlinearity 0.44.

To summarize there are some hints about the universality, and two values seem dominant, 2/5 and 1/3.

Is there a truly universal behavior?

How many universality classes are there?

Understanding Divergence Exponent α

a) Hydrodynamical Arguments

Narayan and Ramaswamy (PRL 89, 200601 (2002) studied a one-dimensional fluid by a renormalization group method, to find $\kappa \propto L^{1/3}$.

This analysis has been further refined to take account of the coupling of thermal modes with viscosity (Lee-Dadswell et al., PRE72, 031202 (2005)). They find two behaviors. If $C_p / C_v > 1$, $\alpha = 1/3$, while if $C_p / C_v = 1$, the behavior is more complex, but asymptotically $\alpha = \frac{1}{2}$.

b) Mode-Coupling Method:

Delfini et al. (PRE 73, 060201 (2006)) find answers that depend on the nonlinearity of the potential. For the cubic potential, $\alpha = 1/3$, while for quartic potential $\alpha = \frac{1}{2}$.

Divergence of Thermal Conductivity in Low Dimensions

From the microscopic point of view, the relaxation occurs due to collisions between modes. The phase space and hence the scattering probability is drastically reduced with the reduction of dimensionality.

In a one-dimensional system, when two modes/particles with momenta p and q collide, due to momentum and energy conservation, the resulting modes after the collision, would have to have the same momenta p and q.

Pereverzev (PRE 68, 056124 (2003)) used Boltzmann equation approach to study relaxation of the energy of a mode with wavevector $\mathbf{q}$. This approach gives a mode relaxation rate, $\gamma_q = \tau_q^{-1} \propto \mathbf{q}^{5/3}$ for the quartic potential. This implies $\alpha = 1/3$

Quantum Calculation of κ

We study the quantum version of the FPU chain. We utilize Kubo formula, which assumes a small thermal gradient and local equilibrium. But we can go beyond the Boltzmann approach in a systematic manner.

$$\kappa = \frac{1}{kT} \int_0^\infty dt \langle J(t)J(0) \rangle$$

In this formulation, key quantity is the dependence of phonon transport relaxation rate

$$\gamma_q \propto q^\beta$$

From this the finite-size results are obtained by limiting the time integral to a finite time of order of chain size L. This yields

$$\kappa \propto L^\alpha ;; \alpha = 1 - 1/\beta$$

Thermal Conductivity for a Quartic Potential

$$H = \sum_k \omega_k a_k^* a_k + \frac{1}{4!N} \sum_{k,p,q,s} V(k,p,q,s) A_k^* A_p^* A_q A_s$$

$$A_k = a_k + a_{-k}^*,$$

$$V(k,p,q,s) = g\Delta(k+p-q-s)\frac{\gamma_{-k}\gamma_{-p}\gamma_q\gamma_s}{(\omega_k\omega_p\omega_q\omega_s)^{1/2}}$$
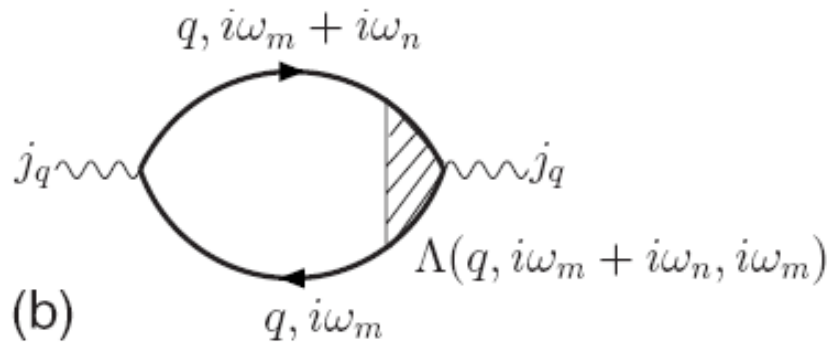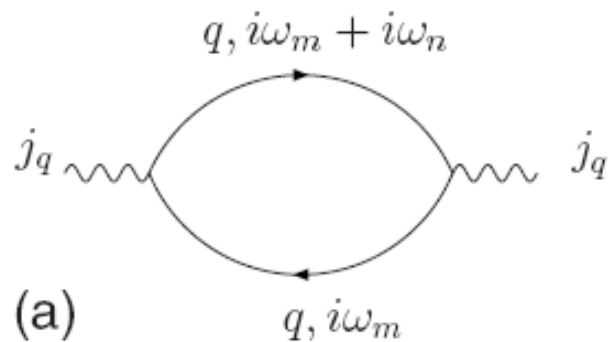
$$\gamma_k = 1 - e^{-ik}, \quad \omega_k = 2\sin k/2, \quad Current$$

$$\Delta(k) = \sum_n \delta_{k,2\pi n} \qquad\qquad J = \sum_k j_k a_k^* a_k; \; j_k = v_k \omega_k$$

Thermal Conductivity for a Quartic Potential

$$W(\tau) = \sum j_q \langle a_q^+(\tau) a_q(\tau) a_p^+(0) a_p(0) \rangle j_p$$

(a)

(b)

One needs to include two features. Phonon life-time and vertex corrections. With just life-time correction, one obtains

$$\kappa = \Sigma \, v_q^2 \, C_q \, \tau_q \; , \quad \tau_q^{-1} = \gamma_q$$

where C_q denotes mode specific heat and τ_q the phonon life time. τ_q is obtained from the phonon self energy $\Sigma(q,\omega)$.

Phonon Relaxation Rate

The self energy diagrams are shown below. Fig. (a) is the basic four phonon collision term. For relaxation rate it leads to corrections that are nonsingular in wave-vector q. The corrections arising from interaction renormalization are regular.
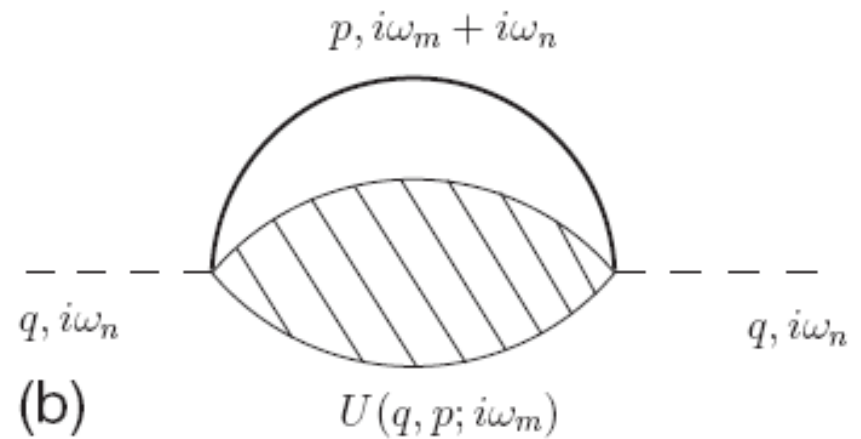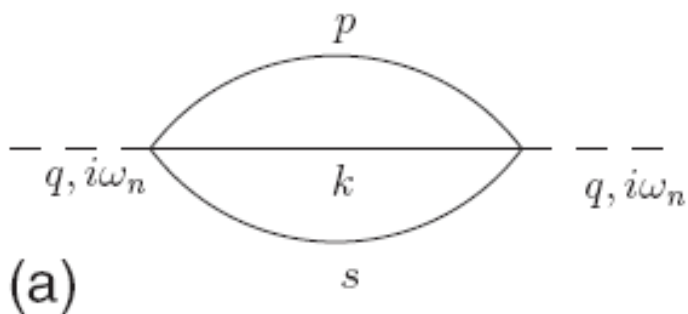
Phonon Relaxation rate

$$\gamma_q = \text{Im } \Sigma.$$

This expression involves energy and momentum conservation. The key point is that two conservations can happen only for Umklapp processes.

$$\gamma_q \propto \omega_q (e^{\beta\omega_q} - 1)\sum_p |U|^2 \frac{n_p \omega_p n(\omega_1)\omega_1[1 + n(\omega_2)]\omega_2}{J(q,p)}$$

$$J(q,p) = [(\cos q/2 + \cos p/2)^2 + 4\sin q/2 \sin p/2]^{1/2}$$

The factor outside the sum is proportional to q^2, but the integral diverges as q goes to zero as $q^{-1/3}$. Thus,

$$\gamma_q \approx T^2 \ q^{5/3}.$$

Next we incorporate the vertex corrections.

Result for the quartic potential

- We have numerically solved the equation for the vertex function, and find that the transport relaxation time or the current relaxation time also has the same wave vector dependence. Thus for the quartic potential $\alpha=2/5$.

- Now the question arises whether alpha has the same value for the other potentials. For example, the cubic potential is physically a larger term. So we consider the cubic potential next.

FPU-Cubic Chain

$$H = \sum_k \omega_k (a_k^* a_k + 1/2) +$$

$$\frac{g_3}{3! \, N^{1/2}} \sum_{k,q,p} v(k,q,p) A_k A_q A_p$$

$$v(p,k,q) = \frac{\gamma_k \gamma_p \gamma_q}{(\omega_k \omega_p \omega_q)^{1/2}} \Delta(k+p+q)$$
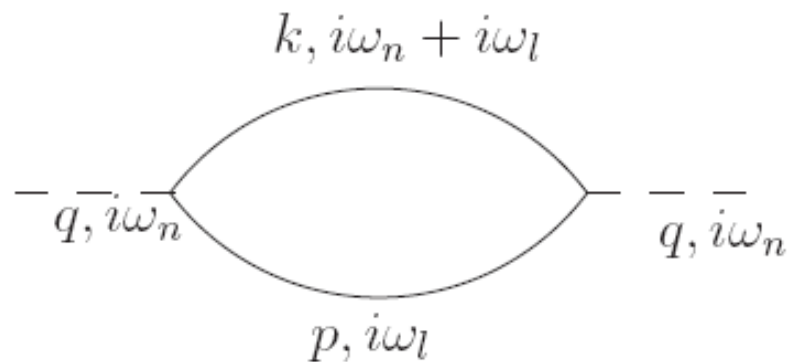
FPU-Cubic Chain

The cubic case is very different from the quartic case. Physically the interaction requires generation of two phonons from one or vice versa. However, the energy dependence is such that momentum and energy conservation cannot be satisfied simultaneously in such processes. Thus the basic diagrams give a zero answer.

This calculation needs to be done self-consistently. This is done by using dressed propagators for internal lines. This leads to an integral equation for the relaxation rate γ_q

$$\gamma_q = Tq^2 \int_0^{2\pi} \frac{dp}{\gamma_p + \gamma_{p+q}}$$

This is a singular integral equation. If we set q=0 , the integral diverges if we take $\gamma_q \sim q^2$. The self-consistent solution is

$$\gamma_q = T^{\frac{1}{2}} q^{\frac{3}{2}}$$
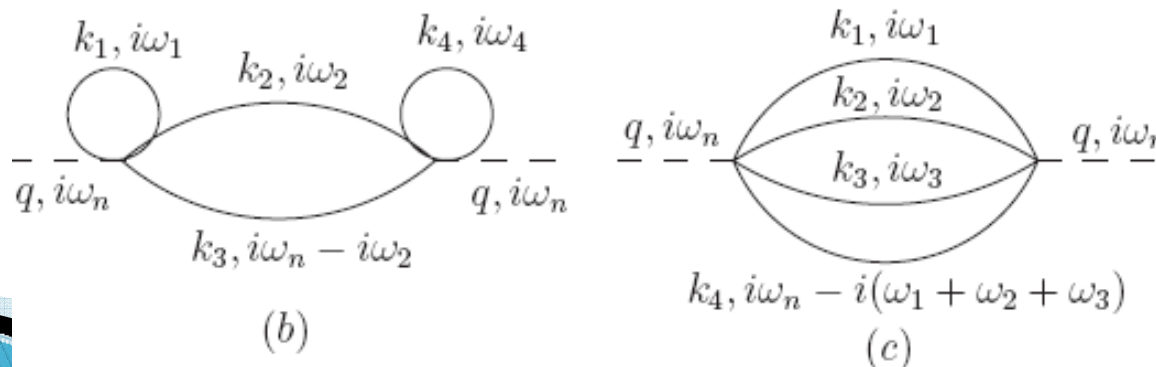
Higher odd power potentials

$V_5 = (g/5! \ N^3) \ \Sigma v(k_1,k_2,k_3,k_4,k_5) A(k_1) \ A(k_2) A(k_3) \ A(k_4) \ A(k_5)$

$v(k_1,k_2,k_3,k_4,k_5) = \Pi_i \ [\gamma(k_i)/\omega \ (k_i)] \ \Delta \ (k_1+k_2+k_3+k_4+k_5)$

Self-Energy Diagrams

$\Gamma_q \sim \beta\omega_q^2$ x collision integral

The collision integral is singular for some processes. It turns out to be regular for the new diagrams (c). (b) gives same the contribution same as cubic. This remains true for higher order odd potentials. Thus there is a universal answer.

(b)

(c)

Higher even power Potentials

Above arguments show that for all odd potentials to leading order in q, $\gamma_q = q^{3/2}$. Higher power odd potentials simply renormalize the cubic potential. The additional processes contribute terms of order q^2. This gives $\alpha = 1/3$.

Generalization to higher order even powers is more tedious, due to involvement of many umklapp processes. However our preliminary results indicate that only one scattering integral corresponding to 4th order potential is singular. The higher orders renormalize the 4th order vertex and contribute terms proportional to q^2. This leads to

$$\gamma_q \propto q^{5/3}$$

Summary

- A systematic evaluation of the conductivity of a quantum chain with quartic nonlinearity has been made in the low phonon density limit. This calculation shows that thermal resistance arises due to Umklapp scattering of phonons.

- The phonon relaxation rate γ_q goes as $q^{5/3}$ and conductivity diverges with chain length as $L^{2/5}$. Preliminary results show this to be true for all even potentials.

- We have also considered chains with nonlinear potentials of odd power. For such potentials, we find a **universal behavior**. γ_q goes as $q^{3/2}$ and conductivity diverges with chain length as $L^{1/3}$.
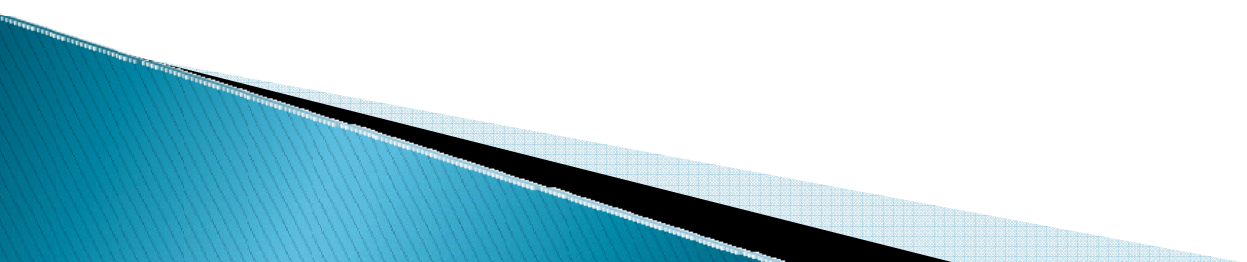
References

Santhosh G. and Deepak Kumar,

Phys. Rev. E 76, 021105 (2007)
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Phys. Rev. E 77, 011113 (2008)
Phys. Rev. E 82, 011130 (2010)

Second law of Thermodynamics

The irreversibility is understood by introducing the thermodynamic attribute of Entropy for the equilibrium states of the system. When the state changes the Entropy increases, except when the change is thermodynamically reversible. **Boltzmann provided microscopic understanding of Entropy and the Second law**
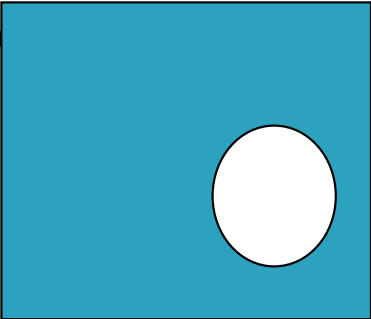
$$S = k_B \ln W$$

W = No. of microscopic states for a given set of macroscopic parameters like energy, volume, magnetization etc.
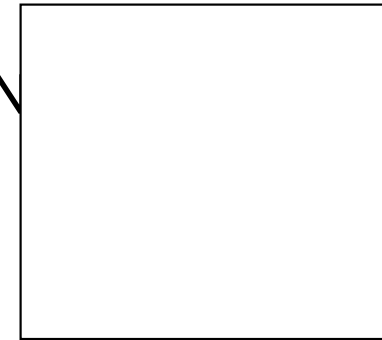
Probability of a state with a given set of macroscopic or thermodynamic parameters is proportional to W.

Irreversibility : Configurations of lower probability go over to configurations of higher probability

low entropy state   high entropy state

Proportional to $(\delta V/V)^N$

Can we not reverse the motions to go from right state to the left state? This is permitted by time reversal. It is possible, but highly improbable for a large system.

Thus the 2nd law is not certain, but it is overwhelmingly probable for large systems.

Understanding Transport

While for equilibrium, Statistical Mechanics provides
the connection between Hamiltonian and thermodynamics,
Non-equilibrium phenomena is much more difficult to derive
from basic dynamical laws.

Have these phenomenological laws, like Fourier's law, been
derived starting from microscopic dynamics? Such transport
laws require the establishment of local equilibrium.

Equilibrium arises due to exchange of energy, momentum etc.
between degrees of freedom due to their interaction. For
example if a particle with large(small) velocity is injected in a
gas it loses(gains) its excess(deficit) energy above (below)
the equilibrium value, by colliding with other particles. Only
if this process occurs sufficiently fast and happens in a
small enough region, would we have local equilibrium.

Numerical Studies

Studies on other systems give exponent α as: Toda lattice 0.4,
Hard sphere gas 0.33, FPU chain with cubic nonlinearity 0.44.

To examine the robustness of these exponent values for vibrational chains, we studied a chain with second-neighbour
couplings. We found a value of $\alpha = 0.4$ at small coupling but
the value rises as the coupling strength increases. This is surprising as the second-neighbour coupling only changes the dispersion of the phonon. The certainity of numerical results is limited by the size of the simulation.

To summarize there are some hints about the universality, and
two values seem dominant, 2/5 and 1/3. **Is there a truly universal behavior?**
How many universality classes are there?

Understanding Divergence Exponent α

Theoretical Approaches

a) Mode-Coupling Method: Constructs a nonlinear equation for the mode Correlation function, $G(q,,t)$. The recent calculation by Delfini et al. (Phys. Rev. E73, 060201)

gives answers that depend on the nonlinearity of the potential. For the cubic potential,

$$G(q,t) \approx \exp(-bq^2\, t^{4/3})$$
$$\alpha = 1/3 \quad (\tau_q^{-1} \propto q^{3/2}),$$

while for the quartic potential

$$G(q,t) \approx \exp(-bq^2\, t)$$
$$\alpha = 1/2 \quad (\tau_q^{-1} \propto q^2),$$

▸

. A fractional value of α implies a non-analytic wave vector dependence of the relaxation rate of the mode $\gamma_q = \tau_q^{-1} \propto q^\beta$ where $\beta = 1/(1-\alpha)$. Here $\beta = 5/3$.

Outline

- Introduction
- Survey of the numerical results
- Theoretical results for the classical chain
- Quantum chain
    - a. Conductivity for the quartic potential
    - b. Mode relaxation for the cubic potential
    - c. Universality for the odd potentials
- Summary
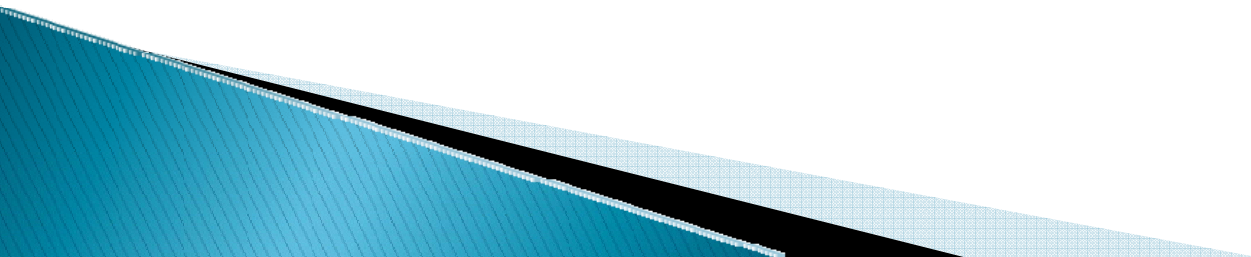
Theoretical Approaches for Mode Relaxation

- Boltzmann equation approach: Studies relaxation of the energy of a mode with wavevector **q** . Pereverzev, Phys. Rev. E68, 056124 (2003) This approach gives a mode relaxation rate, $\gamma_q = \tau_q^{-1} \propto q^{5/3}$ for the quartic nonlinearity

- But the mechanism is very different from mode-coupling theory. Here the result comes from the study of mode relaxation due to scattering from other modes. Umklapp process is responsible and the collision integral has a singularity.

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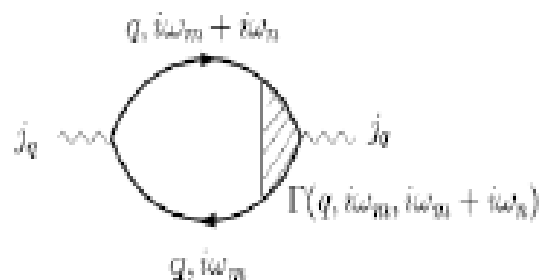appr[...]
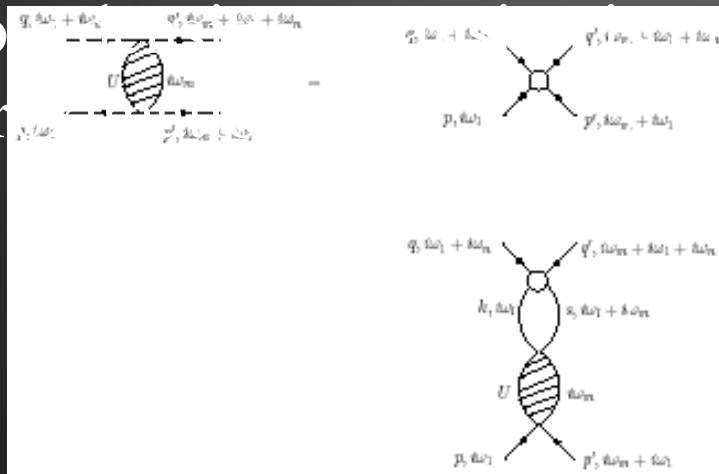
Quantum Calculation of κ

$$\Lambda(q, i w_m + i w_n, i w_m) = j_q - \frac{1}{N\beta} \sum_{q, w_l} U(q, p, q, p; i w_l - i w_m) G(p, i w_l + i w_n) G$$

Where G is the single particle Green's function