

MOCK LECTURE – INTERVIEW

Handout | Mini-lecture on 1D heat flow in a metal

Expected learning outcome. Understanding the meaning of the heat equation.

1. Summary of relevant laws

1.1 The first law of thermodynamics

The first law of thermodynamics is the principle of conservation of energy applied to thermodynamics systems. In a thermodynamic system, the change in internal energy U of a system that does not exchange matter with the environment and does not change its inner composition equals the amount of heat Q transferred to the system and the work W done by the surrounding to the system.

$$\Delta U = Q + W \tag{1}$$

We note that in the absence of work ($W=0$), and in its differential form, the first law of thermodynamics can be written as:

$$dU = \delta Q \tag{2}$$

This identity encapsulates the conservation of energy at a microscopical level for a closed thermodynamic system in the absence of work. Eq. 2 is also useful mathematically. U is a state variable and does not depend on paths of integrals whereas Q is not, hence the inexact differential δ .

1.2 The second law of thermodynamics

The second law of thermodynamics states that without work or changes of chemical composition, heats flow always from a hotter to a colder thermodynamic subsystem. In its differential form, the second law of thermodynamics relates to entropy S of a system.

$$dS \geq \frac{\delta Q}{T} \tag{3}$$

The identity holds only for closed systems and reversible processes. The inequality holds for irreversible processes, for example, the cooling of an object. Generally, for any irreversible process, entropy tends to increase. Macroscopically, a thermodynamic system relaxes onto a more homogeneous state.

1.3 The Fourier's Law

The second law of thermodynamics states that heat flows from an object of higher temperature to one of lower temperature. Empirically, we know that the local heat flow J is inversely proportional to the temperature gradient.

$$\vec{J} = \frac{\Delta Q}{\Delta t} \propto -\vec{\nabla} T \quad (3)$$

The proportionality constant is often denoted with k , *i.e.*, the thermal conductivity [$\text{Js}^{-1}\text{m}^{-1}\text{K}^{-1}$]. We have also shown that in its one-dimensional form, the Fourier's Law is:

$$J_x = \frac{\delta Q}{dt} = -k \frac{dT}{dx} \quad (4)$$

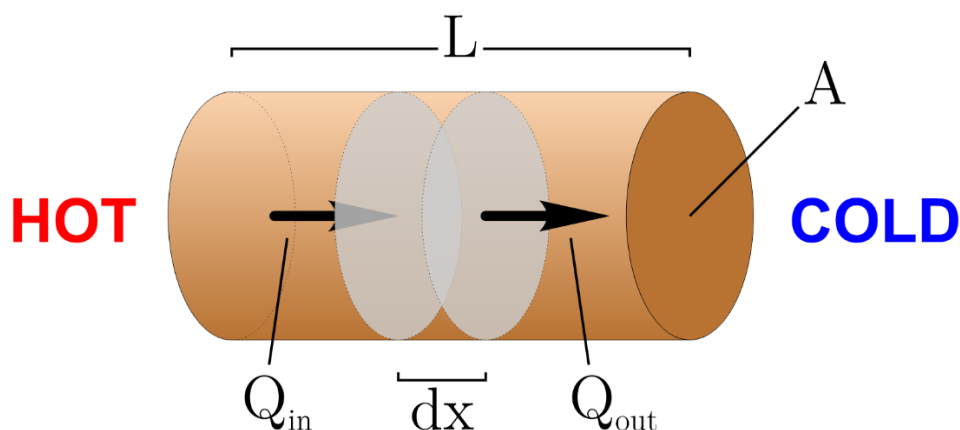
We note that k can be expressed in terms of the geometrical properties of the materials, for example, as per units of length (L) of the material and area (A) through which the heat flow passes (*e.g.*, the cross-section of a metal bar). In these cases, the thermal conductivity is expressed as the product of the thermal conductance κ [$\text{Js}^{-1}\text{K}^{-1}$] to AL^{-1} .

2. One-dimensional heat equation

How does the temperature of a thermodynamic system evolve in space and time? The answer to this question is provided by the heat equation, a partial differential equation. We can derive the heat equation for a one-dimensional system in a simple way considering a number of assumptions.

- Specific heat (c), thermal conductivity (k) and density (ρ) of the material constant and uniform.
- No heat source or sink in the system.
- Perfectly insulated, long thin bar ($L^2 \gg A$).
- The Fourier's Law

For a practical example, let's consider a long bar of copper, perfectly isolated from the environment. Let's focus on an element of volume of the copper bar of thickness dx .



Let's also recall Fourier's Law (eq. 4):

$$\frac{\delta Q}{dt} = -k \frac{dT}{dx}$$

From the Fourier's Law we know that heat will flow from the hot to the cold end of the bar, *i.e.*, there will be a heat flux (Q_{in}) entering and exiting (Q_{out}) the volume element $A dx$.

The net heat transferred into the volume element will be thus:

$$\delta Q = dt \left(-\kappa A \frac{\partial T}{\partial x} \Big|_{x=a} + \kappa A \frac{\partial T}{\partial x} \Big|_{x=a+dx} \right) \quad (5)$$

From the first law of thermodynamics, we know that the inexact differential can be described by the differential of the state variable internal energy U .

$$dU = \kappa A dx \left(\frac{\partial T}{\partial x} \Big|_{x=a+dx} - \frac{\partial T}{\partial x} \Big|_{x=a} \right) \quad (6)$$

The difference in internal energy of the volume element $A dx$ between the times t and $t+dt$ is:

$$dU = c \rho A dx T_{x,t+dt} - c \rho A dx T_{x,t} \quad (7)$$

Where $\rho A dx$ is the mass of the slice of the copper bar under consideration. From Eqs. 6-7 we can then derive the heat equation.

$$c \rho A dx T_{x,t+dt} - T_{x,t} = \kappa A dx \left(\frac{\partial T}{\partial x} \Big|_{x=a+dx} - \frac{\partial T}{\partial x} \Big|_{x=a} \right) \quad (8)$$

Rearranging Eq. 8 we obtain:

$$\frac{T_{x,t+dt} - T_{x,t}}{dt} = \frac{\kappa}{c \rho} \frac{\frac{\partial T}{\partial x} \Big|_{x=a+dx} - \frac{\partial T}{\partial x} \Big|_{x=a}}{dx} \quad (9)$$

Which leads to:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (10)$$

That is the 1D heat equation, where α [m^2s^{-1}] is the thermal diffusivity of the material. The thermal diffusivity is the ratio of the thermal conductance (κ) to the specific heat capacity (c) and the density (ρ). The thermal diffusivity is the speed with which heat flow in a material to minimize temperature inhomogeneities. In substances with high thermal conductance, equilibrium can be reached faster. Materials with high heat capacity ($c\rho$) exhibits more 'inertia'

towards thermalization and they are slower to reach a steady state. They ‘like’ to store heat locally.

	Thermal Conductivity (Js ⁻¹ m ⁻¹ K ⁻¹)	Specific Heat Capacity (Jg ⁻¹ K ⁻¹)	Thermal Diffusivity mm ² s ⁻¹)	Density (kg m ⁻³)
Air	0.024	1	19	1.3
Argon	0.016	0.5	22	1.8
Water	0.59	4.2	0.14	1000
Alcohol	0.1	2.5	0.07	790
Polystyrene	0.03	1.1	0.77	38
Diamond	543	0.51	306	3500
Copper	390	0.39	111	8900
Brass	110	0.38	28	8600
Zinc	120	0.38	40	7100
Aluminium	237	0.89	97	2700

3. General properties of the heat equation

We will learn how to solve the heat equation by using initial (*e.g.*, the heat profile at time $t=0$) and two boundary conditions (*e.g.*, fixed $T(0,t)$ and $T(L,0)$). We can now appreciate the general properties of the heat equations.

The heat equation states that the local temperature change (the first derivative) is directly proportional to the curvature of the temperature profile (the second derivative).

For example, we can infer that at the steady-state (null first derivative):

$$\frac{\partial T}{\partial t} = 0 \Leftrightarrow \frac{\partial^2 T}{\partial x^2} = 0 \Leftrightarrow \frac{\partial T}{\partial x} = \text{const.} \quad (11)$$

The temperature profile will be a line. This means that for a linear material, its longitudinal temperature profile will decrease linearly from the hot to the cold end at steady state, *i.e.* if sufficient time for thermalization is passed and the ends are thermally connected to thermostats.

Away from steady state, the heat equation implies that hot spots will dissipate faster. Temperature inhomogeneity will thus disappear faster favouring the emergence of an homogenous temperature profile. This is indeed what we should expect from a thermodynamic system reaching equilibrium through an irreversible process, resulting in an increase of entropy.

3.1 Are heat waves really waves?

If they look like a wave and they are called waves, they must be waves... or not.

The heat equation is an instance of common PDEs found in physics but it is not an instance of the second order PDE describing waves, the wave equation.

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \quad (12)$$

Which are the differences between the heat equation (Eq. 10) and the wave equation (Eq. 12)?

Note the heat equation is a first order PDE in respect of time but the wave equation has a derivative of second order. This implies numerous differences. Can you infer physical properties of a 'heat wave' from the heat equation in relation to the wave equation?

Let's consider the copper rod. If we hit one end, we generate a longitudinal wave travelling to the opposite end with the equation described by Eq. 12. The sound wave will travel at speed ($v=Y^{0.5}\rho^{0.5}$) proportional to the square root of the ratio between the Young's modulus and the density of the material. Notably, a sound wave can reflect at the end of the rod and, in an ideal material, could travel indefinitely back and forward.

This is not the case for a 'heat wave' for example generated by a pulse of energy injected at one of the two ends of the copper rod. The heat equation describes a dissipative irreversible process. The wave will have maximum amplitude at $t=0$, and at any following time the maximum measurable temperature will be lower.

Also, the wave equation is time-invariant, *i.e.* a wave travelling back in time and a wave travelling forward are equally well described by Eq. 12. The heat equation describes a dissipative process in a mathematically consistent way only starting from the initial conditions.

3.2 What is diffusing in a solid!?

The heat equation is in fact a diffusion equation. If we indicate with ϕ the concentration of a diffusing substance, the change in space (1D case) and time of the substance are described by the diffusion equation:

$$\frac{\partial \phi}{\partial t} = D \frac{\partial^2 \phi}{\partial x^2} \quad (13)$$

Equation 13 is identical to the heat equation. Similarly to the heat equation, the diffusion equation is derived by the use of conservation of mass and the phenomenological law

$$J_x = -D \frac{d\phi}{dx} \quad (14)$$

Equation 14 is the Flick's first law and it is analogous to the Fourier's Law but applied to mass. The Flick's law encapsulate the observation that mass flows from areas of high concentrations

to areas of lower concentration, as the Fourier's Law enunciates for thermal energy encapsulating the principle of the second law of thermodynamics.

However, what does diffuse in a solid? A solid is a rigid body of matter where no diffusion occurs. Heat is the transfer of thermal energy by definition. At the molecular level, heat in a solid is the vibrational energy of molecules, but molecules are locked in their position.

In solid state physics we will learn how to model solids with quasi-particles called 'phonons', quantized lattice vibrations. At room temperature, phonons contribute for the most part of the heat capacity of a solid. We will also learn how to model metals with phonons and free electrons. Free electrons can be treated as an ideal gas of fermions to explain the high conductivity of metals.