

Heat Conduction

So far we have used the fundamental postulate to study experimental phenomena in a particular way. For a given phenomenon, we construct an isolated system with an internal variable. As the isolated system flips from one quantum state to another, the internal variable changes in time. Associated with each value of the internal variable is a subset of the quantum states of the isolated system, and the number of the quantum states in this subset. The fundamental postulate implies that the internal variable evolves in time to increase the number of quantum states in the subset.

This statement leads to an algebraic equation to determine the internal variable in equilibrium, and an ordinary differential equation to evolve the internal variable in time. We have used this procedure to model several phenomena, including

- a half glass of wine (<http://imechanica.org/node/290>),
- two systems in thermal contact (<http://imechanica.org/node/291>),
- two types of phase transition (<http://imechanica.org/node/4878>).

We now wish to study phenomena in which internal variables are represented by *time-dependent fields*. We do not change our perspective on the fundamental postulate. Rather, we change our way to describe internal variables, from using numbers to using fields. This change results in a change in mathematical tools, from algebraic equations and ordinary differential equations to partial differential equations.

Such a change, however, is not as profound as it may appear. Especially in our own time, fields are routinely discretized into numbers, and the computer solves algebraic equations to determine these numbers in equilibrium, or solves ordinary differential equations to evolve these numbers in time. The computer crunches numbers; it knows no partial differential equations.

We begin with a familiar phenomenon: heat conduction. We will first recall the theory of heat conduction presented in undergraduate textbooks. Inside a body is a time-dependent field of temperature. When the field is inhomogeneous, energy will flow from a place of high temperature to a place of low temperature. When the field is homogenous, energy will cease to flow.

We will then show that the above theory is consistent with the fundamental postulate. We would like to use this familiar phenomenon to describe a procedure that will allow us to formulate theories for other phenomena.

A field of material particles. We represent a thermal conductor by a field of material particles. At a macroscopic scale, the conductor is taken to be rigid and stationary, so that each material particle remains fixed in space. We label a material particle by its coordinate \mathbf{x} .

Each material particle is regarded as a system with a single independent variable: energy. Let u be the energy per unit volume. In general, u varies from particle to particle, and also varies with time. The aim of the theory is to evolve the field $u(\mathbf{x}, t)$ over time t .

Conservation of energy. Energy flows from one material particle to

another. Define heat flux by

$$\text{energy flux} = \frac{\text{energy across a plane}}{\text{area} \times \text{time}}$$

The heat flux is a time-dependent vector field, $J_i(\mathbf{x}, t)$. That is, for an element of area dA in the conductor, with unit vector n_i normal to the area, the energy per unit time across the area is $J_i n_i dA$.

Conservation of energy requires that

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} + \frac{\partial J_i(\mathbf{x}, t)}{\partial x_i} = 0.$$

This equation connects the scalar field $u(\mathbf{x}, t)$ to a vector field $J_i(\mathbf{x}, t)$. To evolve these fields, we need more equations.

Heat capacity. Because each material particle is modeled as a system of single independent variable, energy, all other variables of the system depend on energy. In particular, the temperature T of a material particle is a function of the energy. We will not be concerned with phase transition here, so that the temperature and the energy have a 1-to-1 relation. We can write energy as a function of temperature, $u(T)$. This function characterizes the thermodynamics of the material. The heat capacity is defined by

$$c = \frac{\partial u(T)}{\partial T}.$$

The heat capacity defined this way has the unit $\text{JK}^{-1}\text{m}^{-3}$. Heat capacity is material specific and in general varies with temperature, $c(T)$.

Thermal conductivity. In the conductor the temperature varies from one material particle to another material particle, and varies from time to time. That is, the temperature in the conductor is a time-dependent field, $T(\mathbf{x}, t)$. Energy flows from a particle of a high temperature to a particle of a low temperature. This statement is embodied in Fourier's law: the heat flux is proportional to the gradient of the temperature, namely,

$$J_i = -\kappa \frac{\partial T(\mathbf{x}, t)}{\partial x_i},$$

where κ , a positive quantity, is called thermal conductivity. Thermal conductivity is material specific and in general varies with temperature, $\kappa(T)$.

Diffusion equation. A combination of the above three equations gives

$$c(T) \frac{\partial T(\mathbf{x}, t)}{\partial t} = \frac{\partial}{\partial x_i} \left[\kappa(T) \frac{\partial T(\mathbf{x}, t)}{\partial x_i} \right].$$

This partial differential equation evolves the field of temperature, $T(\mathbf{x}, t)$, subject to initial and boundary conditions. The equation is known as the diffusion equation.

The two functions $c(T)$ and $\kappa(T)$ make the diffusion equation nonlinear. For most applications, the variations of the heat capacity and thermal

conductivity are small, and can be treated as constants. Consequently, the diffusion equation becomes

$$\frac{\partial T(\mathbf{x}, t)}{\partial t} = D \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \right) T(\mathbf{x}, t),$$

where

$$D = \frac{\kappa}{c}.$$

The diffusivity D is material specific, and has the unit

$$D = \frac{(\text{length})^2}{\text{time}}.$$

You can estimate the order of magnitude of the diffusivity of a stick by placing one end of the stick above a flame, and use your fingers to feel the temperature at the other end of the stick. The length of the stick, along with the time for the stick to conduct the heat of the flame to your fingers, gives you an estimate the diffusivity.

You must have solved some partial differential equations before, and may not wish to spend time on such activities here. But we should recall salient features of such solutions.

Equilibrium state. When the field of temperature is homogenous, the heat flux vanishes, and the conductor is said to be in an *equilibrium state*.

For example, when heat is added at one part of the conductor, the temperature is nearly homogenous in the conductor if the heat is added over a time scale larger than the time needed for the heat to diffuse across the conductor. The time needed for the heat to diffuse across the conductor increases with the size of the conductor:

$$t \sim \frac{L^2}{D},$$

where L is a characteristic length of the conductor. A representative value of the diffusivity for metals is $D \sim 10^{-4} \text{ m}^2/\text{s}$. For a conductor of size 1 m, the above time scale is 10^4 s. In this example, to add heat and maintain homogenous temperature, heat must be added over a time scale of hours.

Steady state. When the field of temperature is inhomogeneous, but is independent of time, the conductor is said to be in a *steady state*.

For example, a blade of a gas turbine is made of a superalloy, covered with a thermal barrier coating. The coating is made of zirconia, of thickness 200 μm and conductivity $\kappa = 2 \text{ WK}^{-1}\text{m}^{-1}$. The coating maintains a drop in temperature 100 K. In this example, the heat flux is

$$J = \kappa \frac{\text{temperature drop}}{\text{thickness}} = 10^6 \text{ W/m}^2.$$

The energy is produced by combustion of the fuel, and is taken away by a fluid flowing inside the superalloy. The thermal barrier coating maintain the

temperature drop, so that the fuel burns at a high temperature to gain a high efficiency, while the superalloy is maintained at a allowable temperature to sustain mechanical loads.

Transient state. When the field of temperature varies from one material particle to another, and from time to time, the conductor is said to be in a *transient state*.

For example, the field of temperature around us is transient. While the temperature on the surface of the earth suffers a seasonal change, the change in temperature under ground is negligible. You can solve a boundary-initial-value problem to show that the cyclic change in temperature decays with the depth into the ground. However, the essential result can be obtained by a dimensional consideration. The characteristic length for decay is

$$d \sim \sqrt{Dt_{\text{period}}}.$$

A representative value of diffusivity for soil is $D \sim 10^{-6} \text{ m}^2/\text{s}$. The time period of one year is $t_{\text{period}} \sim 10^8 \text{ s}$. Consequently, the depth is about $d \sim 10 \text{ m}$. Cavemen living underground below this level would feel no seasonal change of temperature.

A thermodynamic model of a material particle. We now wish to reformulate the above theory, starting from the fundamental postulate. So far as heat conduction is concerned, this alternative formulation will add nothing new to the theory. This lack of novelty need not disappoint us. The alternative formulation will aid us in formulating theories for more complex phenomena. Besides, it is always good to link theoretical ideas.

Once again we represent a heat conductor by a field of *material particles*. We model each material particle as a system with a single independent variable: energy. For example, the material particle does not deform. Nor does the material particle gain or lose molecules.

Let u be the energy per unit volume, and s be the entropy per unit volume. A thermodynamic model of the material particle is specified by a function

$$s = s(u).$$

For a given material, this function is usually determined experimentally (<http://imechanica.org/node/291>). The temperature of the material particle, T , is given by

$$\frac{1}{T} = \frac{\partial s(u)}{\partial u}.$$

We can also use temperature as an independent variable, and express the energy and the entropy as functions of the temperature, $u(T)$ and $s(T)$. The heat capacity is defined by

$$c = \frac{\partial u(T)}{\partial T}.$$

The heat capacity defined this way has the unit $\text{JK}^{-1}\text{m}^{-3}$. Heat capacity is material specific and in general varies with temperature, $c(T)$.

For a quantity f associated with the material particle, a small change in the quantity is represented by the symbol δf . In practice, the thermodynamics of a material is often described by reporting the experimentally determined function $c(T)$. The energy $u(T)$ can be determined by integrating

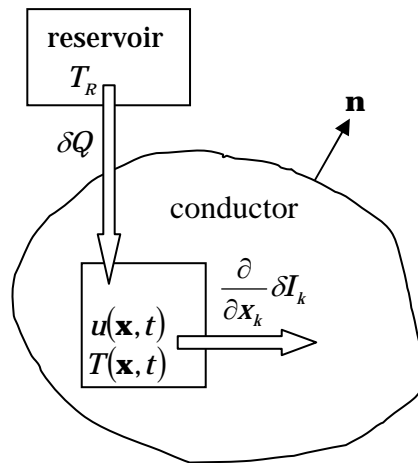
$$\delta u = c(T)\delta T.$$

The entropy $s(T)$ can be determined by integrating

$$\delta s = \frac{c(T)}{T} \delta T.$$

The conductor is taken to be rigid and stationary. We label each material particle by its coordinate \mathbf{x} . The energy density varies from particle to particle, and from time to time. That is, the energy density is a time-dependent field, $u(\mathbf{x}, t)$. So are the entropy density $s(\mathbf{x}, t)$ and temperature $T(\mathbf{x}, t)$.

For a homogenous material, the function $s(u)$ is the same for all material particles and for all time. Once any one of the three fields, $u(\mathbf{x}, t)$, $s(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$, is known, the other two fields can be calculated by invoking the basic relations given above.



Conservation of energy. Each material particle is in thermal contact with a heat reservoir, held at temperature T_R . The temperature of the reservoir, T_R , needs not be the same as that of the material particle, T . The conductor as a whole is in thermal contact with a field of reservoirs, held at a field of temperature, $T_R(\mathbf{x}, t)$. Let an element of the volume of the conductor, dV , receive from a reservoir an amount of energy $Q(\mathbf{x}, t)dV$. Let an element of the surface of the conductor, dA , receive from a reservoir an amount of energy $q(\mathbf{x}, t)dA$.

Let n_k be a unit vector normal to a plane, and let $n_k I_k(\mathbf{x}, t)$ be the amount of energy across unit area of the plane. The conservation of energy requires that

$$\delta u + \frac{\partial}{\partial \mathbf{x}_k} \delta I_k = \delta Q$$

in each element of the volume, and

$$\delta I_k n_k = -\delta q$$

on each element of the surface.

An isolated system with internal variables. The conductor and the field of reservoirs together constitute an isolated system. For this isolated system, we have identified six fields of internal variables:

$$u(\mathbf{x}, t), s(\mathbf{x}, t), T(\mathbf{x}, t), I_k(\mathbf{x}, t), Q(\mathbf{x}, t), q(\mathbf{x}, t).$$

These six fields are subject to the constraints of the thermodynamic model of the material and conservation of energy. Consequently, only some of these fields can vary independently. For example, here is a choice of independent internal variables:

$$I_k(\mathbf{x}, t), Q(\mathbf{x}, t), q(\mathbf{x}, t).$$

That is, once we know the energy added to a material particle from the reservoir and from neighboring material particles, the conservation of energy determines variation of the energy of the material particle, and the thermodynamic model of the material determines the entropy and the temperature of the material particle.

How entropy of the isolated system varies with the internal variables. The isolated system flips among a set of quantum states. A subset of the quantum states with given values of the internal variables constitute a macrostate of the isolated system. We need to count the number of quantum states in each of the macrostates of the composite. That is, we need to relate the entropy of the composite to the independent internal variables.

When the independent internal variables vary by small amounts, the entropy of the field of reservoirs varies by

$$-\int \frac{\delta Q}{T_R} dV - \int \frac{\delta q}{T_R} dA,$$

and the entropy of the conductor varies by

$$\begin{aligned} \int \delta s dV &= \int \frac{\delta u}{T} dV \\ &= \int \frac{1}{T} \left(\delta Q - \frac{\partial}{\partial \mathbf{x}_k} \delta I_k \right) dV \\ &= \int \frac{\delta Q}{T} dV + \int \frac{\delta q}{T} dA + \int \frac{\partial}{\partial \mathbf{x}_k} \left(\frac{1}{T} \right) \delta I_k dV \end{aligned}$$

The above equation expresses the variation in the entropy of the conductor in terms of the variations of the independent internal variables. The last step invokes the divergence theorem, which is appended at the end of these notes.

The sum of the entropy of the conductor and that of the reservoirs gives the entropy of the composite. Consequently, when the independent internal variables vary by small amounts, the entropy of the composite varies by

$$\int \left(\frac{1}{T} - \frac{1}{T_R} \right) \delta Q dV + \int \left(\frac{1}{T} - \frac{1}{T_R} \right) \delta q dA + \int \frac{\partial}{\partial x_k} \left(\frac{1}{T} \right) \delta I_k dV.$$

Vary internal variables to increase the entropy of the isolated system. As the internal variables change, the macrostate also changes. The fundamental postulate implies that the internal variables evolve to increase the number of quantum states in the macrostate.

Each integral in the above expression of the variation in the entropy of macrostate involves an independent field of internal variable variables, $Q(\mathbf{x}, t)$, $q(\mathbf{x}, t)$, and $I_k(\mathbf{x}, t)$. Each field represents a distinct way to transfer energy to or from material particles. The fundamental postulate implies that the entropy of the composite increases for every possible way of variation in the internal variables. Consequently, each integrand must be positive-definite:

$$\begin{aligned} \left(\frac{1}{T} - \frac{1}{T_R} \right) \delta q &\geq 0, \\ \left(\frac{1}{T} - \frac{1}{T_R} \right) \delta Q &\geq 0, \\ \frac{\partial}{\partial x_k} \left(\frac{1}{T} \right) \delta I_k &\geq 0. \end{aligned}$$

Kinetic models. Let us look at these conditions one by one. The first condition may be satisfied in several ways. For example, the surface of the conductor may be in thermal equilibrium with the reservoirs, so that

$$T = T_R.$$

We say that the temperature at the surface of the conductor is prescribed.

As a second way to satisfy the condition, the surface of the conductor may be insulated, $\delta q = 0$. We say that the heat flux at the surface of the conductor is prescribed to be zero.

As a third way to satisfy the condition, we can make the two factors of the product have the same sign. For example, we can set

$$\frac{\partial q(\mathbf{x}, t)}{\partial t} = K(T_R - T).$$

where $K > 0$ is known as the conductance. We say that the interface between the conductor and the reservoir have a finite conductance.

The second condition can be similarly satisfied.

The third condition is satisfied if we assume that the two factors have the same sign. Note that $J_i = \partial I(\mathbf{x}, t) / \partial t$. We can satisfy the inequality if we assume that the heat flux is linear in the temperature gradient:

$$J_i = -\kappa(T) \frac{\partial T(\mathbf{x}, t)}{\partial x_i},$$

with $\kappa(T) > 0$. This relation recovers Fourier's law.

As a generalization, we can satisfy the inequality by assuming that

$$J_i = -\kappa_{ij} \frac{\partial T(\mathbf{x}, t)}{\partial x_j},$$

where κ_{ij} is a symmetric and positive-definite tensor. This model is suitable for anisotropic conductors. Further generalization is possible, but we will not pursue them here.

Divergence theorem. This is a theorem in calculus. Let $f(x_1, x_2, x_3)$ be a function defined in a volume in the space (x_1, x_2, x_3) , and n_i be the unit vector normal to the surface enclosing the volume. The divergence theorem states that

$$\int \frac{\partial f}{\partial x_i} dV = \int f n_i dA.$$

The integral on the left-hand side extends over the volume, and the integral on the right-hand side extends over the surface enclosing the volume.