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1980 J. Phys. A: Math. Gen. 13 767

(http://iopscience.iop.org/0305-4470/13/2/038)

J. Phys. A: Math. Gen., 13 (1980) 767–769. Printed in Great Britain

COMMENT

On the sign of $\ddot{S}$ for thermal conduction

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Received 5 April 1979

Abstract. It is shown that during thermal conduction the second time-derivative of the entropy will be negative if a certain inequality concerning the temperature variation of the specific heat and that of the thermal conductivity is satisfied. Consideration is given to when the inequality will hold.

Over the past few years there has been considerable interest in showing that during the passage to equilibrium for various isolated systems, the second time derivative of the entropy S can never become positive, that is

$$d^2S/dt^2 \leqslant 0 \tag{1}$$

(Harris 1967, 1968a, b, 1971, Maass 1970, McElwain *et al* 1969, Mihaljan 1978, Pritchard 1975, Pritchard *et al* 1974, Ray 1978, Rouse and Simons 1976, Shear 1968, Simons 1969, 1970, 1971a, b, 1972, 1976, West 1978, Yao 1971). Among the systems considered was that of thermal conduction (Simons 1971b). Here the result (1) was proved for the situation where the thermal conductivity K and the specific heat C were both assumed to be independent of temperature T, since this independence greatly simplifies the theoretical treatment. However, there remains, of course, to be considered the physically realistic situation when both K and C depend on T, and it is this which we treat below. A further motivation for this work is the incorrect conclusion recently reached by Mihaljan (1978), based on an incomplete analysis of the problem, that inequality (1) will only hold for thermal conduction if K is proportional to T^{-2}.

Consider heat flow in the x direction through an isolated system bounded by the planes $x = a$ and $x = b$. Then the temperature $T(x, t)$ within the system satisfies the conduction equation

$$CT_t = (KT_x)_x \tag{2}$$

with boundary conditions

$$T_x|_a = T_x|_b = 0, \tag{3}$$

where the subscript notation implies differentiation with respect to the corresponding variable. The rate of entropy production is given by Landau and Lifshitz (1959) in the form

$$S_t = \int_a^b \frac{K}{T^2} T_x^2 \, dx,$$

and hence

$$\ddot{S} = S_{tt} = \int_a^b \left[\frac{2K}{T^2} T_x T_{tx} + T_x^2 T_t \frac{\partial}{\partial T}\left(\frac{K}{T^2}\right)\right] \mathrm{d}x. \tag{4}$$

Now

$$\frac{\partial}{\partial x}\left(\frac{2K}{T^2} T_x T_t\right) = \frac{2K}{T^2} T_x T_{tx} + \frac{2K}{T^2} T_t T_{xx} + \frac{\partial}{\partial T}\left(\frac{2K}{T^2}\right) T_x^2 T_t.$$

On integrating this from $x = a$ to $x = b$ and using the boundary conditions (3), we may eliminate the first term in the integrand of equation (4) to yield

$$\ddot{S} = -\int_a^b \left[\frac{2K}{T^2} T_{xx} + \left(\frac{K}{T^2}\right)_T T_x^2\right] T_t \,\mathrm{d}x$$

$$= -\int_a^b \frac{1}{C}\left\{\frac{2K^2}{T^2} T_{xx}^2 + K_T\left(\frac{K}{T^2}\right)_T T_x^4 + \left[K\left(\frac{K}{T^2}\right)_T + \frac{2KK_T}{T^2}\right] T_x^2 T_{xx}\right\} \mathrm{d}x \tag{5}$$

on substituting for T_t from equation (2). Now, for any function $f(T)$, we have, on integrating 'by parts' and using the boundary conditions (3),

$$\int_a^b f(T) T_x^2 T_{xx} \,\mathrm{d}x = -\frac{1}{3}\int_a^b [f(T)]_T T_x^4 \,\mathrm{d}x, \tag{6}$$

and this may be used to eliminate the term in equation (5) involving $T_x^2 T_{xx}$. Thus we obtain

$$\ddot{S} = -\int_a^b \left\{\frac{2K^2}{CT^2} T_{xx}^2 + \left[\frac{K_T}{C}\left(\frac{K}{T^2}\right)_T - \frac{1}{3}\left(\frac{K}{C}\left(\frac{K}{T^2}\right)_T + \frac{2KK_T}{CT^2}\right)_T\right] T_x^4\right\} \mathrm{d}x, \tag{7}$$

and since the coefficient of T_x^4 in this equation is of uncertain sign, we cannot as yet prove inequality (1). To progress further it is now necessary to assume that both C and K are proportional to some power of T; that is, we take

$$C = C_0 T^c \qquad \text{and } K = K_0 T^k, \tag{8}$$

when equation (7) yields

$$\ddot{S} = -(K_0^2/C_0)\int_a^b [2T^{2k-c-2} T_{xx}^2 + (ck - k^2 + \tfrac{7}{3}k - \tfrac{2}{3}c - 2) T^{2k-c-4} T_x^4] \,\mathrm{d}x. \tag{9}$$

We now use Schwarz's inequality in the form

$$\int_a^b [f(x)]^2 \,\mathrm{d}x \int_a^b [g(x)]^2 \,\mathrm{d}x \geqslant \left|\int_a^b f(x) g(x) \,\mathrm{d}x\right|^2,$$

taking $f(x) = T^{k-\frac{1}{2}c-1} T_{xx}$ and $g(x) = T^{k-\frac{1}{2}c-2} T_x^2$. This gives

$$\int_a^b T^{2k-c-2} T_{xx}^2 \,\mathrm{d}x \int_a^b T^{2k-c-4} T_x^4 \,\mathrm{d}x \geqslant \left[\int_a^b T^{2k-c-3} T_{xx} T_x^2 \,\mathrm{d}x\right]^2$$

$$= \frac{(2k-c-3)^2}{9}\left[\int_a^b T^{2k-c-4} T_x^4 \,\mathrm{d}x\right]^2$$

on using equation (6). Since

$$\int_a^b T^{2k-c-4} T_x^4 \,\mathrm{d}x > 0,$$

this yields

$$\int_a^b T^{2k-c-2} T_{xx}^2 \, dx \geqslant \frac{(2k-c-3)^2}{9} \int_a^b T^{2k-c-4} T_x^4 \, dx,$$

and substituting from here for the first term in the integrand of equation (9) gives (since this term is positive)

$$\ddot{S} \leqslant \frac{K_0^2(k-2c)(k+c+3)}{9C_0} \int_a^b T^{2k-c-4} T_x^4 \, dx. \tag{10}$$

As generally $c \geqslant 0$ it follows that inequality (1) will hold if

$$-(c+3) \leqslant k \leqslant 2c. \tag{11}$$

For k outside this interval, whether or not inequality (1) holds remains undecided.

It follows from inequality (11) that in many—if not most—situations, inequality (1) will be satisfied. Thus it will hold for non-conductors, both at high temperatures where $c = 0$ and $k = -1$, and also at low temperatures where $c = 3$ and $k = 2$ or 3, depending on the principal phonon scattering mechanism (Ziman 1960). However, there is at least one situation for which the inequality (11) is not satisfied. This is the low-temperature situation for an infinite perfect crystal when Umklapp processes predominate. Under these circumstances, $K(T) \propto T^n \exp(\alpha/T)$ with $\alpha > 0$ (Ziman 1960), and it is clear that for sufficiently small T this will correspond to $K(T)$ being proportional to T^k with $k < -(c+3)$, and thus inequality (11) will not then be satisfied. Whether or not inequality (1) is then true remains as yet an open question.

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