Thermal and electrical transport formalism for electronic microstructures with many terminals

1990 J. Phys.: Condens. Matter 2 4869

(http://iopscience.iop.org/0953-8984/2/22/008)

J. Phys.: Condens. Matter **2** (1990) 4869–4878. Printed in the UK

Thermal and electrical transport formalism for electronic microstructures with many terminals

P N Butcher
Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Received 6 February 1990

Abstract. The Landauer–Buttiker formalism for an electronic microstructure with many terminals is extended to account for temperature changes in the reservoirs and heat fluxes in the terminals. Terminal relations are developed in the presence of an arbitrary applied magnetic induction field which becomes uniform in the neighbourhood of each terminal. They use temperature changes in the reservoirs and either chemical potential changes in the reservoirs or charge fluxes in the terminals as independent variables. In both cases formulae for the transport matrices are given in terms of the scattering matrix of the microstructure. Onsager symmetry relations and reciprocity theorems are given for electrical, thermal and thermoelectric configurations. The behaviour of quantum point contacts is outlined.

1. Introduction

In 1957 Landauer [1] proposed a formula for the electrical conductance of a two-terminal electron system. This has been expressed in a way which is convenient for many-terminal systems by Buttiker [2, 3]. The Buttiker formalism directly relates the conductance matrix **G** to the electron scattering matrix **S**. The formalism has been useful for the interpretation of experiments on low-dimensional systems relating to universal fluctuations [4, 5], Aharanov–Bohm oscillations [6], ballistic transport [7–9], the integer quantum Hall effect [10, 11] and its quenching at low magnetic fields [12, 13].

In this paper we derive corresponding formulae for the thermal and thermoelectric transport matrices which are associated with a microstructure. They are the terminal analogues of the local tensors describing thermopower, Peltier effect and thermal conductivity in bulk solids. In the macroscopic regime the local tensors determine the corresponding matrices via the solution of macroscopic conservation equations with appropriate boundary conditions. In the mesoscopic and ballistic regimes this is no longer the case. The thermal and thermoelectric transport matrices are controlled by Schrödinger's equation and, like **G**, they may be directly expressed in terms of **S**.

Universal fluctuations of thermopower have recently been measured [14]. That apart, there is no current experimental data on the thermal and thermoelectric transport matrices of mesoscopic and ballistic systems. Nevertheless, interesting and challenging experiments are easily envisaged and several authors have discussed the theory of thermal and thermoelectric transport in microstructures. Sivan and Imry [15] relate the fluxes of charge and heat in the terminals to chemical potentials and temperatures which are also measured in the terminals in a particular way. Esposito *et al* [16] discuss universal

0953-8984/90/224869 + 10 $03.50

fluctuations of thermopower. Kearney and Butcher [17] comment on that problem and they also discuss the analogue of the Wiedemann–Franz law. Finally, Streda [18] outlines a calculation of the thermopower of a quantum point contact. These discussions are all restricted to two-terminal microstructures in zero applied magnetic induction field.

We present here a general formalism in which the thermal transport matrices are expressed in terms of $\mathbf{S}$ for a microstructure with any number of terminals which is subjected to an applied magnetic induction field. To do so we relate the fluxes of charge and heat in the terminals to chemical potentials and temperatures in the reservoirs feeding the terminals. Buttiker has stressed the overall utility of proceeding in this way in the case of electrical measurements [2, 3]. His arguments are easily extended to thermal and thermoelectric measurements. The resulting formalism may be used to interpret experiments in which chemical potentials and temperatures are measured in the reservoirs. They may also be used to interpret experiments in which these quantities are measured in the terminals provided that the measurement procedures are defined. The results of Sivan and Imry [15], for example, may be recovered by using their definitions.

In the next section we remind the reader about the linear transport formalism for bulk solids. This familiar situation provides guidelines for the development of the corresponding theory for microstructures. In section 3 we outline the salient properties of the electron energy eigenstates in the terminals when a uniform magnetic induction field is present. The scattering matrix is discussed briefly in section 4. With these preliminaries out of the way, the many-terminal transport relations for a microstructure containing non-interacting electrons are easily written down in section 5. We initially given them a non-linear form which relates the fluxes of charge and heat in the terminals to the chemical potentials and temperatures in the reservoirs. Then we linearise the equations by assuming small departures from equilibrium. The formulae for the transport matrices in the linearised equations are given both exactly and as low temperature approximations which are particularly simple and instructive.

In the general linear analysis it is convenient to use the changes of the chemical potentials and temperatures in all the reservoirs as independent variables. However, the fluxes are all controlled by differences of these quantities and the total fluxes of charge and heat into the microstructure both vanish. In section 6 we use these observations to simplify the terminal relations. The simplified equations have the advantage that it is possible to invert them so as to use the charge fluxes in the terminals as independent variables instead of the changes of the chemical potentials in the reservoirs. This is analogous to what is usually done in bulk solids. In section 7, we discuss Onsager symmetry and reciprocity in electrical, thermal and thermoelectric configurations. Finally, in section 8, we outline the behaviour of quantum point contacts and indicate some ways in which the theory might usefully be extended.

2. Local relationships in bulk solids

In bulk solids, linear transport theory is summarised in expressions for the fluxes of charge $\boldsymbol{J}$ and heat $\boldsymbol{Q}$ in terms of the EMF $\boldsymbol{E}$ and the temperature gradient ∇T [19, 20]

$$\boldsymbol{J} = \sigma \boldsymbol{E} + \mathbf{L}\nabla T \tag{1a}$$

$$\boldsymbol{Q} = \mathbf{M}\boldsymbol{E} + \mathbf{N}\nabla T. \tag{1b}$$

In these equations both $\boldsymbol{E}$ and ∇T are supposed to be sufficiently small and slowly-varying for a quasi-static, linear approximation to $\boldsymbol{J}$ and $\boldsymbol{Q}$ to be appropriate. The coefficients in (1) are the conductivity tensor $\boldsymbol{\sigma}$ and thermoelectric and thermal transport tensors $\mathbf{L}$, $\mathbf{M}$ and $\mathbf{N}$. They have the Onsager symmetry properties [20, 21]

$$\boldsymbol{\sigma}(-\boldsymbol{B}) = \tilde{\boldsymbol{\sigma}}(\boldsymbol{B}) \tag{2a}$$

$$\mathbf{L}(-\boldsymbol{B}) = -\tilde{\mathbf{M}}(\boldsymbol{B})/T \tag{2b}$$

$$\mathbf{N}(-\boldsymbol{B}) = \tilde{\mathbf{N}}(\boldsymbol{B}). \tag{2c}$$

in a magnetic induction field $\boldsymbol{B}$ where T is the absolute temperature and $\tilde{\mathbf{P}}$ denotes the transpose of a matrix $\mathbf{P}$. Equation (2) is a consequence of the time-reversal symmetry of the underlying equations of motion of the particles in the solid [21].

Equation (1) is the theoretician's form of the local transport equations. Experimentalists prefer to replace $\boldsymbol{E}$ by $\boldsymbol{J}$ as an independent variable. Then (1) may be arranged in the form

$$\boldsymbol{E} = \boldsymbol{\rho}\boldsymbol{J} + \mathbf{S}\nabla T \tag{3a}$$

$$\boldsymbol{Q} = \boldsymbol{\pi}\boldsymbol{J} - \boldsymbol{\kappa}\nabla T \tag{3b}$$

where

$$\boldsymbol{\rho} = \boldsymbol{\sigma}^{-1} \tag{4a}$$

$$\mathbf{S} = -\boldsymbol{\rho}\mathbf{L} \tag{4b}$$

$$\boldsymbol{\pi} = \mathbf{M}\boldsymbol{\rho} \tag{4c}$$

$$\boldsymbol{\kappa} = \mathbf{M}\boldsymbol{\rho}\mathbf{L} - \mathbf{N} \tag{4d}$$

are respectively the resistivity, thermopower, Peltier and thermal conductivity tensors. These are the quantities which are usually measured in bulk solids. We see from (2) that they have the Onsager symmetry properties

$$\boldsymbol{\rho}(-\boldsymbol{B}) = \tilde{\boldsymbol{\rho}}(\boldsymbol{B}) \tag{5a}$$

$$\mathbf{S}(-\boldsymbol{B}) = \tilde{\boldsymbol{\pi}}(\boldsymbol{B})/T \tag{5b}$$

$$\boldsymbol{\kappa}(-\boldsymbol{B}) = \tilde{\boldsymbol{\kappa}}(\boldsymbol{B}). \tag{5c}$$

3. The electron states in the terminals

We follow Buttiker [2, 3] and suppose that free electrons with effective mass m^* enter the microstructure through ideal terminals in the form of long, straight electron waveguides. To discuss the energy eigenfunctions in a particular terminal it is convenient to introduce a local Cartesian coordinate system, $0xyz$, with $0z$ parallel to the axis of the terminal and z increasing towards the microstructure. The one-electron Hamiltonian is then

$$H = \frac{1}{2m^*}(\boldsymbol{p} + e\boldsymbol{A})^2 + V(x, y) \tag{6}$$

where $\boldsymbol{A}$ is the vector potential and $V(x, y)$ is the potential energy field confining the electrons in the terminal.

We suppose that the local magnetic induction field $\boldsymbol{B}$ is uniform and choose $\boldsymbol{A} = (-B_z y, 0, B_x y - B_y x)$ so that H does not involve z. Then the energy eigenfunctions take the form

$$\psi_{\alpha k}(x, y, z) = \ell^{-1/2} \exp(\mathrm{i}kz)\varphi_{\alpha k}(x, y) \tag{7a}$$

with energies

$$\varepsilon_{\alpha k} = E_\alpha(k) + h^2 k^2 / 2m^*. \tag{7b}$$

In (7*a*) ℓ is the length of the terminal considered and α labels the normalised transverse eigenfunctions $\varphi_{\alpha k}(x, y)$. These are determined, together with the transverse energies $E_\alpha(k)$, by the 2D Schrödinger equation

$$H\varphi_{\alpha k}(x, y) = \varepsilon_{\alpha k}\varphi_{\alpha k}(x, y) \tag{8}$$

in which $p_z = \hbar k$.

To quantise k we introduce periodic boundary conditions over the terminal length ℓ. Then we may verify that the diagonal matrix element $\langle \alpha k | v_z | \alpha k \rangle$ of the longitudinal velocity operator $v_z = (p_z + eA_z)/m^*$ is equal to the group velocity $v_{\alpha k} = \hbar^{-1}\, \mathrm{d}\varepsilon_{\alpha k}/\mathrm{d}k$ (cf [20]). Moreover, the density of states $N_{\alpha k}$ per unit energy range per unit length of the terminal is $N_{\alpha k} = (\pi\, \mathrm{d}\varepsilon_{\alpha k}/\mathrm{d}k)^{-1}$ when we introduce a factor 2 for spin degeneracy.

Hence

$$N_{\alpha k}\langle \alpha k | v_z | \alpha k \rangle = 2h^{-1}. \tag{9}$$

The elegance of the Landau–Buttiker formalism is due to this simple fundamental result.

In the above discussion we use a particular gauge to make the treatment transparent. However, the essential results are all gauge invariant. Thus, suppose that we change to a new gauge in which the vector potential becomes $\boldsymbol{A} = \boldsymbol{A} + \boldsymbol{\nabla}\chi$. Then $\psi_{\alpha k}$ is replaced by $\psi_{\alpha k} \exp(-\mathrm{i}e\chi/\hbar)$ and α and k may still be used to label the eigenfunctions. It is, therefore, easy to verify that $\varepsilon_{\alpha k}$, $N_{\alpha k}$, the diagonal matrix element of the longitudinal velocity operator and the fundamental result (9) remain the same in the new gauge.

4. The scattering matrix

The terminal transport relationships all involve the scattering matrix $\mathbf{S}$ evaluated at some value ε of the one-electron energy. In this section we outline the definition of $\mathbf{S}$ and discuss its symmetry properties.

The case in which $\boldsymbol{B} \to 0$ in the terminals is well known [2, 3]. Then $E_\alpha(k) = E_\alpha$ which is independent of k. We see from (7*b*) that the channels (i.e. eigenfunctions) with $E_\alpha > \varepsilon$ are evanescent and decay to zero away from the microstructure. In the asymptotic regions of the terminals we are therefore concerned only with the propagating channels with $E_\alpha < \varepsilon$. Equation (7*b*) determines $|k|$ for each propagating mode and we may identify an incident wave with $k = |k|$ and $v_{\alpha k} = h|k|/m^*$ and a reflected wave for which both these quantities are negated. The general case in which $\boldsymbol{B} \neq 0$ in the terminals is similar but more complicated because $E_\alpha(k)$ in (7*b*) depends on k in a way which involves the detailed structure of the terminals. Nevertheless, there are still evanescent channels which may be ignored and propagating channels with incident and reflected waves for which we write $k = k_\mathrm{i}$ and $k = k_\mathrm{r}$ respectively. They are distinguished by the sign of $v_{\alpha k}$: $v_{\alpha k_\mathrm{i}} > 0$ and $v_{\alpha k_\mathrm{r}} < 0$.

In the general case it is convenient to write the wave function in the asymptotic regions of the terminals in the form:

$$\psi = \sum_{\alpha} [a_\alpha(\ell/v_{\alpha k_i})^{1/2}\, \psi_{\alpha k_i} + b_\alpha\, (\ell/|v_{\alpha k_r}|)^{1/2}\, \psi_{\alpha k_r}]. \tag{10}$$

In (10) we have generalised the interpretation of α: it now labels a channel in *any* of the terminals and the sum ranges over the propagating modes in *all* the terminals. The square root factors have been introduced to give a convenient normalisation to the coefficients a_α and b_α of the incident and reflected waves. Their contributions to the longitudinal particle flux $\ell^{-1}\langle\psi|v_z|\psi\rangle$ are simply $|a_\alpha|^2$ and $-|b_\alpha|^2$ respectively.

The scattering matrix $\mathbf{S}$ determines the relation imposed by the microstructure between the coefficients $\boldsymbol{a} = \{a_\alpha\}$ of the incident waves and the coefficients $\boldsymbol{b} = \{b_\alpha\}$ of the reflected waves. We write the relation in the form

$$\boldsymbol{b} = \mathbf{S}\boldsymbol{a} \tag{11}$$

where $\boldsymbol{a}$ and $\boldsymbol{b}$ are column matrices. Since particles are conserved we must have (with the normalisation introduced above) $|\boldsymbol{b}|^2 = |\boldsymbol{a}|^2$ for all $\boldsymbol{a}$. Hence $\mathbf{S}$ is unitary, i.e. $\mathbf{S}^{-1} = \mathbf{S}\dagger$. Another important symmetry property of $\mathbf{S}$ follows from the time-reversal symmetry of Schrödinger's equation for the entire microstructure at energy ε. The Hamiltonian has the form (6) with $\boldsymbol{A}$ now describing the entire applied magnetic field $\boldsymbol{B}(\boldsymbol{r})$ and $V(x, y)$ replaced by the entire potential energy field $V(x, y, z)$. Now suppose that $\boldsymbol{B}(\boldsymbol{r})$ is reversed everywhere by changing the sign of $\boldsymbol{A}$. The new wave function for the entire system is the complex conjugate of the old one. Consequently, since complex conjugation interchanges incident and reflected waves, we have the time-reversal symmetry property: $\mathbf{S}(-\boldsymbol{B}) = [\mathbf{S}^{-1}(\boldsymbol{B})]^*$. Finally, when this property is combined with the unitary character of $\mathbf{S}$ we obtain the reciprocity relation $\mathbf{S}(-\boldsymbol{B}) = \mathbf{S}(\boldsymbol{B})$ [2, 3].

5. General terminal transport relations for microstructures

The terminal transport relations involve real quantities. The scattering matrix enters into them through the real matrix $\mathbf{T}$ of transmission and reflection probabilities with elements

$$\mathbf{T}_{\alpha\beta} = |\mathbf{S}_{\alpha\beta}|^2. \tag{12}$$

We see by inspection that $\mathbf{T}_{\alpha\beta}$ is the probability that an electron incident in channel β will appear in channel α, when $\alpha \neq \beta$, or will be reflected in channel β when $\alpha = \beta$. The reciprocity relation for $\mathbf{S}$ which is derived at the end of section 4 implies that $\mathbf{T}$ is transposed when the magnetic induction field is reversed, i.e.

$$\mathbf{T}_{\alpha\beta}(-\boldsymbol{B}) = \mathbf{T}_{\alpha\beta}(\boldsymbol{B}). \tag{13}$$

Moreover, the unitary nature of $\mathbf{S}$ may be exploited easily to show that

$$\sum_{\alpha} \mathbf{T}_{\alpha\beta} = \sum_{\beta} \mathbf{T}_{\alpha\beta} = 1. \tag{14}$$

We make extensive use of (13) and (14) in sections 6 and 7.

Following Buttiker [2, 3] and Sivan and Imry [15] we suppose that the occupation probability $f_\alpha(\varepsilon)$ of the incident wave in channel α is given by a Fermi–Dirac function:

$$f_\alpha(\varepsilon) = \{\exp[(\varepsilon - \mu_\alpha)/k_B T_\alpha] + 1\}^{-1} \tag{15}$$

where μ_α is the chemical potential and T_α is the temperature. Then the total charge flux towards the microstructure in channel α is

$$J_\alpha = -e \int d\varepsilon f_\alpha(\ell N_{\alpha k_i})(v_{\alpha k_i}/l) + e \sum_\beta \int d\varepsilon f_\beta(\ell N_{\beta k_i})(v_{\beta k_i}/\ell) T_{\alpha\beta}$$

$$= -e^{-1} \sum_\beta \int d\varepsilon f_\beta \Gamma_{\alpha\beta} \tag{16a}$$

where we have used (9) and

$$\Gamma_{\alpha\beta} = (2e^2/h)(\delta_{\alpha\beta} - T_{\alpha\beta}). \tag{16b}$$

Similarly, to obtain the total heat flux Q_α flowing towards the microstructure in channel α we have only to divide J_α by $-e$ and insert a factor $(\varepsilon - \mu_\alpha)$ in the integrand of (16*a*). Thus we obtain

$$Q_\alpha = e^{-2} \sum_\beta \int d\varepsilon_\beta \Gamma_{\alpha\beta}(\varepsilon - \mu_\alpha). \tag{16c}$$

In (16) it is left understood that α and β always refer to propagating channels.

To linearise (16) we put

$$\mu_\alpha = \mu - eV_\alpha \tag{17a}$$

and

$$T_\alpha = T - \theta_\alpha \tag{17b}$$

where eV_α and θ_α are small perturbations of the chemical potential and temperature in channel α from equilibrium values μ and T which are common to all channels. Then

$$f_\alpha \simeq f_0 + f_0'[eV_\alpha - (\varepsilon - \mu/T)\theta_\alpha] \tag{18}$$

where f_0 is given by (15) with $\mu_\alpha = \mu$ and $T_\alpha = T$ and f_0' is the energy derivative of f_0. (Minus signs have been used in (17) to enhance the analogy between the transport relations for microstructures and bulk solids). When (18) is substituted into (16) f_0 makes no contribution to J_α and Q_α because of (14). Hence we obtain

$$J_\alpha = \sum_\beta (G_{\alpha\beta} V_\beta + L_{\alpha\beta}\theta_\beta) \tag{19a}$$

$$Q_\alpha = \sum_\beta (M_{\alpha\beta} V_\beta + N_{\alpha\beta}\theta_\beta) \tag{19b}$$

where

$$G_{\alpha\beta} = -\int d\varepsilon f_0' \Gamma_{\alpha\beta} \simeq \Gamma_{\alpha\beta} \tag{20a}$$

$$L_{\alpha\beta} = -\frac{1}{eT} \int d\varepsilon f_0' \Gamma_{\alpha\beta}(\varepsilon - \mu) \simeq L_0 eT\Gamma'_{\alpha\beta} \tag{20b}$$

$$M_{\alpha\beta} = -TL_{\alpha\beta} \simeq -L_0 eT^2 \Gamma'_{\alpha\beta} \tag{20c}$$

$$N_{\alpha\beta} = \frac{1}{e^2 T}\int \mathrm{d}\varepsilon f_0' \Gamma_{\alpha\beta}(\varepsilon - \mu)^2 \simeq -L_0 T \Gamma_{\alpha\beta} \tag{20d}$$

with $L_0 = (\pi k_B/e)^2/3$ denoting the Lorenz number [19]. In each equation in (20) the first formula is exact. The second formula is the leading term in a Sommerfield expansion at low temperatures [19, 20] in which $\Gamma_{\alpha\beta}$ and its energy derivative $\Gamma'_{\alpha\beta}$ are evaluated at $\varepsilon = \mu$.

6. Simplification of the terminal transport relations for a microstructure

The similarity between the terminal relations (19) and the local relations (1) is obvious. However, some care is needed in developing the analogy. The Greek subscripts in (19) label propagating channels. We are more interested in terminals. Each terminal may contain several propagating channels which are all fed from a common reservoir so that they have common values of V_β and θ_β. Moreover, only the total fluxes of charge and heat in each terminal are accessible to measurement. To allow for these facets of the microstructure problem we have only to re-interpret α and β in (19) as terminal labels and replace $\Gamma_{\alpha\beta}$ in (20) by

$$\Gamma_{\alpha\beta} \rightarrow \sum_{\alpha'\beta'} \Gamma_{\alpha'\beta'} \tag{21}$$

where the summation is over all propagating channels α' in terminal α and β' in terminal β. Then the terminal relations may be written as matrix equations:

$$\boldsymbol{J} = \mathbf{G}\boldsymbol{V} + \mathbf{L}\boldsymbol{\theta} \tag{22a}$$

$$\boldsymbol{Q} = \mathbf{M}\boldsymbol{V} + \mathbf{N}\boldsymbol{\theta}. \tag{22b}$$

In (22), with N_t denoting the number of terminals, $\boldsymbol{J}$, $\boldsymbol{Q}$, $\boldsymbol{V}$ and $\boldsymbol{Q}$ are $N_t \times 1$ column matrices with elements J_α, Q_α, V_β and θ_β respectively. The elements of the $N_t \times N_t$ square matrices $\mathbf{G}$, $\mathbf{L}$, $\mathbf{M}$ and $\mathbf{N}$ are defined by (20) and (21).

Equations (22) may be further simplified because (14) and (20) show that the rows and columns of all the transport matrices in them sum to zero. The first property reflects the fact that $\boldsymbol{J}$ and $\boldsymbol{Q}$ are determined only by *differences* of the terminal voltages and temperatures. The second property reflects the fact that

$$\sum_\alpha J_\alpha = \sum_\alpha Q_\alpha = 0$$

because of particle conservation. We are therefore free to choose terminal N_t as a reference (ground) terminal at which we set $V_{N_t} = \theta_{N_t} = 0$. Moreover, we have no need to calculate J_{N_t} and Q_{N_t} because they may be determined subsequently from J_α and Q_α in the other terminals.

To take these observations into account we have only to remove the N_tth row and column from all the matrices in (22). We leave this operation understood. The reduced form of (22) gives a result closely analogous to the theoretician's form (1) of the local transport equations. Moreover, it has the advantage that $\mathbf{G}$ now has an inverse $\mathbf{R} = \mathbf{G}^{-1}$ so that we may rewrite the equations as

$$\boldsymbol{V} = \mathbf{R}\boldsymbol{J} + \mathbf{S}\theta \tag{23a}$$

$$\boldsymbol{Q} = \boldsymbol{\Pi}\boldsymbol{J} - \boldsymbol{\kappa}\boldsymbol{\theta} \tag{23b}$$

which are the analogues of the experimentalist's form (3) of the local transport relations. The $(N_t - 1) \times (N_t - 1)$ matrices $\mathbf{R}$, $\mathbf{S}$, $\mathbf{\Pi}$ and $\boldsymbol{\kappa}$ in (23) are given in terms of those in the reduced form of (22) by (4) with $\mathbf{G}$ and $\mathbf{R}$ replacing $\boldsymbol{\sigma}$ and $\boldsymbol{\rho}$ respectively.

7. Onsager symmetry and reciprocity

The Onsager symmetry of the matrices in (19), in the reduced forms of (22) and in (23) are all dictated by (13). Together with (16*b*) this equation implies that $\Gamma_{\alpha\beta}(-\boldsymbol{B}) = \Gamma_{\beta\alpha}(\boldsymbol{B})$. Consequently, all the matrices in (19) and (22) are transposed when the magnetic induction field is reversed. Thus the Onsager symmetry relations (2*a*) and (2*c*) survive intact in the microstructure while (2*b*) is replaced by $\mathbf{L}(-\boldsymbol{B}) = \tilde{\mathbf{L}}(\boldsymbol{B})$. Equation (20*c*) also implies that $\mathbf{M} = -T\mathbf{L}$ in the microstructure so that we may recast this simple symmetry relation in a more complicated form which is analogous to (2*b*): $\mathbf{L}(-\boldsymbol{B}) = -\tilde{\mathbf{M}}(\boldsymbol{B})/T$.

The Onsager symmetry relations (5) all survive intact in a microstructure. In general (5*b*) cannot be simplified like (2*b*) because $\mathbf{R}$, which replaces $\boldsymbol{\rho}$ in (4), does not commute with $\mathbf{L}$ and $\mathbf{M}$. However, in a two-terminal network all the transport matrices in (23) reduce to scalars and we have the simple relation $\mathbf{\Pi} = -T\mathbf{S}$ in which both $\mathbf{\Pi}$ and $\mathbf{S}$ are even functions of $\boldsymbol{B}$.

Electrical reciprocity is discussed by Buttiker [2, 3]. It rests on the Onsager symmetry relation (2*a*) with $\boldsymbol{\sigma}$ replaced by $\mathbf{G}$. We give a simpler treatment which is easily extended to deal with thermal and thermoelectric reciprocity. Thus we set $\boldsymbol{\theta} = 0$ in the reduced form of (22*a*). Then, we have

$$\tilde{V}(-\boldsymbol{B})\boldsymbol{J}(\boldsymbol{B}) = \tilde{V}(-\boldsymbol{B})\mathbf{G}(\boldsymbol{B})V(\boldsymbol{B}) = \tilde{V}(\boldsymbol{B})\tilde{\mathbf{G}}(\boldsymbol{B})V(-\boldsymbol{B}) = \tilde{V}(\boldsymbol{B})\boldsymbol{J}(-\boldsymbol{B}). \tag{24}$$

Here $V(\pm\boldsymbol{B})$ is related to $\boldsymbol{J}(\pm\boldsymbol{B})$ by (22*a*) in magnetic induction fields $\pm\boldsymbol{B}$ but are otherwise arbitrary. In the second line of (24) we transpose the scalar product and in the last line we use $\mathbf{G}(\boldsymbol{B}) = \mathbf{G}(-\boldsymbol{B})$.

Let us consider a two-terminal network. When terminal 2 is grounded (24) gives

$$V_1(-\boldsymbol{B})/J_1(-\boldsymbol{B}) = V_1(\boldsymbol{B})/J_1(\boldsymbol{B}) \tag{25}$$

i.e. the two-terminal resistance is an even function of $\boldsymbol{B}$. Now consider a four-terminal network. When terminal 4 is grounded (24) gives

$$\sum_{\alpha=1}^{3} V_\alpha(-\boldsymbol{B})J_\alpha(\boldsymbol{B}) = \sum_{\alpha=1}^{3} V_\alpha(\boldsymbol{B})J_\alpha(-\boldsymbol{B}). \tag{26}$$

Suppose that, in the magnetic induction fields $+\boldsymbol{B}$ and $-\boldsymbol{B}$, we connect an ideal voltmeter between terminals 1 and 2 and between terminals 3 and 4 respectively. Then, for $+\boldsymbol{B}$ we have $J_1(\boldsymbol{B}) = J_2(\boldsymbol{B}) = 0$ and for $-\boldsymbol{B}$ we have $J_3(-\boldsymbol{B}) = J_4(-\boldsymbol{B}) = 0$ so that charge conservation gives $J_2(\boldsymbol{B}) = -J_1(\boldsymbol{B})$. Hence (26) reduces to

$$V_3(-\boldsymbol{B})/J_1(-\boldsymbol{B}) = (V_1(\boldsymbol{B}) - V_2(\boldsymbol{B}))/J_3(\boldsymbol{B}) \tag{27}$$

i.e.

$$R_{12,34}(-\boldsymbol{B}) = R_{34,12}(\boldsymbol{B}) \tag{28}$$

in the notation of Buttiker [2, 3]. Here: $R_{\alpha\beta,\gamma\delta}$ denotes a four-terminal resistance which is determined by measuring the voltage drop from γ to δ with an ideal voltmeter (which draws no current) and dividing it by a current which enters through α and leaves through

β. Equation (28) expresses the electrical reciprocity theorem: $R_{\alpha\beta,\gamma\delta}$ is unaltered when the current source and voltmeter are interchanged provided that $\boldsymbol{B}$ is reversed [2, 3].

Since $\mathbf{N}(\boldsymbol{B})$ and $\boldsymbol{\kappa}(\boldsymbol{B})$ have the same Onsager symmetry as $\mathbf{G}(\boldsymbol{B})$ we may immediately write down analagous reciprocity relations for thermal 'resistances' measured when $\boldsymbol{V} = 0$ or $\boldsymbol{J} = 0$ by using a heat flux source and an ideal temperature meter which draws no heat flux. Similarly, since $\mathbf{L}(\boldsymbol{B})$ and $\mathbf{M}(\boldsymbol{B})$ also have the same Onsager symmetry as $\mathbf{G}(\boldsymbol{B})$, we may also write down analagous reciprocity relations for thermoelectric 'resistances' measured (when $\boldsymbol{V} = 0$) by using a current source and an ideal temperature meter which transmits no charge flux and measured (when $\boldsymbol{\theta} = 0$) by using a heat flux source and an ideal voltmeter which transmits no heat flux. These relationships are not readily tested experimentally. Most importantly: when $\boldsymbol{J} = 0$, which is the usual situation in thermopower measurements, no four-terminal reciprocity exists because $\mathbf{S}(-\boldsymbol{B}) \neq \tilde{\mathbf{S}}(\boldsymbol{B})$. In the two-terminal case, however, all the transport matrices, including $\mathbf{S}$, reduce to scalars which are even functions of $\boldsymbol{B}$.

8. Conclusion

The transport relations in the general form (19), in the reduced form of (22), or in the alternative form (23), all give a complete description of the linear electrical, thermal and thermoelectric transport properties of a microstructure. The formulae (20) and (21) for the transport matrices are exact when the microstructure contains independent electrons which do not have any phase-breaking interactions with another system, e.g. phonons. They have the transparent simplicity which is characteristic of the Landauer–Buttiker formalism. Nevertheless, *evaluating* the formulae is complicated when there are many terminals.

We confine our attention here to some brief remarks about the low temperature behaviour of ideal quantum point contacts which have only two terminals and very simple scattering properties [7, 8]. An electron which is incident in terminal 1 is either totally reflected or is totally transmitted to terminal 2. Hence we see from (16*b*) that $\Gamma_{11} = (2e^2/h)N_c$ where N_c is the number of transmitted channels. Hence, (20) and (21) predict the staircase structure for G_{11} which has been observed [7, 8]. More importantly, we may immediately derive the Wiedemann–Franz law $\kappa_{11} = L_0 T G_{11}$ from (20), (21) and (4) so that κ_{11} is expected to show similar behaviour. Finally, as Streda has pointed out [18] equations (20), (21) and (4) also imply that S_{11} will exhibit negative peaks which are associated with the steps in G_{11}. The shape of the peaks has been calculated by Cantrell and Butcher in another connection [22]. Experimental studies of the thermal and thermoelectric behaviour of quantum point contracts would therefore be of great interest.

The theory developed here puts the formulae for the thermal and thermoelectric matrices of a microstructure with many terminals on the same footing as those for the conductance matrix. For simplicity we have ignored spin-splitting, spin–orbit coupling and the effects of periodic crystal fields. Further development of the formalism is required to take account of these effects. The incorporation of electron–phonon coupling would greatly enhance the scope of the theory. Finally, and most importantly, thermal and thermoelectric measurements on microstructures with more than two terminals present an interesting experimental challenge.

References

[1] Landauer R 1957 *IBM J. Res. Dev.* **1** 223
[2] Buttiker M 1986 *Phys. Rev. Lett.* **57** 1761
[3] Buttiker M 1988 *IBM J. Res. Dev.* **32** 317
[4] Stone A D 1985 *Phys. Rev. Lett.* **54** 2692
[5] Washburn S 1988 *IBM J. Res. Dev.* **32** 335
[6] Washburn S and Webb R A 1985 *Adv. Phys.* **35** 375
[7] van Wees B J, van Houten H, Beenakker C W J, Williamson J G, Kouenhoven L P, van der Marel D and Foxon C T 1988 *Phys. Rev. Lett.* **60** 848
[8] Wharan D A, Thornton D J, Newbury R, Pepper M, Ahmed H, Frost J E F, Hasko D J, Peacock D C, Richie D A and Jones G A C *J. Phys. C: Solid State Phys.* **21** L209
[9] Stone A D and Szafer A 1989 *Phys. Rev. Lett.* **62** 300
[10] Buttiker M 1988 *Phys. Rev.* B **38** 9375
[11] Beenakker C W J and van Houten H 1988 *Phys. Rev. Lett.* **60** 2406
[12] Kliczenov G 1989 *Phys. Rev. Lett.* **62** 2993
[13] Buttiker M 1989 *Phys. Rev. Lett.* **62** 229
[14] Galloway T, Gallagher B L, Beton P, Oxley J P, Carter M, Beaumont S P, Thoms S and Wilkinson C D W 1989 *EP2D58 Grenoble, Workbook* p 558
[15] Sivan U and Imry Y 1986 *Phys. Rev.* B **33** 551
[16] Esposito F P, Goodman B and Ma M 1987 *Phys. Rev.* B **36** 4507
[17] Kearney M J and Butcher P N 1988 *J. Phys. C: Solid State Phys.* **21** L265
[18] Streda P 1989 *J. Phys.: Condens. Matter* **1** 1025
[19] Wilson A H 1954 *The Theory of Metals* (Cambridge: Cambridge University Press)
[20] Butcher P N 1973 *Electrons in Crystalline Solids* ed A Salam (Vienna: IAEA)
[21] Lax M 1974 *Symmetry Principles in Solid State and Molecular Physics* (New York: Wiley)
[22] Cantrell D G and Butcher P N 1985 *J. Phys. C: Solid State Phys.* **18** L587