PHYSICAL REVIEW B VOLUME 33, NUMBER 1 1 JANUARY 1986

# Multichannel Landauer formula for thermoelectric transport with application to thermopower near the mobility edge

U. Sivan and Y. Imry
*School of Physics and Astronomy, Tel Aviv University, 69978 Tel Aviv, Israel*

(Received 24 May 1985)

Various thermoelectric linear transport coefficients are defined and calculated for two reservoirs connected with ideal multichannel leads and a segment of an arbitrary disordered system. The reservoirs have different temperatures and chemical potentials. All of the inelastic scattering (and, thus, the dissipation) is assumed to occur only in the reservoirs. The definitions of the chemical potentials and temperature differences across the sample itself (mostly due to elastic scattering) are presented. Subtleties of the thermoelectric effects across the sample are discussed. The associated transport coefficients display deviations from the Onsager relations and from the Cutler-Mott formula for the thermopower (although the deviations vanish for a large number of channels and/or high resistance). The expression obtained is used to predict the critical behavior of the electronic thermopower near the mobility edge. It is shown to satisfy a scaling form in the temperature and separation from the mobility edge.

## I. INTRODUCTION AND DISCUSSION OF THE MODEL

In the studies of conduction in systems with strong elastic scattering,[1,2] or in the case of the quantum transport through small devices at low temperatures, the approach due to Landauer[3,4] has been extremely useful. In the original one-dimensional (1D) or single-channel case, the conductance of noninteracting electrons at a zero temperature, due to a barrier with transmission coefficient $T$ is given by (including spin degeneracy)

$$G=\frac{e^2}{\pi\hbar}\frac{T}{1-T} . \tag{1}$$

The generalization of Eq. (1) to finite temperatures and an analogous formula for the electronic thermal conductivity have been discussed by Engquist and Anderson.[5] The generalization to the many channel case (i.e., arbitrary dimensionality) has been the subject of several papers.[2,6–9] Here we shall adopt the approach of Büttiker *et al.*,[10,11] whose results are similar to those previously obtained by Azbel.[9]

These considerations are especially appropriate for calculating the transport coefficients of a sample due to arbitrary elastic scattering (the generalization including inelastic scattering will be discussed elsewhere[12]).

In this model,[10] described in Fig. 1, the elastic scatterer is fed by two ideal leads, each supporting $N$ conduction channels at the Fermi energy (due to, e.g., $N$ different transverse states of the ideal wire). These leads are driven from left and right by heat (and electron) reservoirs (HR) with chemical potentials $\mu_1,\mu_2$ and temperatures $\theta_1,\theta_2$, respectively.

All elastic processes in the sample are represented by a $2N\times 2N$ transfer matrix $S$ whose transmission $T_{ij},T'_{ij}$ and reflection $R_{ij},R'_{ij}$ coefficients can mix the left-hand side (lhs) and right-hand side (rhs) channels. [$T_{ij}$ ($T'_{ij}$) is the probability of an electron traveling to the right (left) in the $j$th channel on the lhs (rhs) to be transmitted into the $i$th channel on the rhs (lhs), and $R_{ij}$ ($R'_{ij}$) the probability of that electron to be back scattered into the $i$th channel on the lhs (rhs).]

We point out that in the model considered here, the thermalization of the electrons, by inelastic scattering, and hence the Joule energy dissipation occurs only in the outside HR's and not in the system itself.

We assume that the left HR maintains a Fermi distribution with chemical potential $\mu_1$ and temperature $\theta_1$ in the right propagating states in all channels on the lhs of the barrier. Similarly, the distribution of the left propagating states on the rhs is taken to be equal to that in the rhs HR. All other distributions, namely the distributions of left propagating electrons on the lhs and the right propagating electrons on the rhs are now determined only by the barrier properties. No interchannel scattering is taken to occur in the leads.

On the above model we may define a conductance between the outside reservoirs at zero temperature as the total current $I$ divided by the chemical potential difference

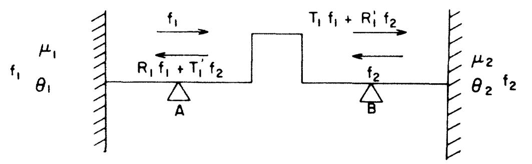

FIG. 1. Schematics of the model: Two HR's with chemical potentials $\mu_1,\mu_2$ and temperatures $\theta_1,\theta_2$ are connected via ideal leads and an arbitrary scatterer, represented by the barrier. The ingoing channels have the distributions of the appropriate HR's, $f_1$ and $f_2$. The distribution in the outgoing channels is determined by the transmission and reflection of the barrier. $A$ and $B$ are the measurement "points" for $\mu_A,\mu_B,\theta_A,\theta_B$.

between them:

$$G_c = \frac{I}{\mu_1 - \mu_2} = \frac{e^2}{\pi\hbar} \sum_{i,j=1}^{N} T_{ij} \; . \tag{2}$$

However, this is *not* the conductance of the sample itself, as $G_c$ includes possible additional contact resistances between the reservoirs and the leads,[10,11] and in general[5,10,11] the actual voltage and temperature drop across the scatterer will differ from $\mu_1 - \mu_2$ and $\theta_1 - \theta_2$ (although these differences may be expected to be small, in typical cases, when the sample's length is much larger than the elastic mean free path). Determining these differences, namely $\mu_A - \mu_B$ and $\theta_A - \theta_B$ in Fig. 1, is the subtle point of all our calculations. The distributions of electrons on both sides of the barrier differ, due to the lack of inelastic and interchannel scattering, from the familiar shifted Fermi distributions (for example the different channels have different chemical potentials). On the other hand, we emphasize that these distributions are *exactly* known.

At zero temperature Büttiker *et al.*[10] define the chemical potentials $\mu_A$ and $\mu_B$ to give the correct particle density in the leads and obtain for the conductance of the sample when all the interchannel scattering in the leads is neglected:

$$G = \frac{I}{\mu_A - \mu_B} = \frac{2e^2}{\pi\hbar} \frac{\left[ \sum_{i=1}^{N} T_i \right] \left[ \sum_{i=1}^{N} v_i^{-1} \right]}{\sum_{i=1}^{N} \left[ (1 + R_i - T_i)/v_i \right]} \; , \tag{3}$$

where $T_i = \sum_j T_{ij}$, $R_i = \sum_j R_{ij}$, and $v_i$ is the Fermi velocity in the current direction in the $i$th channel, defined by $\hbar k_i / m$ ($k_i$ is the longitudinal Fermi wave vector of the $i$th state).

In the case of a finite temperature,[12] the situation becomes more complicated. A possible solution was suggested by Engquist and Anderson,[5] where they introduced two measurement reservoirs (MR) $A$ and $B$, coupled to the leads at points $A$ and $B$, respectively, through two potentiometers (thermometers in the case of temperature measurement). By tuning, for example, the chemical potential of MR $A$ they can find a point where the net current from the lhs lead to reservoir $A$ is equal to the current in the opposite direction. This chemical potential is defined to be the effective chemical potential of the lhs, $\mu_A$. Identical procedure is performed simultaneously on the rhs leading to a chemical potential $\mu_B$. The voltage drop is obtained as $\mu_A - \mu_B$. The temperature measurement is performed similarly by tuning the respective temperatures to yield zero net heat currents between the MR's and the leads.

Apart from neglecting thermoelectric currents (that may be corrected by simultaneous tuning of the temperatures and chemical potentials), the introduction of MR's raises some questions about the energy dependence of their coupling to the system. We will refer to these rather subtle points later.

Another thermodynamic definition of the effective chemical potentials and temperatures is presented here. To do that, we notice that although the intensive parameters in the leads are not well defined, the densities of the extensive ones may be calculated using the known distributions (in particular the particle density and the specific entropy are well defined[13]). Then, we define the effective chemical potential and effective temperature as the parameters that should be assigned to an equilibrium distribution in order to get the same particle density and specific entropy. It turns out that these two conditions (or any other independent pair) determine consistently all other extensive quantities (such as the specific energy). For zero temperature difference, the first condition is actually a manifestation of the Einstein relation between the diffusion coefficient and the conductivity. The conditions for equivalence of the above two definitions of $\mu_A - \mu_B$ and $\theta_A - \theta_B$ will be discussed in Sec. III.

In the next section and Sec. III, we derive and discuss all transport coefficients measured on both the sample itself and between the reservoirs. In particular, we obtain expressions for the thermoelectric coefficients and the thermoelectric power. We show that although the Onsager relation holds among the thermoelectric coefficients defined on the entire system, it breaks down when we consider the differences across the sample itself [a similar result was found in Ref. 14 for the relation $\sigma(H) = \sigma(-H)$]. In the final section we use these results to construct a scaling theory for the thermoelectric power near the metal-insulator localization transition in the metallic phase,[15] for bulk systems. The results are briefly summarized in the concluding section.

## II. MULTICHANNEL DERIVATION OF THE THERMOELECTRIC COEFFICIENTS

The net particle current in the $i$th channel on the lhs is given by

$$J_i^l = \frac{\hbar}{m} \sum_{k_i^L=0}^{\infty} \left[ f_1(k) k_i^L \left[ 1 - \sum_{j=1}^{N} R_{ij}(k_i^L) \right] - f_2(k) k_i^L \sum_{j=1}^{N} T'_{ij}(k_i^L) \right] , \tag{4}$$

where $f_1$ and $f_2$ are the Fermi distributions on the left- and right-hand side HR's, respectively, and $\hbar k_i^L$ the longitudinal momentum of an electron in the $i$th channel.

With $E_i^T$ describing the transverse energy associated with the $i$th channel the dispersion becomes

$$E_i = E_i^T + \frac{(\hbar k_i^L)^2}{2m} \; . \tag{5}$$

The total current on the lhs is calculated by summing over all channels,

$$J^l = \frac{1}{h} \sum_{i=1}^{N} \int_{E_i^T}^{\infty} T'_i (E - E_i^T) [f_1(E) - f_2(E)] dE \; , \tag{6}$$

with

$$T'_i = \sum_{j=1}^{N} T'_{ij}(E_i^L) \; , \tag{7}$$

where the velocity and the density of states $[(\pi\hbar v_i)^{-1}]$ factors canceled.

In the last step we also employed the unitarity of $S$:

$$\sum_{j=1}^{N} R_{ij}+\sum_{j=1}^{N} T'_{ij}=1 \, ,$$
$$\sum_{j=1}^{N} R'_{ij}+\sum_{j=1}^{N} T_{ij}=1 \, . \tag{8}$$

In the linear transport regime $|\mu_1-\mu_2|$ and $|\theta_1-\theta_2|$ are arbitrarily small ($\ll k_B\theta$) and if in addition $k_B\theta$ is small, then one may assume that no transverse level falls in the range of few $k_B\theta$ around $\mu_1+\mu_2/2$, thus $f_1(E)-f_2(E)\equiv 0$ for all $E<E_N^T$ and Eq. (6) may be rewritten as

$$J^{l}=\frac{1}{h}\int_0^\infty \sum_{i=1}^{N} T'_i(E-E_i^T)[f_1(E)-f_2(E)]dE \, . \tag{9}$$

(The above condition also guarantees a constant number of channels in both leads.)

Similar calculations for the rhs and the condition of current conservation yield two symmetries:

$$\sum_{i=1}^{N} T_i=\sum_{i=1}^{N} T'_i$$
and
$$\sum_{i=1}^{N} R_i=\sum_{i=1}^{N} R'_i \, . \tag{10}$$

Next, we calculate the heat current due to chemical potential and temperature gradients. The entropy current going to the right in the $i$th channel on the lhs is given by

$$(J_{si})_R=-\frac{k_B}{h}\int_0^\infty [f_1\ln f_1+(1-f_1)\ln(1-f_1)]dE \, , \tag{11}$$

where the velocity and density of states factors canceled. Notice that the expression in the square bracket is the entropy density of noninteracting electrons, distributed according to an arbitrary nonequilibrium $f_1$.[13] The entropy current to the left, in linear transport approximation is

$$(J_{si})_L=-\frac{k_B}{h}\int_0^\infty [(R_if_1+T'_if_2)\ln(R_if_1+T'_if_2)+(1-R_if_1-T'_if_2)\ln(1-R_if_1-T'_if_2)]dE \, . \tag{12}$$

Subtracting Eq. (12) from Eq. (11), summing over all channels and using Eqs. (10), we finally obtain for the heat current

$$U=\theta J_s=\frac{1}{h}\int_0^\infty \sum_{i=1}^{N} T_i(E-E_i^T)(E-\mu)$$
$$\times[f_1(E)-f_2(E)]dE \, , \tag{13}$$

where $\theta$ and $\mu$ can be taken, in linear-transport approximation, to be the average temperature and chemical potential.

The justification for extending the usual relation $U=\theta J_s$, used in linear-transport theory, to the present case where the distribution of electrons in the leads is different from the conventional one, is as follows. The two HR's are by definition in equilibrium and satisfy the thermodynamic identity,

$$dS_i=\frac{1}{\theta_i}dE_i-\frac{\mu_i}{\theta_i}dn_i \quad (i=1,2) \, ,$$

where $dE_i$ and $dn_i$ are the energy and number of electrons entering the $i$th reservoir, respectively. The only changes in energy and number of particles in the HR's are due to the energy and particle currents between them. Thus,

$$dE_1=-dE_2; \quad dn_1=-dn_2 \, .$$

The *net* entropy production in the whole system is then found to be *quadratic* in the differences:

$$\dot{S}=\left[\frac{1}{\theta_1}-\frac{1}{\theta_2}\right]J_E-\left[\frac{\mu_1}{\theta_1}-\frac{\mu_2}{\theta_2}\right]J \, , \tag{14}$$

while the entropy current *between* the reservoirs, $J_s=J_E/\theta-J\mu/\theta$ is *linear* in the differences ($\theta$ and $\mu$ can be taken as the average temperature and chemical potential). It turns out then, that in linear transport regime, the substitution of $\theta ds$ for the heat transfer is justified. We emphasize however, that the entropy production occurs *only* in the outer HR's and not in the leads nor in the sample. This is an important feature of the approach presented here.

In linear transport it is convenient to cast Eqs. (9) and (13) into a matrix form,

$$\begin{bmatrix} J \\ U \end{bmatrix}=\begin{bmatrix} L_0 & \frac{1}{\theta}L_1 \\ L_1 & \frac{1}{\theta}L_2 \end{bmatrix}\begin{bmatrix} \mu_1-\mu_2 \\ \theta_1-\theta_2 \end{bmatrix} \, , \tag{15}$$

with

$$L_\nu=\frac{1}{h}\int_0^\infty \sum_{i=1}^{N} T_i(E-E_i^T)(E-\mu)^\nu\left[-\frac{\partial f}{\partial E}\right]dE \, ,$$
$$\nu=0,1,2 \, . \tag{16}$$

For later reference we point out that Eq. (15) satisfies the Onsager relation for the transport coefficients between two heat reservoirs (i.e., those defined with $\mu_1-\mu_2$ and $\theta_1-\theta_2$).

As discussed in the Introduction, the subtle point of all transport calculations in this configuration is the definition of the chemical potential and temperature differences across the sample. We choose to define them through the differences in the particle density and the specific entropy, which are well defined. One may view this approach as a generalization of the Einstein relation.

The particle density on the lhs is given by

$$n_L=\tfrac{1}{2}\int_0^\infty \sum_{i=1}^{N} (n_s)_i[(1+R_i)f_1+T'_if_2]dE \, , \tag{17}$$

where $(n_s)_i$ is the density of states in the $i$th channel $[(\pi\hbar v_i)^{-1}]$.

We thus define implicitly the effective chemical potential, $\mu_A$ and effective temperature $\theta_A$ to satisfy two conditions; the first of which is

$$\int_0^\infty \sum_{i=1}^N (n_s)_i f_A dE = \frac{1}{2}\int_0^\infty \sum_{i=1}^N (n_s)_i [(1+R_i)f_1 + T_i' f_2] dE \ , \tag{18}$$

where

$$f_A = \{1+\exp[(E-\mu_A)/k_B\theta_A]\}^{-1} \ .$$

Similarly, we define the effective chemical potential $\mu_B$ and effective temperature $\theta_B$ to give the correct density on the rhs:

$$\int_0^\infty \sum_{i=1}^N (n_s)_i f_B dE = \frac{1}{2}\int_0^\infty \sum_{i=1}^N (n_s)_i [T_i f_1 + (1+R_i')f_2] dE \ . \tag{19}$$

Subtracting Eq. (19) from Eq. (18) we find an implicit relation between $f_A, f_B$ and $f_1, f_2$:

$$\int_0^\infty \sum_{i=1}^N (n_s)_i (f_A - f_B) dE = \int_0^\infty \sum_{i=1}^N (n_s)_i \bar{R}_i (f_1 - f_2) dE \ , \tag{20}$$

where $\bar{R}_i = (R_i + R_i')/2$.

A second relation needed to uniquely determine $\mu_A, \mu_B$ and $\theta_A, \theta_B$ emerges from the conditions on the entropy:

$$\begin{aligned} k_B \int_0^\infty \sum_{i=1}^N (n_s)_i [f_A \ln f_A + (1-f_A)\ln(1-f_A)] dE = {} & k_B \int_0^\infty \sum_{i=1}^N (n_s)_i [f_1 \ln f_1 + (1-f_1)\ln(1-f_1)] dE \\ & + k_B \int_0^\infty \sum_{i=1}^N (n_s)_i [(R_i f_1 + T_i' f_2)\ln(R_i f_1 + T_i' f_2) \\ & + (1-R_i f_1 - T_i' f_2)\ln(1-R_i f_1 - T_i' f_2)] dE \ , \end{aligned} \tag{21}$$

and

$$\begin{aligned} k_B \int_0^\infty \sum_{i=1}^N (n_s)_i [f_B \ln f_B + (1-f_B)\ln(1-f_B)] dE = {} & k_B \int_0^\infty \sum_{i=1}^N (n_s)_i [f_2 \ln f_2 + (1-f_2)\ln(1-f_2)] dE \\ & + k_B \int_0^\infty \sum_{i=1}^N (n_s)_i [(R_i' f_2 + T_i f_1)\ln(R_i' f_2 + T_i f_1) \\ & + (1-R_i' f_2 - T_i f_1)\ln(1-R_i' f_2 - T_i f_1)] dE \ . \end{aligned} \tag{22}$$

Subtracting Eq. (22) from Eq. (21) we obtain in the linear-transport approximation:

$$\int_0^\infty \sum_{i=1}^N (n_s)_i (E-\mu)(f_A - f_B) dE = \int_0^\infty \sum_{i=1}^N (n_s)_i \bar{R}_i (E-\mu)(f_1 - f_2) dE \ , \tag{23}$$

which together with Eq. (20) uniquely determines $\mu_A - \mu_B$ and $\theta_A - \theta_B$.

It is again convenient, in linear transport, to cast Eqs. (20) and (23) into a matrix form:

$$\begin{bmatrix} A_0 & \frac{1}{\theta}A_1 \\ A_1 & \frac{1}{\theta}A_2 \end{bmatrix} \begin{bmatrix} \mu_A - \mu_B \\ \theta_A - \theta_B \end{bmatrix} = \begin{bmatrix} B_0 & \frac{1}{\theta}B_1 \\ B_1 & \frac{1}{\theta}B_2 \end{bmatrix} \begin{bmatrix} \mu_1 - \mu_2 \\ \theta_1 - \theta_2 \end{bmatrix} , \tag{24}$$

where $A_\nu$ and $B_\nu$ are given by

$$A_\nu = \int_0^\infty \sum_{i=1}^N \frac{1}{(E-E_i^T)^{1/2}} (E-\mu)^\nu \left[ -\frac{\partial f}{\partial E} \right] dE \ , \qquad \nu = 0,1,2 \tag{25}$$

and

$$B_\nu = \int_0^\infty \sum_{i=1}^N \frac{\bar{R}_i}{(E-E_i^T)^{1/2}} (E-\mu)^\nu \left[ -\frac{\partial f}{\partial E} \right] dE \ , \qquad \nu = 0,1,2 \ . \tag{26}$$

Substituting Eq. (24) into Eq. (15) we finally obtain the transport matrix of the barrier, with the coefficients given by Eqs. (16), (25), and (26):

$$\begin{bmatrix} J \\ U \end{bmatrix} = \begin{bmatrix} K_0 & \frac{1}{\theta}K_1 \\ \tilde{K}_1 & \frac{1}{\theta}K_2 \end{bmatrix} \begin{bmatrix} \mu_A - \mu_B \\ \theta_A - \theta_B \end{bmatrix} , \tag{27}$$

with

$$K_0 = \frac{L_0(B_2A_0 - B_1A_1) + L_1(A_1B_0 - A_0B_1)}{B_0B_2 - B_1^2} \ , \tag{28a}$$

$$K_1 = \frac{L_0(B_2A_1 - B_1A_2) + L_1(B_0A_2 - B_1A_1)}{B_0B_2 - B_1^2} \ , \tag{28b}$$

$$\tilde{K}_1 = \frac{L_1(B_2A_0 - B_1A_1) + L_2(A_1B_0 - A_0B_1)}{B_0B_2 - B_1^2} \ , \tag{28c}$$

and

$$K_2=\frac{L_1(B_2A_1-B_1A_2)+L_2(B_0A_2-B_1A_1)}{B_0B_2-B_1^2} . \tag{28d}$$

## III. DISCUSSION OF THE RESULTS AT LOW TEMPERATURES

In this section we discuss the temperature dependence of the electrical, thermal, and thermoelectric coefficients at low temperatures, for the case where $T_i(E)$, etc., are smooth functions of the energy.

Expanding Eq. (28a) in a Sommerfeld series we reproduce the many channel formula for the conductivity, presented recently by Büttiker *et al.*,[10] with small correction due to a finite temperature:

$$K_0=\left[1+\frac{\pi^2}{6}(k_B\theta)^2\frac{\partial^2}{\partial E^2}\right]_\mu \times\left[\frac{1}{h}\frac{\left[\sum_{i=1}^{N}T_i\right]\left[\sum_{i=1}^{N}1/(E-E_i^T)^{1/2}\right]}{\sum_{i=1}^{N}[\bar{R}_i/(E-E_i^T)^{1/2}]}\right] . \tag{29}$$

In the single-channel case, Eq. (29) reduces to

$$K_0=\left[1+\frac{\pi^2}{6}(k_B\theta)^2\frac{\partial^2}{\partial E^2}\right]_\mu\frac{1}{h}\frac{T}{R} , \tag{30}$$

which is different from the finite-temperature conductance formula given first by Engquist and Anderson [Eq. (9) in Ref. 5]:

$$(R_{\mathrm{el}}^{\mathrm{EA}})^{-1}=\frac{e^2}{h}\frac{\int_{-\infty}^{\infty}T\left[-\frac{\partial f}{\partial E}\right]dE}{\int_{-\infty}^{\infty}R\left[-\frac{\partial f}{\partial E}\right]dE} . \tag{31}$$

(A similar formula, with velocity corrections, has been recently derived and discussed by Büttiker *et al.*[10])

The discrepancy between Eqs. (30) and (31) results from different definitions of the conductance $G$. In order to perform a conductance measurement, one might set $\theta_1=\theta_2=\theta$ and define $G=J/(\mu_A-\mu_B)$, which would yield the conductance given by Eq. (31) (with small velocity corrections[10]). However, it turns out that in this case a finite-temperature difference will be generated, leading to a thermoelectric component in the measured current $J$ [cf. Eq. (27)]. The proper definition of a pure conductance is $G\equiv K_0$, which might be measured in principle by arranging $\theta_A=\theta_B$ (by selecting the appropriate values of $\theta_1,\theta_2$ and $\mu_1,\mu_2$). To demonstrate that this is indeed the difference between Eqs. (30) and (31), we compute below the thermoelectric contribution for the case $\theta_1=\theta_2$. Substituting $\theta_1=\theta_2$ into Eq. (24) we obtain for the temperature difference across the sample

$$\theta_A-\theta_B=\theta\frac{B_1A_0-B_0A_1}{A_0A_2-A_1^2}(\mu_1-\mu_2) , \tag{32}$$

where $A_\nu,B_\nu$ ($\nu=0,1,2$) are given by Eqs. (25) and (26), respectively. Expanding Eq. (32) in Sommerfeld series we find in lowest order

$$\theta_A-\theta_B=\theta\frac{dR}{dE}(\mu_1-\mu_2) .$$

Thus, even if we set $\theta_1=\theta_2$ it follows that for *any finite* temperature $\theta$, $\theta_A\neq\theta_B$ (as long as $dR/dE\neq0$). To obtain the correction to Eq. (31) due to thermoelectric effects, we solve Eq. (24) for $\theta_A-\theta_B$ in terms of $\mu_A-\mu_B$, assuming $\theta_1=\theta_2$.

Expanding the results in Sommerfeld series we obtain in lowest order

$$\theta_A-\theta_B=\theta\frac{d}{dE}(\ln R)(\mu_A-\mu_B) , \tag{33}$$

and by Eq. (27)

$$J=\left[K_0-K_1\frac{d}{dE}(\ln R)\right](\mu_A-\mu_B) . \tag{34}$$

The expression in the large parentheses is the conductance, $1/R_{\mathrm{el}}^{\mathrm{EA}}$ defined in Ref. 5. It is a straightforward matter to check that the term-$K_1(d/dE)(\ln R)$, where $K_1$ is given by Eq. (36) below, is indeed the difference between Eqs. (30) and (31). Note that this difference is of the same order $[(k_B\theta)^2]$ as the lowest temperature correction to the conductance. We emphasize that although Eq. (30) looks similar to the Sommerfeld expansion of

$$\frac{1}{h}\int\frac{T}{R}\left[-\frac{\partial f}{\partial E}\right]dE ,$$

this is valid only to order $(k_B\theta)^2$ and *not* to the next order, $(k_B\theta)^4$.

Expanding Eq. (28d) we obtain for the heat conductivity:

$$K_2=\frac{\pi^2}{3}(k_B\theta)^2K_0+O((k_B\theta)^4) . \tag{35}$$

Comparing Eqs. (29) and (35) we find that Wiedemann-Franz relation, namely

$$K_2=\frac{\pi^2}{3}(k_B\theta)^2K_0 ,$$

holds only in the lowest order.

An even more interesting result emerges upon calculating the thermoelectric coefficients:

$$K_1=\frac{\pi^2}{3}(k_B\theta)^2\frac{\partial}{\partial E}[(K_0)_{\theta=0}]_\mu+O((k_B\theta)^4) , \tag{36}$$

and

$$\tilde{K}_1=K_1+C(k_B\theta)^4 , \tag{37}$$

where the coefficient $C$ (which depends on the variation of $T_i$, $R_i$, and $v_i$ with energy) is in general nonzero. The result is thus, that although we found in Eq. (15) that the Onsager relation holds for the thermoelectric coefficients between the HR's, it breaks down when we consider the actual voltage and temperature drop across the barrier. We believe this to be due to the purely elastic nature of the scattering in the system itself, i.e., from the lack of any mechanism driving it towards thermal equilibrium except for those in the HR's. This is similar to the effect found in Ref. 14. Notice however, that in many practical systems,[2] the transmittance can be very small, causing the gradients across the barrier to be practically equal to $\mu_1-\mu_2$ and $\theta_1-\theta_2$.

Looking at Eq. (36), we see that to obtain large thermoelectric coefficients (and hence a large thermoelectric power), one needs a zero-temperature conductivity which varies rapidly with energy. One interesting case with such variations is quasi-1D systems,[16] where the transmission exhibits rapid resonance type fluctuations. In this case, while the general expressions of Sec. II are valid, the low-temperature expansion holds only when $k_B\theta$ is much smaller than the scale of variation of $\sigma(E)$. A different case of interest will be discussed in the next section.

Another interesting property is the thermoelectric power defined by

$$s=\frac{1}{e\theta}\frac{K_1}{K_0} . \tag{38}$$

Substituting Eqs. (29) and (36) into Eq. (38) we obtain in the lowest order, the familiar expression for metals:

$$s=\frac{k_B}{e}\frac{\pi^2}{3}k_B\theta\frac{\partial}{\partial E}[\ln(K_0)_{\theta=0}]_\mu . \tag{39}$$

Comparing Eqs. (28a) and (28b) with the general, physically plausible expression, given by Cutler and Mott,[17]

$$s=\frac{k_B}{e}\frac{\int_0^\infty \sigma(E)\frac{E-\mu}{k_B\theta}\left[-\frac{\partial f}{\partial E}\right]dE}{\int_0^\infty \sigma(E)\left[-\frac{\partial f}{\partial E}\right]dE} , \tag{40}$$

we see that the last one holds strictly only in the lowest order. It also holds, as can easily be seen, for the simpler transport coefficients of Eq. (15). Thus our procedure provides justification for Eq. (40) in appropriate limits.

The next and last remark is concerned with the chemical potential and temperature measurement. As mentioned previously, one way to perform it, is by introducing two measurement reservoirs $A$ and $B$, and tune their chemical potentials and temperatures to yield a zero net heat and particle currents between them and the system (note that the coupling of the reservoirs to the system should be weak enough so as not to perturb its electron distribution). In the golden rule approximation, zero net particle current implies:

$$\int_0^\infty \sum_{i=1}^N (n_s)_i n_A \frac{|V|^2}{\hbar}(f_A-f_B)dE = \int_0^\infty \sum_{i=1}^N (n_s)_i n_A \frac{|V|^2}{\hbar}\bar{R}_i(f_1-f_2)dE , \tag{41}$$

where $V$ is the matrix element describing the coupling between the MR's and the system and $n_A$ is the density of states of the reservoirs. Similarly, zero net heat current gives

$$\int_0^\infty \sum_{i=1}^N (n_s)_i n_A \frac{|V|^2}{\hbar}(E-\mu)(f_A-f_B)dE = \int_0^\infty \sum_{i=1}^N (n_s)_i n_A \frac{|V|^2}{\hbar}\bar{R}_i(E-\mu)(f_1-f_2)dE . \tag{42}$$

Comparing Eqs. (41) and (42) to the previously derived conditions, Eqs. (20) and (23), we find that they are identical if $n_A(|V|^2/\hbar)$ is independent of energy and channel number $i$. It seems then, that an ideal measurement process should satisfy the above condition or otherwise we find differences in the extensive parameters between the system and the measurement reservoirs. Moreover, such a measurement will depend on details of the coupling to the system and the structure of the specific apparatus. A weaker condition, more plausible in real systems, which might be sufficient in the case of a large number of channels is that there exist no *systematic* variation of $n_A(|V|^2/\hbar)$ with energy. We expect that purely random variations would cancel out.

## IV. CRITICAL BEHAVIOR OF THE METALLIC THERMOPOWER NEAR THE MOBILITY EDGE

One of the advantages of a multichannel Landauer-type formula is that it may be used to create and justify the scaling theory for the transport in disordered systems, by looking at the size dependence of the appropriate coefficients.[2,6,18] In this section we shall use our theory for the thermoelectric coefficients to derive an expression for the thermopower in terms of the energy-dependent conductivity $\sigma(E)$. In the derivation we employ the now accepted assumptions for the scaling behavior[18] of $\sigma(E)$ near the mobility edge $E_M$ to obtain the scaling of the electronic thermopower, $S(\theta,E_F-E_M)$ as a function of the temperature $\theta$ and separation from the mobility edge [the usual localization metal-insulator (MI) transition is obtained when $E_F\rightarrow E_M$] in the metallic phase. This expression is valid for an arbitrary amount of disorder as long as hopping and inelastic processes are neglected and it holds in the whole metallic phase (as long as $E_F$ is within the region of extended states).

Our assumptions are as follows. We treat only the electronic contribution and neglect the phonon part of the heat current. Phonon-drag effects, that may be crucial for the thermopower of pure metals, are neglected since the disorder is also assumed to severely limit the phonon mean free path.

We have discussed in this paper two types of transport coefficients: those between the outside HR's [defined by Eq. (15)] and those on the system itself [defined by Eq. (27)]. The former include the effects of the contact resistances with and the electron thermalization in the reservoirs while the latter include mostly elastic scattering in the sample itself. Fortunately, the differences between these two types of coefficients become small in the limit of a large number of channels and/or weak transmission. Both of those conditions are relevant near the MI transition at low temperatures. Thus, in this section we use the simpler coefficients of Eq. (15). This enables us to use the

Cutler-Mott[17] expression, Eq. (40) for the thermopower. However, instead of using the assumptions[15,19] of minimum metallic conductivity for $\sigma(E)$, we invoke the result of the scaling theory[18] that in the vicinity of $E_M$

$$\sigma(E)=a(E-E_m)^x,\quad E\geq E_m \tag{43}$$

where the exponent $x$ is currently believed to be around unity and $a$ is some constant. Substituting Eq. (43) into Eq. (40) we obtain in the lowest order in temperature $(k_B\theta \ll E_F-E_M)$:

$$s=\frac{k_B}{e}\frac{\pi}{3}\frac{k_B\theta}{E_F-E_m}\,, \tag{44}$$

while for high temperatures $(k_B\theta \gg E_F-E_m)$ we find

$$s=\frac{k_B}{e}\left[\text{const}-\frac{E_F-E_m}{k_B\theta}\right]. \tag{45}$$

Notice however, that the latter limit may be inconsistent with the neglect of inelastic processes. Equations (44) and (45) imply that $S$ can be scaled to depend not on $k_B\theta$ and $E_F-E_M$ separately, but on a single variable $k_B\theta/(E_F-E_M)$.

In the metallic phase, the neglect of inelastic scattering is valid on length scales smaller than the phase coherence length $L_\phi$ [given in usual cases[20] by $(D\tau_{\text{in}})^{1/2}$, $D$ being the diffusion coefficient and $\tau_{\text{in}}$ the inelastic scattering time for the electrons]. On the other hand, the thermal smearing involved in the evaluation of our results [e.g., Eq. (16), etc.] uses energies $|E-E_F|\lesssim k_B\theta$ and thus length scales,[21] $(\hbar D/|E-E_F|)^{1/2}\gtrsim(\hbar D/k_B\theta)^{1/2}$. Since $\tau_{\text{in}}$ is typically larger than $\hbar/k_B\theta$ by at least one to two orders of magnitude, most of the latter scales are smaller than $L_\phi$ so that our assumption is consistent.

Once the transport coefficients are evaluated for scales up to $L_\phi$, their behavior for macroscopic samples is obtained by using[18,20,22] classical combination rules. Since the thermopower $S$ is given via Eq. (38), by a ratio of two transport coefficients, both proportional, in three dimensions, to the system's length, it turns out to be scale independent from $L_\phi$ on.

We believe that the above remarks, for systems where the disorder is sufficiently effective to make the effects of the phonons relatively unimportant, make our assumptions appear rather plausible. It would, thus, be extremely interesting to check our results in this section, namely Eqs. (44) and (45), experimentally near the MI transition in bulk systems.

## V. SUMMARY AND CONCLUSIONS

We presented a comprehensive theory for linear thermal and electrical transport for noninteracting electrons between two reservoirs connected via ideal multichannel leads and an arbitrary disordered sample. Both temperature and chemical potential differences are assumed between the two reservoirs. There are two types of transport coefficients: those [Eq. (15)] defined between the two reservoirs and those [Eq. (27)] defined across the sample itself. The former include the various impedances due to the connections of the leads to the reservoirs as well as the effects of electron thermalization by inelastic scattering in the reservoirs. The latter include only the effects of *elastic* scattering in the sample (and the neglect of interchannel interference, justified by the phase randomization of the electrons in the reservoirs).

The definitions of temperature and chemical potential differences across the sample are discussed along with some subtleties in the suggested (conceptual) way to measure them. Although the thermoelectric coefficients defined between the reservoirs satisfy the Onsager relation, the coefficients defined across the sample itself violate it. Similarly, only the thermopower resulting from the former coefficients satisfies exactly the Cutler-Mott expression [Eq. (40)]. Correction to the multichannel conductance formula for a finite temperature[12] is given as well. The results are used to make a prediction for the thermopower near the localization MI transition in bulk systems from the metallic side at not overly high temperatures.

This theory can be straightforwardly generalized to go beyond the linear transport approximation. A generalization to include inelastic scattering in the sample[12] is very much called for as well. We are currently attempting to further understand the thermoelectric phenomena in the hopping regime.

## ACKNOWLEDGMENTS

Instructive discussions with R. Landauer, M. Büttiker, and A. D. Stone are gratefully acknowledged. This research was partially supported by the fund for basic research administrated by the Israeli Academy for Sciences and Humanities.

---

[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).

[2] P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B **22**, 3519 (1980).

[3] R. Landauer, IBM J. Res. Dev. **1**, 223 (1957).

[4] R. Landauer, Philos. Mag. **21**, 863 (1970).

[5] H. L. Engquist and P. W. Anderson, Phys. Rev. B **24**, 1151 (1981).

[6] P. W. Anderson, Phys. Rev. B **23**, 4828 (1981).

[7] P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).

[8] D. C. Langreth and E. Abrahams, Phys. Rev. B **24**, 2978 (1981).

[9] M. Ya. Azbel, J. Phys. C **14**, L225 (1981).

[10] M. Büttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B **31**, 6207 (1985).

[11] R. Landauer, in *Localization, Interaction, and Transport Phenomena in Impure Metals, Braunschweig, 1984,* Vol. 61 of *Springer Series in Solid State Sciences,* edited by G. Bergmann, Y. Bruynseraede, and B. Kramer (Springer, Heidelberg, 1985), p. 38.

[12] M. Büttiker and Y. Imry J. Phys. C **18**, L467 (1985); M. Büttiker (unpublished).

[13] L. D. Landau and E. M. Lifschitz, *Statistical Physics* (Pergamon, New York, 1959), p. 54.

[14] M. Büttiker and Y. Imry, J. Phys. C (to be published).

[15] N. F. Mott, *Metal-Insulator Transitions* (Taylor and Francis, London, 1974), and references listed therein.

[16]M. Ya. Azbel and P. Soven, Phys. Rev. **27**, 831 (1983).

[17]M. Cutler and N. F. Mott, Phys. Rev. **181**, 1336 (1969).

[18]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).

[19]N. F. Mott, Philos. Mag. **31**, 217 (1975).

[20]D. J. Thouless, Phys. Rev. Lett. **39**, 1167 (1977).

[21]Y. Imry and Z. Ovadyahu, Phys. Rev. Lett. **49**, 841 (1982).

[22]Y. Imry, Phys. Rev. Lett. **44**, 469 (1980); Y. Imry, in *Percolation, Localization and Superconductivity,* edited by A. M. Goldman and S. A. Wolf (Plenum, New York, 1984), p. 189.