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1984 J. Phys. A: Math. Gen. 17 1745

(http://iopscience.iop.org/0305-4470/17/8/028)

J. Phys. A: Math. Gen. 17 (1984) 1745–1754. Printed in Great Britain

On the hopping conductivity in the presence of a magnetic field

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Received 21 October 1983, in final form 15 December 1983

Abstract. It is shown that, for hopping systems, even in the presence of a magnetic field, the Kubo approach for zero frequency gives the same DC conductivity tensor as the generalised stationary Miller–Abrahams approach. In general, the result relies on certain assumptions of macroscopic homogeneity about the system, which for periodic lattices turn out to hold exactly.

1. Introduction

Although the generalisation of the hopping rate equation in the presence of a magnetic field dates back to Holstein (1961), its derivation, using either Green function techniques (Böttger and Bryksin 1977a, b) or the master equation approach (Aldea and Bányai 1980), is fairly recent.

The purpose of the present paper is to compare two ways of extracting the DC conductivity tensor of such a hopping model in the presence of a magnetic field. One alternative is to study, using the standard Kubo theory, the transitory regime in an isolated system in the limit of infinite volume and large times. In the second one, external sources are applied to boundaries in order to obtain a steady flow state. This way one gets a generalisation of the well known Miller–Abrahams scheme. The equivalence of the two approaches is by no means immediate. It seems that certain assumptions of macroscopic homogeneity enter essentially into the proof. In the absence of a magnetic field, for periodical lattices the proof is given by Bányai and Gartner (1980), using the translational invariance of the system.

The presence of the magnetic field $\boldsymbol{H}$ brings in specific complications because essential surface effects must be taken into account. But for a system with a free surface the translational invariance is lost and one has to turn to other means of demonstration.

Throughout the paper, several properties of the system are assumed to hold. They reflect, more or less transparently, the macroscopic homogeneity of the microscopically non-homogeneous system. Every assumption of this kind is proved to hold rigorously for periodic lattices.

Let us consider a finite domain Ω of the space to which a given array of sites, labelled by the index i, is confined. Each site is characterised by its position $\boldsymbol{x}_i$ and energy ε_i. The $\Omega \to \infty$ limit, which will be currently invoked below, implies that this set of sites is the restriction to Ω of an infinite one, extending in the whole space. In the presence of a constant, homogeneous magnetic field $\boldsymbol{H}$ and for small deviation of the average site occupation numbers $\bar{n}_i$ from their equilibrium values $f_i = f(\varepsilon_i)$ (f being the Fermi function) one gets the linearised form of the rate equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta_i = -\sum_{j\in\Omega}\Gamma^{\Omega}_{ij}(\eta_j + e\beta f_j(1-f_j)V_j) \tag{1}$$

where $\eta_i = \bar{n}_i - f_i$, $\beta = 1/kT$, e is the electron charge, $j \in \Omega$ is short for $\boldsymbol{x}_j \in \Omega$, V_j is the (self-consistent) electric potential on the site j, and

$$\Gamma^{\Omega}_{ij} = M^{\Omega}_{ij}/f_j(1-f_j), \qquad M^{\Omega}_{ij} = \delta_{ij}\sum_{k\in\Omega}\mathcal{W}^{\Omega}_{kj} - \mathcal{W}^{\Omega}_{ij}. \tag{2}$$

In the absence of the magnetic field, as is well known, the matrix $\mathcal{W}^{\Omega}_{ij}$ is symmetrical, independent of Ω and related in a simple way to the phonon-induced hopping transition rates W_{ij} (that are assumed rapidly decreasing with $|\boldsymbol{x}_i - \boldsymbol{x}_j|$)

$$\mathcal{W}^{\Omega}_{ij}|_{\boldsymbol{H}=0} = f_i(1-f_j)W_{ij} \equiv \mathcal{W}^{\mathrm{S}}_{ij} = \mathcal{W}^{\mathrm{S}}_{ji} \geqslant 0.$$

It follows that $M^{\Omega}|_{\boldsymbol{H}=0}$ is positive definite.

A homogeneous magnetic field $\boldsymbol{H}$ (in the linear approximation with respect to this field) introduces an additional antisymmetric and Ω-dependent piece $\mathcal{W}^{\Omega,\mathrm{A}}_{ij}$ in the matrix $\mathcal{W}^{\Omega}_{ij}$ (Böttger and Bryksin 1977a, b, Aldea and Bányai 1980, Butcher and Kumar 1980) coming from the corresponding modifications of the transition rates. This antisymmetric part can be written as

$$\mathcal{W}^{\Omega,\mathrm{A}}_{ij} = \sum_{k\in\Omega} A_{ijk} \tag{3}$$

where

$$A_{ijk} = e[(\boldsymbol{x}_i - \boldsymbol{x}_k)\times(\boldsymbol{x}_j - \boldsymbol{x}_k)]\boldsymbol{H}\mathcal{U}_{ijk}.$$

$\mathcal{U}_{ijk}$ is positive, Ω-independent, rapidly decreasing with the distance between $\boldsymbol{x}_i$, $\boldsymbol{x}_j$, $\boldsymbol{x}_k$ and totally symmetric with respect to the permutation of the indices i, j, k. That makes A_{ijk} totally antisymmetric (due to the presence of the oriented area of the triangle $\boldsymbol{x}_i$, $\boldsymbol{x}_j$, $\boldsymbol{x}_k$ in its definition). $\mathcal{W}^{\Omega,\mathrm{A}}_{ij}$ is Ω-dependent, but this dependence becomes weaker the further we are from the boundaries of Ω. The explicit form of $\mathcal{U}_{ijk}$ in terms of the electron–phonon interaction may be found in the above-mentioned papers.

2. The steady flow

Let us start with some simple considerations concerning the macroscopic equations of the steady flow. If the system is infinite, homogeneous, with DC conductivity tensor σ, one has

$$\boldsymbol{j} = -\sigma\nabla V, \qquad \nabla\boldsymbol{j} = I, \tag{4}$$

where V is the electric potential, $\boldsymbol{j}$ the current density and I the external current source needed to maintain the steady flow. Since our microscopic model lacks an unambiguous definition of the current density, we eliminate $\boldsymbol{j}$ from (4) to get

$$\nabla\sigma\nabla V = -I \tag{5}$$

or, in Fourier transform,

$$\boldsymbol{k}\sigma\boldsymbol{k}\hat{V} = -\hat{I}.$$

It is obvious that only the symmetric part of σ is involved, and the interesting $\boldsymbol{H}$-dependent (Hall) effect is lost. Therefore, we are compelled to consider systems with free surface, where boundary conditions of the type

$$I_\Sigma = -\boldsymbol{n}\boldsymbol{j}|_\Sigma = \boldsymbol{n}\sigma(\nabla V)_\Sigma \tag{6}$$

appear. I_Σ is the external source concentrated on the surface Σ of the domain Ω, $\boldsymbol{n}$ being the outward normal of Σ. We mention also the relation ($|\Omega|$ = the volume of the domain Ω)

$$\frac{1}{|\Omega|}\int_\Omega \boldsymbol{x}I\,\mathrm{d}v + \frac{1}{|\Omega|}\int_\Sigma \boldsymbol{x}I_\Sigma\,\mathrm{d}s = -\frac{1}{|\Omega|}\int_\Omega \boldsymbol{j}\,\mathrm{d}v$$

which is based on (4) for the bulk term and (6) for the surface term. For the particular case of the steady flow in a constant electric field $\boldsymbol{E}$, $\boldsymbol{j}$ is also constant whence $I = 0$ and one is left with

$$|\Omega|^{-1}\int_\Sigma \boldsymbol{x}I_\Sigma\,\mathrm{d}s = -\boldsymbol{j}. \tag{7}$$

Turning now back to the microscopic problem, it is clear that in order to have a solution of the problem corresponding to a stationary flow one has to modify the rate equation (1) by an external source term (Bányai and Aldea 1979). The steady state is then given by

$$I_i = e^2\beta\sum_{j\in\Omega} M_{ij}^\Omega U_j = e^2\beta\sum_{j\in\Omega}\mathcal{W}_{ij}^\Omega(U_i - U_j) \tag{8}$$

where $U_j = \eta_j/e\beta f_j(1-f_j) + \mathcal{V}_j$ is the local electrochemical potential. Equation (8) looks formally like the original Miller–Abrahams equation, but its interpretation as a resistance network is no longer valid for $\boldsymbol{H} \neq 0$ since $\mathcal{W}_{ij}^\Omega$ is no longer symmetric. For the infinite, periodic system equation (8) is readily solved by discrete Fourier transforms (Bányai and Gartner 1980). For systems with free surfaces the idea is to guess a particular solution for U which gives through (8) a set of external sources coupled only in a narrow strip at the boundaries, and is zero in the bulk. This is done as follows.

Since the infinite macroscopic system, described by (5) with the sources at infinity, has the constant field solution $V = -\boldsymbol{x}\boldsymbol{E}$ it is assumed that its microscopic counterpart (8) with sources at infinity

$$0 = \sum_j M_{ij}U_j \tag{9}$$

admits the solution

$$U_j = -(\boldsymbol{x}_j + \boldsymbol{\alpha}_j)\boldsymbol{E} = -\boldsymbol{y}_j\boldsymbol{E}. \tag{10}$$

The exact homogeneous field (linear potential) solution is not expected to hold down to the microscopic scale, and $\boldsymbol{\alpha}_j$ takes into account the local departures, but it is assumed that $\boldsymbol{\alpha}_j/|\boldsymbol{x}_j|$ becomes negligible for large $|\boldsymbol{x}_j|$, to ensure the correct (linear) asymptotic behaviour.

This assumption will be proved to hold for periodic lattices with a periodic and therefore also bounded function of site. (The absence of superscript Ω in (9) means Ω = infinity.)

Introducing the solution (10) in (8) for the finite volume,

$$I_i = -e^2\beta\sum_{j\in\Omega} M_{ij}^\Omega \boldsymbol{y}_j\boldsymbol{E},$$

it is clear that the non-vanishing external sources I_i are needed near the surface to compensate for the flow between Ω and the rest of the infinite system in (9). This compensation decreases rapidly with the distance from the boundary of Ω. (This is the microscopic counterpart of the macroscopic constant field case, where only I_Σ is present.)

The identification between the macroscopical and microscopical entities is done by (see (7))

$$\boldsymbol{j} = -\lim_{\Omega\to\infty} \frac{1}{|\Omega|} \sum_{i\in\Omega} \boldsymbol{x}_i I_i = \lim_{\Omega\to\infty} \frac{e^2\beta}{|\Omega|} \sum_{i,j\in\Omega} \boldsymbol{x}_i M_{ij}^{\Omega}(\boldsymbol{y}_j \boldsymbol{E})$$

whence the DC conductivity tensor is

$$\sigma_{\mu\nu} = \lim_{\Omega\to\infty} \frac{e^2\beta}{|\Omega|} \sum_{i,j\in\Omega} x_i^\mu M_{ij}^\Omega y_j^\nu, \qquad \mu, \nu = 1, 2, 3. \tag{11}$$

Here $|\Omega|$ is the number of sites in the domain Ω.

Since the sum over j is non-zero only for i in the neighbourhood of the surface, replacing x_i^μ by y_i^μ gives rise to a difference which tends to zero as Ω tends to infinity (e.g. if α_i^μ is bounded it decays as the surface divided by the volume):

$$\sigma_{\mu\nu} = \lim_{\Omega\to\infty} \frac{e^2\beta}{|\Omega|} \sum_{i,j\in\Omega} y_i^\mu M_{ij}^\Omega y_j^\nu, \qquad \mu, \nu = 1, 2, 3,$$

or, using the definition of M^Ω (equations (2) and (3)) and after some simple algebraic manipulations:

$$\sigma_{\mu\nu} = e^2\beta \lim_{\Omega\to\infty} |\Omega|^{-1} \left(\tfrac{1}{2} \sum_{i,j\in\Omega} \mathscr{W}_{ij}^{S}(y_i^\mu - y_j^\mu)(y_i^\nu - y_j^\nu) + \tfrac{1}{3} \sum_{i,j,k\in\Omega} A_{ijk}(y_i^\mu - y_k^\mu)(y_j^\nu - y_k^\nu) \right). \tag{12}$$

The first term of (12) is obviously the symmetric part of σ while the second is its antisymmetric part. The last one can be written, using the totally antisymmetric tensor $\varepsilon_{\mu\nu\rho}$, as

$$\sigma_{\mu\nu}^{A} = \sum_{\rho} \varepsilon_{\mu\nu\rho} h_\rho$$

with

$$\boldsymbol{h} = e^2\beta \lim_{\Omega\to\infty} \frac{1}{|\Omega|} \frac{1}{6} \sum_{i,j,k\in\Omega} A_{ijk}[(\boldsymbol{y}_i - \boldsymbol{y}_k)\times(\boldsymbol{y}_j - \boldsymbol{y}_k)].$$

The sign of the Hall effect is given by the sign of

$$\begin{aligned}\boldsymbol{H}\cdot\boldsymbol{h} &= e^2\beta \lim_{\Omega\to\infty} \frac{1}{|\Omega|} \frac{1}{6} \sum_{i,j,k\in\Omega} A_{ijk}[(\boldsymbol{y}_i - \boldsymbol{y}_k)\times(\boldsymbol{y}_j - \boldsymbol{y}_k)]\cdot\boldsymbol{H} \\ &= e^2\beta \lim_{\Omega\to\infty} \frac{1}{|\Omega|} \frac{1}{6} \sum_{i,j,k\in\Omega} \mathscr{U}_{ijk}\{[(\boldsymbol{x}_i - \boldsymbol{x}_k)\times(\boldsymbol{x}_j - \boldsymbol{x}_k)]\boldsymbol{H}\} \\ &\quad \times\{[(\boldsymbol{y}_i - \boldsymbol{y}_k)\times(\boldsymbol{y}_j - \boldsymbol{y}_k)]\boldsymbol{H}\}.\end{aligned} \tag{13}$$

3. The Kubo approach

It is known that the Kubo-type approach to the hopping conduction problem, which uses (1) (Brenig *et al* 1971, Butcher 1972), gives rise to the following expression for the conductivity tensor

$$\sigma_{\mu\nu} = e^2\beta \lim_{z\to 0} \lim_{\Omega\to\infty} \frac{1}{|\Omega|} \sum_{i,j\in\Omega} x_i^\mu \left(\frac{z\Gamma^\Omega}{z+\Gamma^\Omega}\right)_{ij} f_j(1-f_j)x_j^\nu$$

(z tends to zero along the imaginary axis of the complex plane $z = \mathrm{i}\omega$ and $\lim_{z\to 0}$ is in fact the zero-frequency limit).

The only new ingredient is again the magnetic field dependent part of Γ^Ω (see also Aldea and Bányai 1980).

Defining the matrix p by

$$p_{ij} = \delta_{ij} f_j(1-f_j) = \delta_{ij} p_i, \qquad p_i > 0,$$

and noting (see (2)) that $\Gamma^\Omega p = M^\Omega$, one gets

$$\sigma_{\mu\nu} = e^2\beta \lim_{z\to 0} \lim_{\Omega\to\infty} \left[\frac{1}{|\Omega|} \sum_{i,j\in\Omega} x_i^\mu M_{ij}^\Omega x_j^\nu - \frac{1}{|\Omega|} \sum_{i,j\in\Omega} x_i^\mu \left(M^\Omega \frac{1}{zp+M^\Omega} M^\Omega\right)_{ij} x_j^\nu\right]. \tag{14}$$

Our purpose is to show the equivalence of (14) with the Miller–Abrahams result (11), and to this end we proceed in two steps.

(i) Firstly, we shall prove that the second term in (14) can be rewritten as

$$-e^2\beta \lim_{z\to 0} \lim_{\Omega\to\infty} \frac{1}{|\Omega|} \sum_{i\in\Omega} \sum_{j} x_i^\mu \left(M^\Omega \frac{1}{zp+M} M\right)_{ij} x_j^\nu$$

(where again the $\Omega = \infty$ quantities are written without superscript).

For the sake of simplicity we shall consider here only the finite-range case. This amounts to the existence of a distance d such that

$$\begin{aligned} \mathscr{W}_{ij}^{\mathrm{S}} &= 0 \qquad \text{for } |\boldsymbol{x}_i - \boldsymbol{x}_j| > d, \\ A_{ijk} &= 0 \qquad \text{for } \max\{|\boldsymbol{x}_i - \boldsymbol{x}_j|, |\boldsymbol{x}_i - \boldsymbol{x}_k|, |\boldsymbol{x}_j - \boldsymbol{x}_k|\} > d. \end{aligned} \tag{15}$$

The more general case of rapidly decreasing $\mathscr{W}_{ij}^{\mathrm{S}}$ and A_{ijk} can be treated essentially by using the same argument.

The frame of the subsequent discussion is the space l_∞ of bounded sequences defined on our infinite array of sites, with the usual norm of the uniform convergence (Kato 1966).

An infinite matrix T defines a bounded operator, as usual, by

$$(T\lambda)_i = \sum_j T_{ij}\lambda_j$$

if and only if (Kato 1966)

$$\|T\| = \sup_i \sum_j |T_{ij}| < \infty. \tag{16}$$

This is true for our operator M, provided

$$\sum_{j(\neq 1)} \mathscr{W}_{ij}^{\mathrm{S}} < C_1 \qquad \text{and} \qquad \sum_{j,k} |A_{ijk}| < C_2 \tag{17}$$

with C_1, C_2 i-independent constants. These conditions ensure the boundedness of

$\sum_{j(\neq i)} \mathscr{W}_{ij}$. The operator M^Ω can be regarded as acting in l_∞ too, with $M^\Omega_{ij}=0$ if either $i\notin\Omega$ or $j\notin\Omega$. It is obviously bounded, since it is finite dimensional, but what is more important, using (17) again, one readily finds a constant C so that

$$\|M^\Omega\| < C \qquad \text{for every } \Omega.$$

In other words, the set of operators $\{M^\Omega\}_\Omega$ is uniformly bounded.

The sequence $x^\mu = \{x_i^\mu\}_i$ is not bounded, but $\{(M^\Omega x^\mu)_i\}_i$ and $\{(Mx^\mu)_i\}_i$ are, because they involve only coordinate differences, e.g.

$$(Mx^\mu)_i = \sum_j \mathscr{W}_{ij}(x_i^\mu - x_j^\mu),$$

for points with $|\boldsymbol{x}_i - \boldsymbol{x}_j| < d$. As before, for $\{(M^\Omega x^\mu)_i\}_i$ a uniform bound is available.

Let us now turn to the more difficult operators $(zp+M^\Omega)^{-1}$ and $(zp+M)^{-1}$. Both are bounded for Re $z \geqslant 0$, $z \neq 0$, as seen in the following representation:

$$\frac{1}{zp+M} = \sum_{n\geqslant 0}\left(\frac{1}{zp+\Delta}W\right)^n \frac{1}{zp+\Delta} \tag{18}$$

where Δ is the diagonal part of M,

$$\Delta_{ij} = \delta_{ij}\sum_k \mathscr{W}_{ik} = \delta_{ij}\Delta_i,$$

and $W = \Delta - M$ has the transition rates $\mathscr{W}_{ij}$ as matrix elements. The expansion (18) is convergent because (see (16))

$$\left\|\frac{1}{zp+\Delta}W\right\| = \sup_i \frac{1}{|zp_i+\Delta_i|}\sum_j \mathscr{W}_{ij} = \sup_i \frac{\Delta_i}{|zp_i+\Delta_i|} < 1.$$

Strictly speaking the last inequality holds only if p_i cannot approach zero, which amounts to the boundedness of the set of site energies $\{\varepsilon_i\}_i$. The same kind of argument proves that $(zp+M^\Omega)^{-1}$ is uniformly bounded.

With these prerequisites let us turn to our problem and show that, indeed,

$$\begin{aligned}\frac{1}{|\Omega|}\sum_{i,j} x_i^\mu \left(M^\Omega \frac{1}{zp+M^\Omega}M^\Omega\right)_{ij} x_j^\nu &- \frac{1}{|\Omega|}\sum_{i,j} x_i^\mu\left(M^\Omega\frac{1}{zp+M}M\right)_{ij} x_j^\nu \\ &= \frac{1}{|\Omega|}\sum_{i,j} x_i^\mu\left(M^\Omega\frac{1}{zp+M^\Omega}\right)_{ij}[(M^\Omega - M)x^\nu]_j \\ &\quad - \frac{1}{|\Omega|}\sum_{i,j,l} x_i^\mu\left(M^\Omega\frac{1}{zp+M^\Omega}\right)_{ij}(M^\Omega-M)_{jl}\left(\frac{1}{zp+M}Mx^\nu\right)_l\end{aligned} \tag{19}$$

tends to zero as $|\Omega|\to\infty$. The following observations are in order. The quantity

$$\sum_i x_i^\mu\left(M^\Omega\frac{1}{zp+M^\Omega}\right)_{ij}$$

appearing in both terms of (19) is zero for $j\notin\Omega$ and uniformly bounded otherwise. On the other hand both

$$\sum_l (M^\Omega - M)_{jl}x_l^\nu \qquad \text{and} \qquad \sum_l (M^\Omega-M)_{jl}\left(\frac{1}{zp+M}Mx^\nu\right)_l$$

are strictly vanishing for j not belonging to the strip Σ of width d along the surface of Ω. Indeed, equations (15) show that the difference between M^Ω_{jl} and M_{jl} becomes strictly zero for either j or l sufficiently far from the surface of Ω. Therefore both terms in the RHS of (19) involve summations restricted to the strip Σ over uniformly bounded quantities, and tend to zero as $|\Sigma|/|\Omega|$.

(ii) It is not obviously clear whether the $z \to 0$ limit in the Kubo type formula exists. The difficulty comes from the fact that M is not invertible and

$$\left(\frac{1}{zp+M} Mx^{\nu}\right)_i$$

may have no meaning as $z \to 0$. Nevertheless, M is present in the numerator too, so one hopes that the singularity is cancelled out.

Therefore, the second step relies on the assumption (which will be rigorously proved for periodic lattices) that

$$\lambda_i^{\nu} = \lim_{z\to 0} \left(\frac{1}{zp+M} Mx^{\nu}\right)_i \tag{20}$$

exists, and moreover, it can be performed in the expression of σ before the infinite-volume limit. This inversion of the order of limits is true for instance if the convergence in (20) is uniform with respect to i (l_∞ convergence).

We show next that, under these conditions, the assumption contained in (10) becomes true with $\boldsymbol{\alpha}_i = -\boldsymbol{\lambda}_i$. To this end consider

$$\begin{aligned}(M\boldsymbol{\lambda})_i &= \lim_{z\to 0}\left(M\frac{1}{zp+M} M\boldsymbol{x}\right)_i \\ &= (M\boldsymbol{x})_i - \lim_{z\to 0} zp_i \left(\frac{1}{zp+M} M\boldsymbol{x}\right)_i = (M\boldsymbol{x})_i.\end{aligned}$$

Therefore $\boldsymbol{y}_i = \boldsymbol{x}_i - \boldsymbol{\lambda}_i$ satisfies $(M\boldsymbol{y})_i = 0$ for every i. Since $\{\boldsymbol{\lambda}_i\}_i$ is obtained as an l_∞ limit, it is bounded. This shows that $\boldsymbol{y}_i$ has the required asymptotic behaviour, which completes the proof of our statement.

Collecting now the results, one may cast $\sigma_{\mu\nu}$ of (14) into the form

$$\begin{aligned}\sigma_{\mu\nu} &= e^2\beta \lim_{\Omega\to\infty} \frac{1}{|\Omega|} \sum_{i,j\in\Omega} x_i^{\mu} M_{ij}^{\Omega} x_j^{\nu} - e^2\beta \lim_{\Omega\to\infty}\frac{1}{|\Omega|}\sum_{i,j\in\Omega} x_i^{\mu} M_{ij}^{\Omega} x_j^{\nu} \\ &= e^2\beta \lim_{\Omega\to\infty}\frac{1}{|\Omega|}\sum_{i,j\in\Omega} x_i^{\mu} M_{ij}^{\Omega} y_j^{\nu}\end{aligned}$$

which is exactly (11), as desired.

4. Periodic lattices

We consider a periodic lattice, whose Bravais lattice vectors are denoted by $\boldsymbol{r}$, and having N sites per cell. The positions inside the cell are given by the set of vectors $\{\boldsymbol{\xi}_s\}_{1\leq s\leq N}$. This way the site index i is replaced by the set $(\boldsymbol{r}, s)$ and

$$\boldsymbol{x}_s(\boldsymbol{r}) = \boldsymbol{r} + \boldsymbol{\xi}_s, \qquad s = 1, 2, \ldots, N.$$

The translational invariance of the problem implies

$$\varepsilon_s(\boldsymbol{r}) = \varepsilon_s,$$

$$\mathscr{W}^{S}_{ss'}(\boldsymbol{r},\boldsymbol{r}')=\mathscr{W}^{S}_{ss'}(\boldsymbol{r}-\boldsymbol{r}',0)\equiv\mathscr{W}^{S}_{ss'}(\boldsymbol{r}-\boldsymbol{r}'),$$
$$A_{ss's''}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'')=A_{ss's''}(\boldsymbol{r}-\boldsymbol{r}'',\boldsymbol{r}'-\boldsymbol{r}''),$$
$$M_{ss'}(\boldsymbol{r},\boldsymbol{r}')=M_{ss'}(\boldsymbol{r}-\boldsymbol{r}').$$

As immediate consequences we have the periodicity and thus the boundedness of the quantities in (17) and of $p_s(\boldsymbol{r})=p_s$.

We turn now to the proof of (20) (which contains also the proof of (10)). Because of the translation invariance of the problem it is useful to use discrete Fourier transforms

$$\tilde{M}(\boldsymbol{k})=\sum_{\boldsymbol{r}}M(\boldsymbol{r})\,\mathrm{e}^{\mathrm{i}\boldsymbol{kr}}$$

where $\boldsymbol{k}$ runs through the Brillouin zone of the lattice. In this representation $\tilde{M}(\boldsymbol{k})$ are $N\times N$ diagonal blocks of M so that the whole problem becomes N-dimensional. The zero eigenvalue of M belongs to $\tilde{M}(0)$, and is non-degenerate with the eigenvector denoted by $|1\rangle$ having all its N components equal to 1. It is easy to see that

$$M\boldsymbol{x}=\tilde{M}(0)|\boldsymbol{\xi}\rangle+\mathrm{i}(\nabla_{\boldsymbol{k}}\tilde{M})(0)|1\rangle$$

where $|\boldsymbol{\xi}\rangle$ has the components $(\boldsymbol{\xi}_s)_s$.

The quantity of interest becomes

$$\frac{1}{zp+M}M\boldsymbol{x}=\frac{1}{zp+\tilde{M}(0)}[\tilde{M}(0)|\boldsymbol{\xi}\rangle+\mathrm{i}(\nabla_{\boldsymbol{k}}\tilde{M})(0)|1\rangle]. \tag{21}$$

The $z\to 0$ limit of (21) is analysed using the perturbation theory with respect to z. Using the notations m_α, P_α ($\alpha=1,2,\ldots,N$) for the eigenvalues and eigenprojectors of $\tilde{M}(0)$ and knowing that

$$m_1=0,\qquad P_1=|1\rangle\langle 1|/\langle 1|1\rangle,$$

the only singular term in the $z\to 0$ limit can arise from the perturbation of m_1 and is

$$\frac{1}{z\langle 1|p|1\rangle}|1\rangle[\langle 1|\tilde{M}(0)|\boldsymbol{\xi}\rangle+\mathrm{i}\langle 1|(\nabla_{\boldsymbol{k}}\tilde{M})(0)|1\rangle].$$

Since the first term is obviously zero, the essence of the proof is to show that

$$\mathrm{i}\langle 1|(\nabla_{\boldsymbol{k}}\tilde{M})(0)|1\rangle=-\sum_{s,s'}M_{ss'}(\boldsymbol{r})\boldsymbol{r}=0.$$

For the symmetric part of M it is obviously true using inversion symmetry arguments ($M^{S}_{ss'}(\boldsymbol{r})=M^{S}_{s's}(-\boldsymbol{r})$). For the antisymmetric part one has to show that

$$\sum_{\substack{ss's''\\ \boldsymbol{rr}'}}\boldsymbol{r}A_{ss's''}(\boldsymbol{r},0,\boldsymbol{r}')=\sum_{\boldsymbol{r},\boldsymbol{r}'}\boldsymbol{r}a(\boldsymbol{r},0,\boldsymbol{r}')=0 \tag{22}$$

where

$$a(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'')=\sum_{ss's''}A_{ss's''}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'').$$

Since $a(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'')$ is a completely antisymmetric, translation invariant quantity, one has successively

$$\sum_{\boldsymbol{r},\boldsymbol{r}'}\boldsymbol{r}a(\boldsymbol{r},0,\boldsymbol{r}')=\sum_{\boldsymbol{r},\boldsymbol{r}'}\boldsymbol{r}a(\boldsymbol{r}-\boldsymbol{r}',-\boldsymbol{r}',0)=-\sum_{\boldsymbol{r},\boldsymbol{r}'}\boldsymbol{r}a(\boldsymbol{r}-\boldsymbol{r}',0,-\boldsymbol{r}')$$
$$=-\sum_{\boldsymbol{r},\boldsymbol{r}'}(\boldsymbol{r}-\boldsymbol{r}')a(\boldsymbol{r},0,\boldsymbol{r}')=-2\sum_{\boldsymbol{r},\boldsymbol{r}'}\boldsymbol{r}a(\boldsymbol{r},0,\boldsymbol{r}')$$

which shows that (22) is true. Therefore the $z \to 0$ limit exists and the calculations give

$$|\boldsymbol{\lambda}\rangle = -|\boldsymbol{\alpha}\rangle = \lim_{z\to 0} \frac{1}{zp+\tilde{M}(0)} [\tilde{M}(0)|\boldsymbol{\xi}\rangle + \mathrm{i}(\nabla_{\boldsymbol{k}}\tilde{M})(0)|1\rangle]$$

$$= |\boldsymbol{\xi}\rangle + G[\mathrm{i}(\nabla_{\boldsymbol{k}}\tilde{M})(0)|1\rangle] + \Lambda|1\rangle$$

where

$$G = \sum_{\alpha\neq 1} \frac{1}{m_\alpha} P_\alpha$$

and Λ is a constant. In fact Λ is irrelevant since it represents a constant shift of the potential in (10). Up to this term we obtain

$$\boldsymbol{y}_s(\boldsymbol{r}) = \boldsymbol{r} - \sum_{s'} (G\mathrm{i}(\nabla_{\boldsymbol{k}}\tilde{M})(0))_{ss'}$$

independent of the actual positions of the sites in the cell. For periodic lattices the infinite-volume limit for the conductivity (12) is readily performed and gives

$$\sigma_{\mu\nu} = e^2\beta \left(\tfrac{1}{2} \sum_{\substack{ss'\\ \boldsymbol{r}}} \mathscr{W}^{\mathrm{S}}_{ss'}(\boldsymbol{r})(y^\mu_s(\boldsymbol{r}) - y^\mu_{s'}(0))(y^\nu_s(\boldsymbol{r}) - y^\nu_{s'}(0)) \right.$$
$$\left. + \tfrac{1}{3} \sum_{\substack{ss's''\\ \boldsymbol{r}\boldsymbol{r}'}} A_{ss's''}(\boldsymbol{r}, \boldsymbol{r}', 0)(y^\mu_s(\boldsymbol{r}) - y^\mu_{s''}(0))(y^\nu_{s'}(\boldsymbol{r}') - y^\nu_{s''}(0)) \right).$$

For simple Bravais lattices G is equal to zero, so that

$$\boldsymbol{y}(\boldsymbol{r}) = \boldsymbol{x}(\boldsymbol{r}) = \boldsymbol{r}.$$

In this case the sign of the Hall effect is electronic, because (13) becomes

$$\boldsymbol{Hh} = e^3\beta\tfrac{1}{6} \sum_{\boldsymbol{r},\boldsymbol{r}'} \mathscr{U}(\boldsymbol{r}, \boldsymbol{r}', 0)[(\boldsymbol{r}\times\boldsymbol{r}')\boldsymbol{H}]^2.$$

Unfortunately, in general (13) does not allow a simple prediction for the sign of the Hall effect. Indeed, the triangles $(\boldsymbol{x}_i, \boldsymbol{x}_j, \boldsymbol{x}_k)$ and $(\boldsymbol{y}_i, \boldsymbol{y}_j, \boldsymbol{y}_k)$ have, in general, non-parallel normals, and one can easily find cases in which $\boldsymbol{H}$ has opposite sign projections on them. This allows for arbitrary sign in some of the terms of (13), according to the direction of $\boldsymbol{H}$.

Another interesting peculiarity of simple lattices is the fact that it shows very clearly the importance of the surfaces in the Hall effect. Because in simple lattices the problem is always inversion invariant, we have

$$A(\boldsymbol{r}, \boldsymbol{r}', \boldsymbol{r}'') = A(-\boldsymbol{r}, -\boldsymbol{r}', -\boldsymbol{r}'').$$

Therefore we have

$$A(\boldsymbol{r}, 0, \boldsymbol{r}') = A(-\boldsymbol{r}, 0, -\boldsymbol{r}') = -A(0, -\boldsymbol{r}, -\boldsymbol{r}') = -A(\boldsymbol{r}, 0, \boldsymbol{r}-\boldsymbol{r}')$$

and in the expression of

$$\mathscr{W}^{\mathrm{A}}(\boldsymbol{r}) = \sum_{\boldsymbol{r}'} A(\boldsymbol{r}, 0, \boldsymbol{r}')$$

the terms with $\boldsymbol{r}'_1$ and $\boldsymbol{r}'_2 = \boldsymbol{r} - \boldsymbol{r}'_1$ cancel out pairwise so that $\mathscr{W}^{\mathrm{A}}(\boldsymbol{r})$ is identically zero. Therefore any information about the magnetic field is lost on the infinite system. On the other hand, for a finite system, and close to the surface, the cancellation does not take place if one of the terms involves points outside the domain Ω.

5. Concluding remarks

Although in the Kubo version the conductivity seems to depend on the matrices Γ, p and the site locations $\boldsymbol{x}_i$, while the stationary flow problem is formulated only in terms of the matrix M, it was shown that the two approaches are equivalent in the case of periodic lattices. Many steps of the proof do not depend essentially on the periodicity and were given directly for more general systems. Other steps had to be replaced by certain assumptions.

It is obvious that some hypotheses are needed in order to ensure that the system is macroscopically homogeneous. It is felt that the assumptions we made are of this character.

The formula one gets for the conductivity (12) is easily and transparently obtained in the Miller–Abrahams framework, while in the Kubo-type approach a more complicated argument is needed.

As emerged from the analysis, the magnetic field dependent part of σ is highly sensitive to the handling of the surface contribution.

Taking from the very beginning the infinite system leads to incorrect results as shown in § 4.

In what concerns the sign of the Hall effect one cannot predict a unique answer. For Bravais lattices it is electronic, but other cases cannot be ruled out.

Our result (12) was first obtained by Butcher and Kumar (1980). As far as the Hall effect was concerned they essentially used the $\omega \to 0$ limit of the Kubo formula, linearised with respect to $\boldsymbol{H}$ (which amounts to taking for our set $\{y_i\}_i$ in (13) only its $\boldsymbol{H}=0$ value). For the identification of the symmetric part of the DC conductivity tensor the $\omega \to 0$ limit for the Joule heating of the Miller–Abrahams resistor network was computed. The homogeneity was achieved by a configurational average of the disordered system, and the $\omega \to 0$ limit of the relevant quantities was assumed to exist.

We showed here that both the Kubo and the Miller–Abrahams approach give the same result for both the symmetric and the antisymmetric part of σ DC, and tried to restrict to a minimum of explicit assumptions, for the rigorous proof of the results.

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