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The Bloch Equation at Low Temperatures

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Abstract. The Bloch equation (linear Boltzmann equation for fermions) may be written as $L_x f = g_0$ where L_x is a bounded self-adjoint operator and x the normalized inverse temperature. For sufficiently large x the inverse of L_x exists and is bounded. This leads to the x^5 -law for the electrical conductivity.

1. Introduction

Let \mathcal{H} be the Hilbert space of complex-valued functions on the reals with scalar product

$$(f, g) = \int dy \rho(y) \overline{f(y)} g(y) \quad (1.1)$$

where the density ρ is given by

$$\rho(y) = e^y (e^y + 1)^{-2} = (2 \cosh(y/2))^{-2} \quad (1.2)$$

(integrals extend over \mathbb{R} if not otherwise indicated). Define the Bloch operator L_x by

$$(L_x f)(y) = \int dz \theta(x^2 - z^2) K_1(y, z) \{px^2 f(y) - (px^2 - z^2) f(y + z)\} \quad (1.3)$$

for all $f \in \mathcal{H}$ such that $L_x f \in \mathcal{H}$.

The kernels $K_n (n \in \mathbb{N})$ are given by

$$K_n(y, z) = z^{2n} (e^y + 1) \{(e^{y+z} + 1) |1 - e^{-z}|^{-1}\} \quad (1.4)$$

θ is the step function, p a positive constant and $x^{-1} = T/T_0$ the temperature normalized with a suitable reference temperature T_0 .

The Bloch equation, i.e. the linearized Boltzmann equation for electrons (with isotropic energy momentum dispersion) interacting with phonons reads now

$$L_x f = g_0 \quad (1.5)$$

with $g_0(y) = 1$ (this is equation (82) of [1] via the identification $c = pPx^5f$, $pQ = 1$). Remark that $g_0 \in \mathcal{H}$ with $\|g_0\| = 1$.

Assuming existence and uniqueness of the solution f_x of (1.5) the static electric conductivity is given by

$$\sigma(x) = cx^5(f_x, g_0) \quad (1.6)$$

with a constant c independent of x .

It will be shown that L_x is a bounded self-adjoint operator which has a bounded inverse for sufficiently large x . Hence, the solution of (1.5) is given by $f_x = L_x^{-1}g_0$. Furthermore, L_x^{-1} has a limit as x tends to infinity. The corresponding limit of (f_x, g_0) is calculated explicitly, yielding

$$\lim_{x \rightarrow \infty} (f_x, g_0) = (240\zeta(5))^{-1} \quad (1.7)$$

where ζ denotes Riemann's Zeta function. In view of (1.6) this means that the conductivity behaves like x^5 for large x (T^{-5} — law of Bloch [2]).

The proof of these assertions involves an intermediate step consisting of the discussion of a simpler problem,

$$M_x f = g_0 \quad (1.8)$$

where M_x is obtained from (1.3) by omitting the step function. In Section 2 the problems (1.8) and (1.5) are treated, whereas Section 3 is devoted to an extension of (1.5) by including impurity scattering.

2. The Bloch Equation

Let $\hat{\mathcal{H}}$ denote the Hilbert space $L^2(\mathbb{R})$ with the usual scalar product. $\hat{\mathcal{H}}$ and \mathcal{H} , introduced in Section 1, are isomorphic via

$$\hat{f}(y) = (Uf)(y) = \sqrt{\rho(y)}f(y). \quad (2.1)$$

To any operator O in \mathcal{H} corresponds $\hat{O} = UOU^{-1}$ in $\hat{\mathcal{H}}$.

For $n \in \mathbb{N}$ we define the operator B_n in \mathcal{H} by

$$(B_n f)(y) = \int dz K_n(y, z)f(y + z) \quad (2.2)$$

where K_n is given by (1.4). The corresponding operator \hat{B}_n in $\hat{\mathcal{H}}$ is given by

$$\hat{B}_n \hat{f} = b_n * \hat{f} \quad (2.3)$$

(* denoting convolution) with

$$b_n(y) = \frac{1}{2}y^{2n}|\operatorname{csch}(y/2)|. \quad (2.4)$$

By Young's inequality we have

$$\|\hat{B}_n\| \leq \|b_n\|_1. \quad (2.5)$$

Actually, equality holds in (2.5) due to the fact that b_n is even and non-negative. Evaluation of the r.h.s. of (2.5) yields

$$\|b_n\|_1 = 2(2n)! (2^{2n+1} - 1)\zeta(2n + 1). \quad (2.6)$$

The operators \hat{B}_n are self-adjoint and their spectra are absolutely continuous as they are unitarily equivalent to multiplication by real analytic functions.

In view of (1.3) we also introduce operators $B_{n,x}$ in \mathcal{H} :

$$(B_{n,x} f)(y) = \int dz \theta(x^2 - z^2) K_n(y, z)f(y + z). \quad (2.7)$$

They correspond to $\hat{B}_{n,x}$ in $\hat{\mathcal{H}}$ which are defined as convolution with $b_{n,x}$ where

$$b_{n,x}(y) = \theta(x^2 - y^2)b_n(y). \quad (2.8)$$

By arguments identical to those given above the operators $\hat{B}_{n,x}$ and $\hat{B}_n - \hat{B}_{n,x}$ are self-adjoint, have absolutely continuous spectra and satisfy

$$\|\hat{B}_{n,x}\| = \|b_{n,x}\|_1 \quad (2.9)$$

and

$$\|\hat{B}_n - \hat{B}_{n,x}\| = \|b_n - b_{n,x}\|_1, \quad (2.10)$$

respectively. A simple estimate shows that the r.h.s. of (2.10) vanishes exponentially fast as x tends to infinity. Hence, we have

Lemma 1. \hat{B}_n is the norm-limit of $\hat{B}_{n,x}$ where \hat{B}_n and $\hat{B}_{n,x}$ are defined as convolution by b_n and $b_{n,x}$, respectively, with b_n and $b_{n,x}$ given by (2.4) and (2.8).

Let

$$a = B_1 g_0 \quad (2.11)$$

and

$$a_x = B_{1,x} g_0. \quad (2.12)$$

We define operators A and A_x by

$$(Af)(y) = a(y)f(y) \quad (2.13)$$

and similarly for A_x for those $f \in \mathcal{H}$ where the r.h.s. of (2.13) is in \mathcal{H} . As a and a_x are real A and A_x are self-adjoint.

The Bloch equation (1.5) with L_x given by (1.3) may now be written as

$$\{px^2(A_x - B_{1,x}) + B_{2,x}\}f = g_0 \quad (2.14)$$

whereas the simplified Bloch equation (1.8) is obtained by dropping the index x on A , $B_{n,x}$ in (2.14).

From (2.7) and (2.12) we obtain, after some manipulation

$$a_x(y) = 2 \int_0^x dz z^2 \phi(y, z) \operatorname{csch} z \quad (2.15)$$

with

$$\phi(y, z) = (1 - \tanh^2(z/2) \tanh^2(y/2))^{-1}. \quad (2.16)$$

This leads to

$$a_x(-y) = a_x(y) \quad (2.17)$$

and

$$\frac{d}{dy} a_x(y) = \int_0^x dz z^2 \phi^2(y, z) \psi(y) \psi(z) \quad (2.18)$$

with

$$\psi(y) = \sinh(y/2) \operatorname{sech}^3(y/2) \quad (2.19)$$

i.e. (for $y > 0$ as we shall always assume)

$$\frac{d}{dy} a_x(y) > 0 \quad \text{for } y > 0. \quad (2.20)$$

Hence, a_x increases monotonically from

$$a_x(0) = 2 \int_0^x dz z^2 \operatorname{csch} z > 0 \quad (2.21)$$

to

$$a_x(\infty) = \int_0^\infty dz z^2 \coth(z/2) \quad (2.22)$$

as y varies from 0 to ∞ . The limiting value (2.22) may be written as

$$a_x(\infty) = (x^3/3) + 4\zeta(3) - 2 \int_x^\infty dz z^2 e^{-z} (1 - e^{-z})^{-1} \quad (2.23)$$

where the last term decreases exponentially fast as x tends to infinity. Actually, $a_x(y)$ becomes ‘flat’ at $y \approx x$ for large x as is seen from

$$a_x(x) = (x^3/3) - x^2 \ln 2 + (\pi^2 x/6) + 2.5\zeta(3) + r(x)$$

where the remainder

$$r(x) = \int_x^\infty dz (x - z)^2 (e^z + 1)^{-1} + e^{-x} \int_0^x dz z^2 (e^z + e^{-z})^{-1}$$

decreases exponentially fast as x tends to infinity. From (2.20)–(2.22) it follows that A_x has an absolutely continuous spectrum consisting of the interval $[a_x(0), a_x(\infty)]$, i.e. A_x is bounded.

Now, $a(y)$ and $da(y)/dy$ are obtained from (2.15) and (2.18), respectively, by replacing the upper limit of integration by ∞ . Hence, (2.17) and (2.20) hold also for $a(y)$. It follows that $a(y)$ increases monotonically from

$$a(0) = 2 \int_0^\infty dz z^2 \operatorname{csch} z = 7\zeta(3) \quad (2.24)$$

to infinity. The spectrum of A is absolutely continuous and consists of the interval $[a(0), \infty)$, i.e. A is unbounded. From (2.15) and (2.18) and their analogues for $a(y)$ it follows that

$$a(y) > a_x(y)$$

and

$$\frac{d}{dy} a(y) > \frac{d}{dy} a_x(y), \quad y > 0,$$

whence

$$0 < a_x(y)^{-1} - a(y)^{-1} < a_x(\infty)^{-1}. \quad (2.25)$$

According to their spectral properties A and A_x have bounded inverses which satisfy by (2.25)

$$\|A^{-1} - A_x^{-1}\| = a_x(\infty)^{-1}. \quad (2.26)$$

As, in view of (2.23), the r.h.s. of (2.26) is $O(x^{-3})$ for large x we have

Lemma 2. A_x^{-1} converges in norm to A^{-1} where A_x^{-1} and A^{-1} are defined as multiplication by $a_x(y)^{-1}$ and $a(y)^{-1}$ with a and a_x given by (2.11) and (2.12), respectively.

The following lemma concerns the combinations $A_x - B_{1,x}$ and $A - B_1$ which occur in (2.14) and its simplified version. Remark that $A_x - B_{1,x}$ is bounded and self-adjoint whereas $A - B_1$ is unbounded and self-adjoint on the domain $D(A)$ of A .

Lemma 3. The operators $A_x - B_{1,x}$ and $A - B_1$ are positive and zero is a simple eigenvalue with eigenvector g_0 .

Proof. For $f \in \mathcal{H}$

$$((A_x - B_{1,x})f)(y) = \int dz \theta(x^2 - (z - y)^2) K_1(y, z - y) \{f(y) - f(z)\} \quad (2.27)$$

and

$$(f, (A_x - B_{1,x})f) = \frac{1}{2} \int dy \int dz \theta(x^2 - (z - y)^2) H(y, z) |f(y) - f(z)|^2 \quad (2.28)$$

with

$$H(y, z) = (y - z)^2 \{(e^y + 1)(e^z + 1) |e^{-y} - e^{-z}|\}^{-1}. \quad (2.29)$$

From (2.27) it follows that g_0 is an eigenvector belonging to the eigenvalue zero whereas (2.29) shows that g_0 is simple and $A_x - B_{1,x}$ positive. Dropping the subscripts x and the θ -functions in (2.27) and (2.28) and choosing $f \in D(A)$ yields the proof for $A - B_1$.

Lemma 4. The operators B_n are A -compact.

Proof. This is equivalent with \hat{A} -compactness of \hat{B}_n . As b_n and $1/a$ belong to \mathcal{H} we obtain

$$\|\hat{B}_n \hat{A}^{-1}\|_{HS} = \|b_n\| \|1/a\|,$$

i.e. $\hat{B}_n \hat{A}^{-1}$ is a Hilbert-Schmidt operator, hence compact.

Corollary. Let B be a finite real linear combination of $\{B_n\}$. The operator $A + B$ is self-adjoint on $D(A)$ and its essential spectrum coincides with that of A , i.e.

$$\sigma(A + B) = \sigma_d(A + B) \cup [a(0), \infty)$$

where σ and σ_d denote spectrum and discrete spectrum (set of isolated eigenvalues of finite multiplicity), respectively. The only possible accumulation point of σ_d is $a(0)$. Especially, zero is an isolated eigenvalue of $A - B_1$.

Proof. The statements of the corollary follow [3] from Lemma 4 (and Lemma 3). Let $\rho(X)$ denote the resolvent set of the operator X .

Lemma 5. For sufficiently large x and arbitrary $\lambda \in \mathbb{R}$

$$z \in \rho(A - \lambda B_1) \Rightarrow z \in \rho(A_x - \lambda B_{1,x}) \quad (2.30)$$

and

$$\text{norm-lim}_{x \rightarrow \infty} (z - A_x + \lambda B_{1,x})^{-1} = (z - A + \lambda B_1)^{-1}. \quad (2.31)$$

Proof. According to [3] it is sufficient to prove (2.31) for $z = i$. Let

$$\Delta_x(\lambda) = (i - A + \lambda B_1)^{-1} - (i - A_x + \lambda B_{1,x})^{-1}$$

and $\Delta_x = \Delta_x(0)$. Repeated use of the resolvent equation yields

$$\begin{aligned}\Delta_x(\lambda) &= \Delta_x - \lambda(i - A_x + \lambda B_1)^{-1} B_1 \Delta_x - \lambda \Delta_x B_1 (i - A + \lambda B_1)^{-1} \\ &\quad + \lambda^2 (i - A_x + \lambda B_1)^{-1} B_1 \Delta_x B_1 (i - A + \lambda B_1)^{-1} \\ &\quad - \lambda (i - A_x + \lambda B_1)^{-1} (B_1 - B_{1,x}) (i - A_x + \lambda B_{1,x})^{-1}\end{aligned}$$

leading to the estimate

$$\|\Delta_x(\lambda)\| \leq (1 + \|\lambda B_1\|)^2 \|\Delta_x\| + \|\lambda (B_1 - B_{1,x})\|.$$

Together with Lemma 1 and Lemma 2 the result follows.

Corollary. Zero is an isolated eigenvalue of $A_x - B_{1,x}$ for x sufficiently large.

Now, by (a trivial generalization of) Theorem 5 of [4]

$$\{px^2(A_x - B_{1,x}) + B_{2,x}\}^{-1} = (g_0, B_{2,x}g_0)^{-1}P - \kappa E_x F_x(\kappa)G_x \quad (2.32)$$

where

$$F_x(\kappa) = \sum_{n=0}^{\infty} (\kappa F_x)^n \quad (2.33)$$

with $\kappa^{-1} = px^2$ and

$$\begin{aligned}E_x &= S_x - (g_0, B_{2,x}g_0)^{-1} P B_{2,x} S_x \\ S_x &= \text{norm-lim}_{z \rightarrow 0} (z - A_x + B_{1,x})^{-1} (P - I) \\ F_x &= -B_{2,x} E_x \\ G_x &= (g_0, B_{2,x}g_0)^{-1} B_{2,x} P - I.\end{aligned} \quad (2.34)$$

P is the projector on the subspace spanned by g_0 . Similarly, we have

$$\{px^2(A - B_1) + B_2\}^{-1} = (g_0, B_2g_0)^{-1}P - \kappa E F(\kappa)G \quad (2.35)$$

with the r.h.s. defined by formulae obtained from (2.33) and (2.34) by dropping the subscript x . All operators on the r.h.s. of (2.32) and (2.35) are bounded and the latter are the norm limits of the former. Hence, the series (2.33) converges absolutely for $x > x_0$ with x_0 suitably chosen.

From (2.32) it follows that the solution of equation (2.14) is given by

$$f_x = (g_0, B_{2,x}g_0)^{-1}g_0 - \kappa E_x F_x(\kappa)G_x g_0 \quad (2.36)$$

leading to

$$\lim_{x \rightarrow \infty} (g_0, f_x) = (g_0, B_2g_0)^{-1} \quad (2.37)$$

with

$$(g_0, B_2g_0) = 240\zeta(5). \quad (2.38)$$

Remark. The operators $\hat{B}_{n,x}$ do not depend analytically on x . They are norm continuous but their derivatives $\hat{B}'_{n,x}$ are only strongly continuous. A simple calculation yields

$$\hat{B}'_{n,x} = b_n(x)\{\hat{U}(x) + \hat{U}(-x)\} \quad (2.39)$$

where $\hat{U}(x)$ is the one-parameter group of translations,

$$(\hat{U}(x)\hat{f})(y) = \hat{f}(y - x) \quad (2.40)$$

which is strongly but not norm continuous. However, \hat{g}_0 is an analytic vector of $\hat{U}(x)$, i.e. $\hat{U}(x)\hat{g}_0$ depends analytically on x . Hence, the same is true for $\hat{B}_{n,x}\hat{g}_0$. This is a first step towards answering the open question whether f_x (or at least (f_x, g_0)) depends analytically on x . The case is different for the solution of the simplified Bloch equation where the analogue of (2.35) immediately exhibits analyticity in $(x_0, \infty]$ with $px_0^2 = \|F\|$.

3. The Modified Bloch Equation

If the electrons not only interact with phonons but also with randomly distributed impurities the Bloch equation (1.5) has to be modified in the following way [5]:

$$L_x f + c\sigma_0^{-1}x^5 f = g_0 \quad (3.1)$$

where σ_0 is a positive constant (the constant c is the same as in equation (1.6)). If the electron-phonon interaction is turned off (3.1) reduces to

$$c\sigma_0^{-1}x^5 f = g_0 \quad (3.2)$$

with the solution

$$f_x = c^{-1}\sigma_0 x^{-5} g_0. \quad (3.3)$$

Inserting (3.3) into (1.6) yields

$$\sigma(x) = \sigma_0, \quad (3.4)$$

i.e. the conductivity becomes temperature independent if it is based only on impurity scattering. Setting

$$h = c\sigma_0^{-1}x^5 f \quad (3.5)$$

in (3.1) and (1.6) leads to

$$(c^{-1}\sigma_0 x^{-5} L_x + I)h = g_0 \quad (3.6)$$

and

$$\sigma(x) = \sigma_0(h, g_0). \quad (3.7)$$

Equation (3.6) may be written as (compare with equation (2.14))

$$(C_x + c^{-1}\sigma_0 x^{-5} B_{2,x})h = g_0 \quad (3.8)$$

where

$$C_x = I + c^{-1}\sigma_0 p x^{-3} (A_x - B_{1,x}) \quad (3.9)$$

is a positive bounded operator with lower bound 1 which is a simple eigenvalue and g_0 the associated eigenvector (Lemma 3). For sufficiently large x this eigenvalue is isolated (Corollary to Lemma 5). Hence, $\|C_x^{-1}\| \leq 1$ for all $x > 0$. As $C_x^{-1}g_0 = g_0$ we obtain from (3.8)

$$(I + c^{-1}\sigma_0 x^{-5} C_x^{-1} B_{2,x})h = g_0. \quad (3.10)$$

The operator $C_x^{-1}B_{2,x}$ is uniformly bounded by $\|B_2\|$. Therefore, (3.10) may be solved by the Neumann series for sufficiently large x (e.g. $x^5 > c^{-1}\sigma_0 \|B_2\|$):

$$h = g_0 + \sum_{n=1}^{\infty} (-c^{-1}\sigma_0 x^{-5} C_x^{-1} B_{2,x})^n g_0. \quad (3.11)$$

Inserting (3.11) into (3.7) yields

$$\sigma(x) = \sigma_0 \{1 - c^{-1} \sigma_0 x^{-5} (g_0, B_{2,x} g_0) + s(x)\} \quad (3.12)$$

with

$$s(x) = \sum_{n=2}^{\infty} (-c^{-1} \sigma_0 x^{-5})^n (g_0, (C_x^{-1} B_{2,x})^n g_0) \quad (3.13)$$

which is $O(x^{-10})$ as $x \rightarrow \infty$. Introducing the resistivity $\rho(x) = 1/\sigma(x)$ we get

$$\rho(x) = \rho_0 + \rho_1(x) + \rho_2(x) \quad (3.14)$$

where $\rho_0 = 1/\sigma_0$ is the impurity resistivity, $\rho_1(x)$ the phonon resistivity given by (1.6) and (2.35) and $\rho_2(x)$ the so-called deviation from Matthiessen's rule. From (2.35) and (3.12)–(3.14) it follows that $\rho_2(x) = O(x^{-7})$ as $x \rightarrow \infty$.

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