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

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

where the density ρ is given by

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

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

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

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

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

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

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

$$L_x f = g_0 \tag{1.5}$$

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

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

$$\sigma(x) = cx^5(f_x, g_0) \tag{1.6}$$

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

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

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,

$$M_x f = g_0 \tag{1.8}$$

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

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

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

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

$$(B_n f)(y) = \int dz K_n(y, z) f(y + z) \tag{2.2}$$

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

$$\hat{B}_n \hat{f} = b_n * \hat{f} \tag{2.3}$$

($*$ denoting convolution) with

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

By Young's inequality we have

$$\|\hat{B}_n\| \leqslant \|b_n\|_1. \tag{2.5}$$

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

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

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 $\mathscr{H}$:

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

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

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

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

$$\|\hat{B}_{n,x}\| = \|b_{n,x}\|_1 \tag{2.9}$$

and

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

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

$$a = B_1 g_0 \tag{2.11}$$

and

$$a_x = B_{1,x} g_0. \tag{2.12}$$

We define operators A and A_x by

$$(Af)(y) = a(y)f(y) \tag{2.13}$$

and similarly for A_x for those $f \in \mathscr{H}$ where the r.h.s. of (2.13) is in $\mathscr{H}$. 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

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

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

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

with

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

This leads to

$$a_x(-y) = a_x(y) \tag{2.17}$$

and

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

with

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

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

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

Hence, a_x increases monotonically from

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

to

$$a_x(\infty) = \int_0^x dz z^2 \coth(z/2) \tag{2.22}$$

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

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

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

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

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

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

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

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

whence

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

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

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

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 $f \in \mathscr{H}$

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

and

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

with

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

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 $\hat{\mathscr{H}}$ 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 $\lambda \in \mathbb{R}$

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

and

$$\operatorname*{norm-lim}_{x\to\infty}(z - A_x + \lambda B_{1,x})^{-1} = (z - A + \lambda B_1)^{-1}. \tag{2.31}$$

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

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

leading to the estimate

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

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]

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

where

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

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

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

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

$$\{px^2(A - B_1) + B_2\}^{-1} = (g_0, B_2 g_0)^{-1}P - \kappa EF(\kappa)G \tag{2.35}$$

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

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

leading to

$$\lim_{x\to\infty} (g_0, f_x) = (g_0, B_2 g_0)^{-1} \tag{2.37}$$

with

$$(g_0, B_2 g_0) = 240\zeta(5). \tag{2.38}$$

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

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

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

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

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]:

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

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

$$c\sigma_0^{-1}x^5 f = g_0 \tag{3.2}$$

with the solution

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

Inserting (3.3) into (1.6) yields

$$\sigma(x) = \sigma_0, \tag{3.4}$$

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

$$h = c\sigma_0^{-1}x^5 f \tag{3.5}$$

in (3.1) and (1.6) leads to

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

and

$$\sigma(x) = \sigma_0(h, g_0). \tag{3.7}$$

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

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

where

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

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, $\|C_x^{-1}\| \leqslant 1$ for all $x > 0$. As $C_x^{-1}g_0 = g_0$ we obtain from (3.8)

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

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. $x^5 > c^{-1}\sigma_0\|B_2\|$):

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

Inserting (3.11) into (3.7) yields

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

with

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

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

$$\rho(x) = \rho_0 + \rho_1(x) + \rho_2(x) \tag{3.14}$$

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 $x \to \infty$.

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