The Faraday effect revisited: General theory

Cornean, Horia Decebal; Nenciu, Gheorghe; Pedersen, Thomas Garm

Publication date:
2005

Document Version
Publisher's PDF, also known as Version of record

Link to publication from Aalborg University

Citation for published version (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

? Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
? You may not further distribute the material or use it for any profit-making activity or commercial gain
? You may freely distribute the URL identifying the publication in the public portal

Take down policy
If you believe that this document breaches copyright please contact us at vbn@aub.aau.dk providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from vbn.aau.dk on: January 01, 2020
The Faraday effect revisited: General theory

by

H. D. Cornean, G. Nenciu and T. G. Pedersen

R-2005-24

June 2005
The Faraday effect revisited: General theory

14th of June 2005

Horia D. Cornean\textsuperscript{1}, Gheorghe Nenciu\textsuperscript{2 3}, Thomas G. Pedersen \textsuperscript{4}

Abstract

This paper is the first in a series revisiting the Faraday effect, or more generally, the theory of electronic quantum transport/optical response in bulk media in the presence of a constant magnetic field. The independent electron approximation is assumed. For free electrons, the transverse conductivity can be explicitly computed and coincides with the classical result. In the general case, using magnetic perturbation theory, the conductivity tensor is expanded in powers of the strength of the magnetic field $B$. Then the linear term in $B$ of this expansion is written down in terms of the zero magnetic field Green function and the zero field current operator. In the periodic case, the linear term in $B$ of the conductivity tensor is expressed in terms of zero magnetic field Bloch functions and energies. No derivatives with respect to the quasimomentum appear and thereby all ambiguities are removed, in contrast to earlier work.

1 Introduction

In sharp contrast with the zero magnetic field case, the analysis of properties of electrons in periodic or random potentials subjected to external magnetic fields is a very challenging problem. The difficulty is rooted in the singular nature of the magnetic interaction: due to a linear increase of the magnetic vector potential, the naive perturbation theory breaks down even at arbitrarily small fields.

To our best knowledge, only the periodic case has been considered in connection with the Faraday effect for bulk systems. The first full scale quantum computation was done by Laura M. Roth \cite{Roth} (for a review of earlier attempts we direct the reader to this paper). The physical experiment starts by sending a monochromatic light wave, parallel to the $0z$ direction and linearly polarized in the plane $x0z$. When the light enters the material, the polarization plane can change; in fact, there exists a linear relation between the angle $\theta$ of rotation of

\textsuperscript{1}Dept. Math., Aalborg University, Fredrik Bajers Vej 7G, 9220 Aalborg, Denmark; e-mail: cornean@math.aau.dk
\textsuperscript{2}Dept. Theor. Phys., University of Bucharest, P. O. Box MG11, RO-76900 Bucharest, Romania;
\textsuperscript{3}Inst. of Math. “Simion Stoilow” of the Romanian Academy, P. O. Box 1-764, RO-014700 Bucharest, Romania; e-mail: Gheorghe.Nenciu@imar.ro
\textsuperscript{4}Dept. Phys. and Nanotech., Pontoppidanstræde 103, 9220 Aalborg, Denmark; e-mail: tgp@physics.aau.dk
the plane of polarisation per unit length and the transverse component of the conductivity tensor $\sigma_{xy}$ (see formula (1) in [1]). The material is chosen in such a way that when the magnetic field is zero, this transverse component vanishes. When the magnetic field $B$ is turned on, the transverse component is no longer zero. For weak fields one expands the conductivity tensor to first order in $B$ and obtains a formula for the Verdet constant.

Therefore the central object is $\sigma_{xy}(B)$, which depends among other things on temperature, density of the material, and frequency of light. Using a modified Bloch representation, Roth was able to obtain a formula for $\frac{d\sigma_{xy}}{dB}(0)$, and studied how this first order term behaves as a function of frequency, both for metals and semiconductors.

However, the theory in [1] is not free of difficulties. First, it seems almost hopeless to estimate errors or to push the computation to higher orders in $B$. Second, even the first order formula contains terms which are singular at the crossings of the Bloch bands. Accordingly, at the practical level this theory only met a moderate success and alternative formalisms have been used, as for example the celebrated Kohn-Luttinger effective many band Hamiltonian (see [2, 3, 4] and references therein), or tight-binding models [5]. Since all these methods have limited applicability, a more flexible approach was still needed.

In the zero magnetic field case, a very successful formalism (see e.g. [6, 7, 8, 9] and references therein) is to use the Green function method. This is based on the fact that the traces involved in computing various physical quantities can be written as integrals involving Green functions. The main aim of our paper is to develop a Green function approach to the Faraday effect, i.e. for the conductivity tensor when a magnetic field is present. Let us point out that the use of Green functions (albeit different from the ones used below) goes back at least to Sondheimer and Wilson [10] in their theory of diamagnetism of Bloch electrons. Aside from the fact that the Green function (i.e. the integral kernel of the resolvent or the semigroup) is easier to compute and control, the main point is that by factorizing out the so called ”nonintegrable phase factor” (or ”magnetic holonomy”) from the Green function, one can cope with the singularities introduced by the increase at infinity of the magnetic vector potentials. In addition, (as it has already been observed by Schwinger [11] in a QED context) after factorizing out the magnetic holonomy one remains with a gauge invariant quantity which makes the problem of gauge fixing irrelevant. The observation (going back at least to Peierls [12]) that one can use these magnetic phases in order to control the singularity of the magnetic perturbation has been used many times in various contexts (see e.g. [10, 13]). We highlight here the results of Nedoluha [14] where a Green function approach for the magneto-optical phenomena at zero temperature and with the Fermi level in a gap has been investigated.

But the power of this method has only recently been fully exploited in [15, 16], and developed as a general gauge invariant magnetic perturbation theory in [17]. Applied to the case at hand, this theory gives an expansion of the conductivity tensor in terms of the zero magnetic field Green functions. Moreover, it is free of any divergencies. A key ingredient in controlling divergencies is
the exponential decrease of the Green functions with the distance between the arguments, for energies outside the spectrum [18, 19]. We stress the fact that since no basis is involved, periodicity is not needed and the theory can also be applied to random systems. Finite systems and/or special geometries (layers) are also allowed.

The content of the paper is as follows. In Section 2 we give a derivation of the conductivity tensor from first principles. We include it for two reasons. The first reason is to point out that this coincides with various formulas used before, and in addition to show that in the low frequency limit it coincides (as it should) with a formula of Streda [20] for the Integral Quantum Hall Effect (IQHE). In particular, if we consider the transverse component of the conductivity tensor at low magnetic field, zero temperature, zero frequency, with the Fermi level in a spectral gap of the system without magnetic field, then for periodic systems (under the proviso that exponentially localized Wannier function exist), this component vanishes (see also [21], [22] for related results). We stress that this result holds for the whole \( \sigma_{xy}(B) \) as long as the magnetic field is not too large, not just for \( \frac{d\sigma_{xy}}{dB}(0) \). The vanishing of its first order correction was in fact claimed in formula (50) in [1]. The second reason is that for further mathematical developments we need a form involving a contour integral over complex energies.

Section 3 contains the exact quantum computation of \( \sigma_{xy}(B) \) for free electrons; in spite of the fact that such a result might be known (and it is known at zero frequency), we were not able to find it in the literature. Interestingly enough, the quantum computation gives the same result as the well known classical computation (when the relaxation time is infinite). Section 4 contains the argument that the use of magnetic phases allows one to take the limit of large systems. The core of the paper is contained in Section 5 which includes the derivation of \( \frac{d\sigma_{xy}}{dB}(0) \). As in the zero magnetic field case, its formula only contains zero magnetic field Green functions and current operators. Section 6 deals with periodic systems, and the result of the previous section is written down in terms of zero magnetic field Bloch functions and bands. At the end we have some conclusions.

The main goal of this paper is to present the strategy, state the results concerning the Verdet constant, and to outline future theoretical and practical problems. Detailed proofs will be given elsewhere.

2 Preliminaries. The conductivity tensor in the linear response regime

We begin by fixing the notation used in the description of independent electrons subjected to a constant magnetic field. The units are chosen so that \( \hbar = 1 \). Since we consider spin 1/2 particles, the one particle Hilbert space for a non-confined particle is

\[
\mathcal{H}_\infty = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)
\]
with the standard scalar product. Accordingly, all operators below and their integral kernels are 2 × 2 matrices in the spin variable. We choose the constant magnetic field of strength $B$ to be oriented along the $z$-axis. Then the one particle Hamiltonian with the spin-orbit coupling included is (see e.g. [1])

$$H_\infty(B) = \frac{1}{2m}P(B)^2 + V + g\mu_BB_3,$$

(2.1)

with

$$P(B) = -i\nabla - ba + \frac{1}{2mc^2}s \wedge (\nabla V) = P(0) - ba$$

(2.2)

where $a(x)$ is an arbitrary smooth magnetic vector potential which generates a magnetic field of intensity $B = 1$ i.e. $\nabla \wedge a(x) = (0, 0, 1)$. The most frequently used magnetic vector potential is the symmetric gauge:

$$a_0(x) = \frac{1}{2}n_3 \wedge x.$$  

(2.3)

where $n_3$ is the unit vector along $z$ axis.

In the periodic case we denote by $L$ the underlying Bravais lattice, by $\Omega$ its elementary cell and by $\Omega^*$ the corresponding Brillouin zone. $|\Omega|$ and $|\Omega^*|$ stand for the volumes of the elementary cell and Brillouin zone respectively. In the absence of the magnetic field one has the well known Bloch representation in terms of Bloch functions:

$$\Psi_j(x, k) = \frac{1}{\sqrt{|\Omega^*|}} e^{ik \cdot x} u_j(x, k), \quad x \in \mathbb{R}^3$$

(2.4)

where $u_j(x, k)$ are the normalised to one eigenfunctions of the operator

$$h(k)u_j(x, k) = \lambda_j(k)u_j(x, k)$$

(2.5)

$$h(k) = \frac{1}{2m} \left( -i\nabla_p + \frac{1}{2mc^2}s \wedge (\nabla V) + k \right)^2 + V,$$

$$= \frac{1}{2m}(p + k)^2 + V, \quad k \in \Omega^*,$$

$$p = -i\nabla_p + \frac{1}{2mc^2}s \wedge (\nabla V),$$

(2.6)

defined in $L^2(\Omega) \oplus L^2(\Omega)$ with periodic boundary conditions. We label $\lambda_j(k)$ in increasing order. We have to remember that, as functions of $k$, $\lambda_j(k)$ and $u_j(x, k)$ are not differentiable at the crossing points. Since the $\Psi_j(x, k)$'s form a basis of generalized eigenfunctions, the Green function (i.e. the integral kernel of the resolvent) writes as:

$$G_\infty^{(0)}(x, y; z) = \int_{\Omega^*} \sum_{j \geq 1} \frac{|\Psi_j(x, k)|^2}{\lambda_j(k) - z} d\k.$$  

(2.7)
and it is seen as a matrix in the spin variables. The above formula has to be understood in the formal sense since the series in the right hand side is typically not absolutely convergent, and care is to be taken when interchanging the sum with the integral. Notice however that $G_\infty^{(0)}(x, x'; z)$ is a well behaved matrix valued function.

We consider a system of noninteracting electrons in the grandcanonical ensemble. More precisely, we consider a box $\Lambda_1 \subset \mathbb{R}^3$, which contains the origin, and a family of scaled boxes

$$
\Lambda_L = \{ x \in \mathbb{R}^3 : x/L \in \Lambda_1 \}.
$$

The thermodynamic limit will mean $L \to \infty$, that is when $\Lambda_L$ fills the whole space. The one particle Hilbert space is $H_L := L^2(\Lambda_L) \oplus L^2(\Lambda_L)$. The one particle Hamiltonian is denoted by $H_L(B)$ and is given by (2.1) with Dirichlet boundary conditions (i.e. the wavefunction in the domain of $H_L(B)$ vanishes on the surface $\partial \Lambda_L$). We assume that the temperature $T = 1/(k\beta)$ and the chemical potential $\mu$ are fixed by a reservoir of energy and particles. We work in a second quantized setting with an antisymmetric Fock space denoted by $\mathcal{F}_L$.

Denote the operators in the Fock space with a hat and borrow some notation from the book of Bratelli and Robinson [23]: if $A$ is an operator defined in $H_L$, we denote by $\hat{A} = d\hat{\square}(A)$ its second quantization in the Fock space. At $t = -\infty$ the system is supposed to be in the grandcanonical equilibrium state of temperature $T$ and chemical potential $\mu$, i.e. the density matrix is

$$
\hat{\rho}_c = \frac{1}{\text{Tr}(e^{-\beta K})} e^{-\beta K}, \quad (2.8)
$$

where

$$
\hat{K}_\mu = d\Gamma(H_L(B) - \mu \cdot \text{Id}) \quad (2.9)
$$

is the “grandcanonical Hamiltonian”.

The interaction with a classical electromagnetic field is described by a time dependent electric potential

$$
V(x, t) := (e^{i\omega t} + e^{-i\omega t})eE \cdot x, \quad t \leq 0, \quad x \in \Lambda_L. \quad (2.10)
$$

so the total time dependent one-particle Hamiltonian is

$$
H(t) = H_L(B) + V(t). \quad (2.11)
$$

Notice that $e$ near $E$ is the positive elementary charge. Here we take $\text{Im} \ \omega < 0$ which plays the role of an adiabatic parameter, and insures that there is no interaction in the remote past. Finally, the one-particle current operator is as usual

$$
\mathbf{J} = -e i[H_L(B), \mathbf{X}] = -\frac{e}{m} \mathbf{P}(B), \quad (2.12)
$$

where $\mathbf{X}$ is the multiplication by $x$. We assume that the state of our system is now described by a time-dependent density matrix, $\hat{\rho}(t)$, obtained by evolving $\hat{\rho}_c$ from $-\infty$ up to the given time, i.e.

$$
i\partial_t \hat{\rho}(t) = [\hat{H}(t), \hat{\rho}(t)], \quad \hat{\rho}(-\infty) = \hat{\rho}_c. \quad (2.13)$$
Going to the interaction picture and using the Dyson expansion up to the first order, one gets
\[ \hat{\rho}(t = 0) = \hat{\rho}_e - i \int_{-\infty}^{0} [d\Gamma(\hat{V}(s), \hat{\rho}_e)] ds + O(E^2), \]  
(2.14)
where
\[ \hat{V}(s) := e^{i s H_L(B)} V(s) e^{-i s H_L(B)}. \]  
(2.15)
The current density flowing through our system at \( t = 0 \) is given by (see (2.14)):
\[ j = \frac{1}{|\Lambda_L|} \text{Tr}_{F_L} \left( \hat{\rho}(0) \hat{J} \right) = \frac{1}{|\Lambda_L|} \text{Tr}_{F_L} \left( \hat{\rho}_e \hat{J} \right) - \frac{i}{|\Lambda_L|} \text{Tr}_{F_L} \left( \int_{-\infty}^{0} [d\Gamma(\hat{V}(s), \hat{\rho}_e)] \hat{J} ds \right) + O(E^2). \]  
(2.16)
In evaluating the r.h.s. of (2.16) we use the well known fact that traces over the Fock space can be computed in the one-particle space (see Proposition 5.2.23 in [23]):
\[ \text{Tr}_{F_L} \{ \hat{\rho}_e d\Gamma(A) \} = \text{Tr}_{H_L} \{ f_{FD}(H_L(B)) A \}, \]  
(2.17)
where \( f_{FD} \) is the Fermi-Dirac one-particle distribution function:
\[ f_{FD}(x) := \frac{1}{e^{\beta(x-\mu)} + 1}, \quad x \in \mathbb{R}, \beta > 0, \mu \in \mathbb{R}. \]  
(2.18)
Plugging (2.17) into (2.16), the identity \([d\Gamma(A), d\Gamma(B)] = d\Gamma([A, B])\), the invariance of trace under cyclic permutations and ignoring the quadratic correction in \( E \) one arrives at
\[ j = \frac{1}{|\Lambda_L|} \text{Tr}_{F_L} \{ f_{FD}(H_L(B)) \hat{J} \} - \frac{i}{|\Lambda_L|} \frac{e}{m} \text{Tr}_{H_L} \left( \int_{-\infty}^{0} [\hat{V}(s), P(B)] f_{FD}(H_L(B)) ds \right). \]  
(2.19)
The first term in (2.19) is always zero because of the identity (trace cyclicity again)
\[ \text{Tr}_{H_L} \{ f_{FD}(H_L(B)) [H_L(B), X] \} = \text{Tr}_{H_L} \{ [f_{FD}(H_L(B)), H_L(B)] X \} = 0, \]  
(2.20)
which is nothing but the fact that the current vanishes on an equilibrium state. Using (2.10) and (2.15) one can write
\[ j_\alpha = \sum_{\beta=1}^{3} \{ \sigma_{\alpha\beta}(\omega) + \sigma_{\alpha\beta}(-\omega) \} E_\beta, \quad \alpha \in \{1, 2, 3\}, \quad \Re(\omega) < 0, \]  
(2.21)
where the conductivity tensor is given by
\[ \sigma_{\alpha\beta}(B, \omega) = \frac{e^2}{m} \text{Tr}_{H_L} \int_{-\infty}^{0} [e^{i s H_L(B)} x_\beta e^{-i s H_L(B)}, P_\alpha(B)] f_{FD}(H_L(B)) e^{i s \omega} ds. \]  
(2.22)
Performing an integration by parts, using the formulas $i[H_L(B), x_\beta] = P_\beta(B)/m$ and $i[P_\alpha(B), x_\beta] = \delta_{\alpha\beta}$ one arrives at
\[
\sigma_{\alpha\beta}(B, \omega) = \frac{1}{|\Lambda_L|} \frac{e^2}{im\omega} \delta_{\alpha\beta} \text{Tr}(f_{FD}(H_L(B))) \tag{2.23}
\]
\[
+ \frac{i}{m} \text{Tr} \int_{-\infty}^{0} e^{is(\omega + H_L(B))} P_\beta(B) e^{-isH_L(B)} [P_\alpha(B), f_{FD}(H_L(B))] |ds|,
\]
and this coincides (at least at the formal level) with formula (5) in [1]. Notice that from now on, we write just $\text{Tr}$ when we perform the trace, since we only work in the one-particle space.

Since we are interested in the Faraday effect, and we assume that the magnetic field $B$ is parallel with the $z$ axis, we will only consider the transverse conductivity $\sigma_{12}(B, \omega)$. Hence the first term vanishes. We now perform the integral over $s$ with the help of Stone’s formula followed by a deformation of the contour (paying attention not to hit the singularities of $f_{FD}(z)$ or to make the integral over $s$ divergent
\[
f_{FD}(H_L(B))e^{is(H_L(B)+\eta)} = \frac{i}{2\pi} \int_{\Gamma_\omega} f_{FD}(z)e^{is(z+\eta)}(H_L(B) - z)^{-1}dz. \tag{2.24}
\]
where $\eta$ is either 0 or $\omega$, the contour is counter-clockwise oriented and given by
\[
\Gamma_\omega = \{x \pm id : a \leq x < \infty\} \bigcup \{a + iy : -d \leq y \leq d\} \tag{2.25}
\]
with
\[
d = \min \left\{ \frac{\pi}{2\beta}, \frac{|\text{Im}\omega|}{2} \right\}, \tag{2.26}
\]
and $a + 1$ lies below the spectrum of $H_L(B)$. As a final result one gets
\[
\sigma_{12}(B, \omega) = \frac{e^2}{2\pi m^2 \omega |\Lambda_L|} \cdot \text{Tr} \int_{\Gamma_\omega} f_{FD}(z) \{P_1(B)(H_L(B) - z)^{-1}P_2(B)(H_L(B) - z - \omega)^{-1}
\]
\[
+ z \rightarrow z - \omega \} dz =: \frac{e^2}{m^2 \omega} \eta_L(B, \omega)
\]
where “$z \rightarrow z - \omega$” means a similar term where we exchange $z$ with $z - \omega$.

Now one can see that by inserting the eigenbasis of $H_L(B)$ one obtains the well-known formula derived from semi-classical radiation theory (see e.g. formula (4) in [1]).

### 2.1 The zero frequency limit and IQHE

We end this section with a few important remarks about (2.27).

First, one can show that in the limit $\omega \rightarrow 0$ it coincides with a formula used in the theory of the integer quantum Hall effect (see formula (6) in [20]).
Second, in the limit of an infinitely large domain, zero frequency, zero temperature and for the Fermi energy in a spectral gap, we can show (see also [20]) that we get the Widom-Streda formula:

$$\sigma_{12}(B,0) = ec \left. \frac{\partial N(B,E)}{\partial B} \right|_{E=E_F}$$

where $N(B,E)$ is the integrated density of states up to energy $E$. The above derivative has to be understood in a somehow special sense. If we denote by $B_1$ the $B$ multiplying the spin matrix $\sigma_3$ in our Hamiltonian (2.1), and with $B_2$ the $B$ near $a$, then in fact we have

$$\sigma_{12}(B,0) = ec \left. \frac{\partial N(B_1,B_2,E)}{\partial B_2} \right|_{E=E_F, B_1=B_2=B}.$$  

(2.29)

Note that Streda did not consider spin in his work [20].

Now consider the periodic case, and assume that at $B=0$ all the bands below the Fermi level have exponentially localized Wannier functions. Then according to [19], exponentially localized magnetic Wannier functions still exist for $B$ not too large. Since they are labelled by the same set of indices as in the zero magnetic field case (i.e. the lattice $\mathcal{L}$), it follows that $N(B_1,B_2,E)$ does NOT vary with $B_1$ and $B_2$ if these two parameters lie in a not too large interval around zero. Thus the partial derivative with respect to $B_2$ of $N(B_1,B_2,E)$ must be identically zero on a whole interval. Hence $\sigma_{12}(B,0)$ equals zero, and so does its Taylor expansion at zero in any order in $B$.

In particular, this explains Roth’s result (formula (50) in [1]) for the first order correction in $B$ at zero frequency.

3 Gauge invariance and existence of the thermodynamic limit

Up to now the system was confined in a box $\Lambda_L$. As is well known (see e.g. [1]) a direct evaluation of (2.27) (or previous formulas equivalent to it including formula (4) in Roth’s paper) is out of reach: the eigenvalues and eigenstates of $H(B)$ are rather complicated (even in the thermodynamic limit $\Lambda_L \to \mathbb{R}^3$) and at the same time the Bloch representation is plagued by singular matrix elements of the magnetic vector potential. Roth used a modified magnetic Bloch representation in [24] and derived a formula for the linear term in $B$ of (2.27) in terms of the zero magnetic field Bloch representation. Still, her procedure is not free of difficulties since it involves $\nabla_k u_j(x,k)$ which might not exist at crossing points. In addition, it seems almost hopeless to control the errors or to push computations to the second order in $B$ which would describe the Cotton-Mouton effect for example.

In what follows, we shall outline another route of evaluating (2.27) which is mathematically correct, systematic, and completely free of the above difficulties. There are two basic ideas involved. The first one (going back at least to
Sondheimer and Wilson [10] in their theory of diamagnetism) consists in writing
the trace in (2.27) as integrals over \( \Lambda_L \) of corresponding integral kernels. This
is nothing but the well known Green function approach (see e.g. [25]) which
has been very successful in computing optical and magneto-optical properties
of solids (see e.g. [6], [7], [8]) in the absence of an external magnetic field. The
point is that the integral kernels are on one hand easier to control and compute,
and on the other hand they do not require periodicity. Moreover, this approach
proved to be essential in deriving rigorous results concerning the diamagnetism
of free electrons [16, 26] and actually we expect the methods of the present
paper to simplify the theory of diamagnetism of Bloch electrons as well.

However, when applying Green function approach in the presence of an exter-
nal magnetic field one hits again the divergencies caused by the linear increase
of the magnetic vector potential: naively, at the first sight \( a_L(B, \omega) \) is not bounded
in the thermodynamic limit \( L \to \infty \) but instead grows like the second power of
\( L \). It was already observed in [26] that these divergent terms vanish identically
due to some identities coming from gauge invariance.

This is indeed the case and the main point of this paper is to show, following
the developments in [15], [16], [17], that factorizing the so called “nonintegrable
phase factor” from the Green function (the integral kernel of \( (H_L(B) - \zeta)^{-1} \))
allows, at the same time, to eliminate the divergencies coming from the increase
of the magnetic vector potential and to obtain a controlled expansion in powers
of \( B \). In addition, this leads to expressions of \( a_L(B, \omega) \) which are manifestly
gauge invariant.

For an arbitrary pair of points \( x, y \in \Lambda_L \) consider the “magnetic phase”
associated with the magnetic vector potential \( a(u) \) defined as the path integral
on the line linking \( y \) and \( x \):

\[
\phi_a(x, y) = \int_y^x a(u) \cdot du. \tag{3.1}
\]

The magnetic phase satisfies the following crucial identity: for every fixed \( c \)
\[
e^{-ib\phi_a(x, c)} P(B)e^{ib\phi_a(x, c)} = P(0) - bA(x - c). \tag{3.2}
\]

where \( A(x) = \frac{1}{2} n_3 \wedge x \), i.e. irrespective of the choice of \( a(x) \),

\[
A(x - c) = \frac{1}{2} n_3 \wedge (x - c) \tag{3.3}
\]
is the symmetric (transverse, Poincaré) gauge with respect to \( c \).

Write now the Green function (as a \( 2 \times 2 \) matrix in the spin space)
\[
G_L(x, y; \zeta) = (H_L - \zeta)^{-1}(x, y) \tag{3.4}
\]
in the factorized form
\[
G_L(x, y; \zeta) = e^{ib\phi_a(x, y)}K_L(x, y; \zeta). \tag{3.5}
\]
It is easy to check that while $G_L(x, y; \zeta)$ is gauge dependent, $K_L(x, y; \zeta)$ is gauge independent i.e. the whole gauge dependence of $G_L(x, y; \zeta)$ is contained in the phase factor $e^{ib\phi_a(x, y)}$. Plugging the factorisation (3.5) into the integrand of the r.h.s. of (2.27), using (3.2) and (3.3), one obtains that its integral kernel writes as

$$A_{s,s}^L(x, x') = e^{ib\phi_a(x, x')}$$

(3.6)

$$\cdot \int_{\Omega} dz f_{DF}(z) \sum_{\sigma=1}^2 \int_{\Lambda_L} dy e^{ib\phi(x, y)} \{[(P_1(x(0) - bA_1(x - y))K_L(x, y; \zeta)]_{s,\sigma}

\cdot [(P_2(y(0) - bA_2(x - y))K_L(y, x'; z + \omega)]_{s,\sigma} + z \rightarrow z - \omega\},$$

where

$$\Phi(x, y, x') = \phi_a(x, y) + \phi_a(y, x') + \phi_a(x', x)$$

is the flux of the magnetic field $(0,0,1)$ through the triangle $\Delta(x, y, x')$. Now the fact that there are no long range divergencies in the formula for $A_{s,s}(x, x')$ follows from the exponential decay of Green functions [18] (see also [19]): for $\zeta$ outside the spectrum of $H$ there exists $m(\zeta) > 0$ such that as $|x - y| \rightarrow \infty$

$$|K_L(x, y; \zeta)| = |G_L(x, y; \zeta)| \sim e^{-m(\zeta)|x-y|}.$$ 

It can be proved (the technical details which are far from being simple will be given elsewhere) that $A_{s,s}^L(x, x')$ is jointly continuous and moreover outside a thin region near the surface of $\Lambda_L$ one can replace it by the integral kernel $A_{s,s}^\infty(x, x')$ of the corresponding operator on the whole $\mathbb{R}^3$. Accordingly, up to surface corrections:

$$a_L(B, \omega) \approx -\frac{1}{2\pi|\Lambda|} \sum_{s=1}^2 \int_{\Lambda_L} A_{s,s}^\infty(x, x)dx.$$

(3.7)

Notice that due to the fact that $\Phi(x, y, x) = \phi_a(x, x) = 0$ the phase factors appearing in (3.6) reduce to unity in (3.7).

In the periodic case, from the fact that in the symmetric gauge the Hamiltonian $H_\infty(B)$ commutes with the magnetic translations (actually one can define magnetic translations for an arbitrary gauge, just first make the gauge transformation relating $a(x)$ to $A(x)$) generated by $\mathcal{L}$, it follows that for $\gamma \in \mathcal{L}$ we have:

$$K_\infty(x + \gamma, y + \gamma; \zeta) = K_\infty(x, y; \zeta),$$

which implies that

$$A_{s,s}^\infty(x + \gamma, x + \gamma) = A_{s,s}^\infty(x, x)$$

is periodic with respect to $\mathcal{L}$, hence up to surface corrections:

$$a_L(B, \omega) \approx a(B, \omega) = -\frac{1}{2\pi|\Omega|} \sum_{s=1}^2 \int_{\Omega} A_{s,s}^\infty(x, x)dx.$$

(3.8)
Therefore, the transverse conductivity writes as

$$\sigma_{12}(B, \omega) = \frac{e^2}{m^2\omega} a(B, \omega)$$

(3.9)

with $a(B, \omega)$ given by the r.h.s. of (3.8).

4 A closed formula for free electrons

If $V = 0$ it turns out that the conductivity tensor can be explicitly computed for all values of $B$ and $\omega$. The formula does not depend on whether we work in two or three dimensions. More precisely, we will show in this section that

$$\sigma_{12}(B, \omega) = \frac{e^3 n}{m^2 c \omega^2} - \frac{B^2 e^2}{m^2 c^2},$$

(4.1)

where $n = n(T, \mu, B)$ is the grandcanonical density. The formula (4.1) is well known in classical physics and goes back at least to Drude but we are not aware of a full quantum derivation. The coincidence of classical and quantum formulas can be understood taking into account that the Hamiltonians involved (choose the symmetric gauge) are quadratic and it is known that for this class of operators classical and quantum computations coincide in many instances. While it is possible to derive (4.1) by using the explicit form of the Green function or alternatively of eigenvalues and eigenprojectors for the Landau Hamiltonian (see e.g. [27]) we shall obtain it below only using resolvent and commutation identities.

Let us only notice that when $\omega = 0$ we reobtain formula (18) in [20], while for a fixed frequency we get

$$\frac{\partial \sigma_{12}}{\partial B}(0, \omega) = \frac{e^3 n}{m^2 c \omega^2}$$

which is "the high frequency limit" or what Roth also calls "the free electron Faraday effect" in formula (51) from [1].

We begin by listing a few identities which are valid for a free electron on the entire space.

$$i[P_1(B), P_2(B)] = \frac{B e}{c}$$

$$i[H_\infty(B), P_1(B)] = -\frac{B e}{m c} P_2(B),$$

$$i[H_\infty(B), P_2(B)] = \frac{B e}{m c} P_1(B),$$

$$[H_\infty(B), [H_\infty(B), P_1(B)]] = \frac{B^2 e^2}{m^2 c^2} P_1(B),$$

(4.2)

$$[H_\infty(B), [H_\infty(B), P_2(B)]] = \frac{B^2 e^2}{m^2 c^2} P_2(B).$$
Next, since in this case $A_{s,s}^\infty(x, x)$ does not depend upon $x$ one has

$$a(B, \omega) = -\frac{1}{2\pi} \sum_{s=1}^{2}$$

\begin{align*}
\left\{ \int_{\Gamma_\omega} dz f_{FD}(z) \left[ P_1(B)(H_\infty(B) - z)^{-1}P_2(B)(H_\infty(B) - z - \omega)^{-1} \\
+ z \to z - \omega_1 \right] \right\} (\vec{0}, s; \vec{0}, s).
\end{align*}

(4.3)

Commuting $(H_\infty(B) - z - \omega)^{-1}$ with $P_2(B)$ in the first term, and $P_1(B)$ with $(H_\infty(B) - z + \omega)^{-1}$ in the second one, we obtain

$$a(B, \omega) = -\frac{1}{2\pi|\Omega|} \sum_{s=1}^{2}$$

\begin{align*}
\left\{ \int_{\Gamma_\omega} dz f_{FD}(z) \left[ P_1(B)(H_\infty(B) - z)^{-1}(H_\infty(B) - z - \omega)^{-1}P_2(B) \\
+ P_1(B)(H_\infty(B) - z)^{-1}(H_\infty(B) - z - \omega)^{-1} \\
\cdot [H_\infty(B), P_2(B)](H_\infty(B) - z - \omega)^{-1} \\
+ (H_\infty(B) - z + \omega)^{-1}P_1(B)P_2(B)(H_\infty(B) - z)^{-1} \\
+ (H_\infty(B) - z + \omega)^{-1}[H_\infty(B), P_1(B)] \\
\cdot (H_\infty(B) - z + \omega)^{-1}P_2(B)(H_\infty(B) - z)^{-1} \right] \right\} (\vec{0}, s; \vec{0}, s)
\end{align*}

(4.4)

Now $I + III$ can easily be computed. Indeed, by cyclic permutations one can cluster the two resolvents and then by the resolvent identity

$$\begin{align*}
(A - z_1)^{-1}(A - z_2)^{-1} &= (z_1 - z_2)^{-1}[(A - z_1)^{-1} - (A - z_2)^{-1}],
\end{align*}
$$

(4.5)

one obtains four terms. Two of them vanish after the integration over $z$ due to the analyticity of the integrand while the other two give

$$I + III = \frac{1}{2\pi} \sum_{s=1}^{2}$$

\begin{align*}
\left\{ \int_{\Gamma_\omega} dz f_{FD}(z) \frac{1}{\omega}[P_2(B), P_1(B)](H_\infty(B) - z)^{-1} \right\} (\vec{0}, s; \vec{0}, s)
\end{align*}

(4.6)

\begin{align*}
= B \frac{e}{\omega} \sum_{s=1}^{2} \{f_{FD}(H_\infty(B))\} (\vec{0}, s; \vec{0}, s) =: B \frac{e}{\omega} n(T, \mu, B).
\end{align*}

(4.7)
In an analogous manner

\[ III + IV = \frac{1}{2\pi \omega} \sum_{s=1}^{2} \left\{ \int_{\Gamma_{\omega}} dz f_{FD}(z) \right. \]

\[ \left. \cdot \{(H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{s}(B)](H_{\infty}(B) - z - \omega)^{-1} P_{1}(B) \right. \]

\[ \left. - (H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{1}(B)](H_{\infty}(B) - z + \omega)^{-1} P_{2}(B) \}\right\} \}

\[ \{0, s; 0, s\}. \]

At this point we commute \([H_{\infty}(B), P_{2}(B)]\) with \((H_{\infty}(B) - z - \omega)^{-1}\) in the first term, and \([H_{\infty}(B), P_{1}(B)]\) with \((H_{\infty}(B) - z + \omega)^{-1}\) in the second term and use (3.3) again. Some of the terms vanish after performing the integration over \(z\) and the remaining ones write as:

\[ - \frac{1}{\omega} (H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{s}(B)]P_{1}(B) \]

\[ - \frac{1}{\omega} (H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{1}(B)](H_{\infty}(B) - z - \omega)^{-1} P_{1}(B) \]

\[ - \frac{1}{\omega} (H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{1}(B)]P_{2}(B) \]

\[ - \frac{1}{\omega} (H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{1}(B)](H_{\infty}(B) - z + \omega)^{-1} P_{2}(B). \]

Taking into account (4.2) the first and the third terms in (4.9) combine to

\[ - \frac{1}{\omega} (H_{\infty}(B) - z)^{-1}[H_{\infty}(B), P_{1}(B)]P_{2}(B) \]

which after integration over \(z\) is proportional to

\[ f_{FD}(H_{\infty}(B))[H_{\infty}(B), P_{s}(B)P_{2}(B)], \]

and vanish by the argument leading to (2.20). It follows that we only remain with the second and fourth terms in (4.9). Using (4.2), they become:

\[ - \frac{B^2 e^2}{m^2 c^2 \omega^4} (H_{\infty}(B) - z)^{-1} P_{2}(B)(H_{\infty}(B) - z - \omega)^{-1} P_{1}(B) \]

\[ - \frac{B^2 e^2}{m^2 c^2 \omega^4} (H_{\infty}(B) - z)^{-1} P_{1}(B)(H_{\infty}(B) - z + \omega)^{-1} P_{2}(B). \]

Using once more the cyclicity of the trace and comparing with the starting point (4.3), we obtain the remarkable identity

\[ II + IV = \frac{B^2 e^2}{m^2 c^2 \omega^4} a(B, \omega). \]

Putting together (4.4), (4.6), and (4.11), we obtain the equation:

\[ a(B, \omega) = \frac{B e}{c \omega} n + \frac{B^2 e^2}{m^2 c^2 \omega^4} a(B, \omega), \]

which gives (4.1) (see (3.9)).
5 Magnetic perturbation theory and the linear term in $B$

When $V \neq 0$ it is no longer possible to obtain a closed formula for $\sigma_{12}(B, \omega)$. Since in most physical applications the external magnetic field can be considered weak, an expansion in $B$ up to the first or second order would be sufficient. In this section we show that $a_L(B, \omega)$ has an expansion in $B$ to any order and write down the expressions of the first two terms. The first one gives the transverse conductivity at zero magnetic field and the second which is linear in $B$ provides the Verdet constant. From (3.6) and (3.7) (in what follows by $tr$ we mean the trace over the spin variable):

$$a_L(B, \omega) = -\frac{1}{2\pi|\Lambda_L|} \int_{\Lambda_L} dx \left( \text{tr} \int_{\Gamma_u} dz f_{FD}(z) \right)$$

(5.1)

$$\cdot \int_{\Lambda_L} du \left\{ (P_{x,1}(0) - bA_1(x - u))K_L(x, u;z) \right\}$$

$$\cdot \left\{ [(P_{u,2}(0) - bA_2(u - x'))K_L(u, x'; z + \omega)] + [(P_{x,1}(0) - bA_1(x - u))K_L(x, u; z - \omega)] \right\}$$

$$\cdot \left\{ [(P_{u,2}(0) - bA_2(u - x'))K_L(u, x'; z)] \right\} \bigg|_{x = x'}$$

Let us mention here that one cannot interchange the order of the above integrals. First one performs the integral with respect to $u$, then the integral in $z$, then we can put $x = x'$ since the resulting kernel is smooth, and finally one integrates with respect to $x$ over $\Lambda_L$.

When considering the expansion in $b$ of $a_L(B, \omega)$ we are left with the problem of the expansion of $K_{\Lambda_L}(x, y; \zeta)$. This expansion is provided by the magnetic perturbation theory as developed in [19]. Following the steps in [19] in the case at hand one obtains:

$$K_L(x, y; z) = G^{(0)}_L(x, y; z)$$

$$+ \frac{b}{m} \int_{\Lambda_L} G^{(0)}_L(x, u; z) \left[ P_u(0) - A(u - y)G^{(0)}_L(u, y; z) \right] du$$

$$+ \frac{bgc}{e} \int_{\Lambda_L} G^{(0)}_L(x, u; z) \sigma_3 G^{(0)}_L(u, y; z) du + O(b^2)$$

$$= G^{(0)}_L(x, y; z) + bG^{(orbit)}_L(x, y; z) + bG^{(spin)}_L(x, y; z) + O(b^2).$$

The above integrands are matrices in the spin variable, that is why the spin does not appear explicitly. The error term $O(b^2)$ can also be fully controlled with the magnetic perturbation theory (actually arbitrary order terms can be computed; see [19] for details). Plugging the expansion (5.2) into (5.2) and collecting the terms of zero and first order one obtains

$$a_L(B, \omega) = a_L(0, \omega) + ba_L(1)(\omega) + O(b^2),$$

(5.3)
where the zeroth order term is:

\[ a_L(0, \omega) = -\frac{1}{2\pi|\Lambda_L|} \int_{\Lambda_L} dx \left\{ \text{tr} \int_{\Gamma_\omega} dz f_{FD}(z) \right\} \]

while the first order correction reads as:

\[ a_{L,1}(\omega) = a_{L,1}^{\text{orbit}}(\omega) + a_{L,1}^{\text{spin}}(\omega), \]

where

\[ a_{L,1}^{\text{orbit}}(\omega) = -\frac{1}{2\pi|\Lambda_L|} \int_{\Lambda_L} dx \left\{ \text{tr} \int_{\Gamma_\omega} dz f_{FD}(z) \right\} \]

\[ \cdot \left\{ A_1(x-u)G_L^{(0)}(x; u; z) \right\} \left[ P_{u,2}(0)G_L^{(0)}(u, x'; z + \omega) \right] \]

\[ - \left[ P_{x,1}(0)G_L^{(0)}(x, u; z) \right] \left[ A_2(u-x')G_L^{(0)}(u, x'; z + \omega) \right] \]

\[ + \left[ P_{x,1}(0)G_L^{(\text{orbit})}(x, u; z) \right] \left[ P_{u,2}(0)G_L^{(0)}(u, x'; z + \omega) \right] \]

\[ + \left( z \to z - \omega \right) \}] \left|_{x=x'} \right., \]

\[ a_{L,1}^{\text{spin}}(\omega) = -\frac{1}{2\pi|\Lambda_L|} \int_{\Lambda_L} dx \left\{ \text{tr} \int_{\Gamma_\omega} dz f_{FD}(z) \right\} \]

\[ \cdot \left\{ P_{x,1}(0)G_L^{(\text{spin})}(x, u; z) \right\} \left[ P_{u,2}(0)G_L^{(0)}(u, x'; z + \omega) \right] \]

\[ + \left[ P_{x,1}(0)G_L^{(0)}(x, u; z) \right] \left[ P_{u,2}(0)G_L^{(\text{spin})}(u, x'; z + \omega) \right] \]

\[ + \left( z \to z - \omega \right) \}] \left|_{x=x'} \right.. \]

Now consider the expression \( A(x-y)G_L^{(0)}(x, y; z) \) appearing in the formula for \( a_{L,1}(\omega) \). Observing that it represents a commutator (see (3.3)) one has the identity

\[ A(x-y)G_L^{(0)}(x, y; z) = \left( \frac{1}{2} n_3 \wedge (x-y) \right) G_L^{(0)}(x, y; z) \]

\[ = \left( \frac{1}{2} n_3 \wedge \left[ X, (H_L(0) - z)^{-1} \right] \right) (x, y) \]

\[ = -\frac{i}{2m} \{(H_L(0) - z)^{-1}(n_3 \wedge P)(H_L(0) - z)^{-1}\}(x, y). \]

where \( X \) denotes the multiplication operator with \( x \). By a straightforward (but somewhat tedious) computation one arrives at:

\[ a_{L,1}(\omega) = a_{L,1}^{\text{orbit,1}}(\omega) + a_{L,1}^{\text{orbit,2}}(\omega) + a_{L,1}^{\text{spin}}(\omega) \]

(5.9)

15
where

\[ a_{L,1}^{\text{orbit},1}(\omega) = \frac{i}{4\pi m|\Lambda_L|} \int_{\Lambda_L} dx \left\{ \text{tr} \int_{\mathcal{C}_\omega} dz f_{FD}(z) \right\} \tag{5.10} \]

\[
\cdot \left[ \sum_{\alpha=1}^2 P_\alpha(0)(H_L(0) - z)^{-1} P_\alpha(0)(H_L(0) - z - \omega)^{-1}
+ \sum_{\alpha=1}^2 P_\alpha(0)(H_L(0) - z)^{-1} P_\alpha(0)(H_L(0) - z + \omega)^{-1}
- \sum_{\alpha=1}^2 P_\alpha(0)(H_L(0) - z)^{-1} P_\alpha(0)(H_L(0) - z)^{-1} \right] \{x, x\},
\]

\[ a_{L,1}^{\text{orbit},2}(\omega) = \frac{i}{4\pi m^2|\Lambda_L|} \int_{\Lambda_L} dx \left\{ \text{tr} \int_{\mathcal{C}_\omega} dz f_{FD}(z) \right\} \tag{5.11} \]

\[
\cdot \left\{ -P_1(0)(H_L(0) - z)^{-1} P_1(0)(H_L(0) - z)^{-1}
+ P_2(0)(H_L(0) - z)^{-1} P_2(0)(H_L(0) - z + \omega)^{-1}
- P_1(0)(H_L(0) - z + \omega)^{-1} P_1(0)(H_L(0) - z + \omega)^{-1}
+ P_2(0)(H_L(0) - z + \omega)^{-1} P_2(0)(H_L(0) - z)^{-1}
- P_1(0)(H_L(0) - z)^{-1} P_2(0)(H_L(0) - z - \omega)^{-1}
+ P_1(0)(H_L(0) - z - \omega)^{-1} P_1(0)(H_L(0) - z)^{-1}
- P_2(0)(H_L(0) - z - \omega)^{-1} P_2(0)(H_L(0) - z - \omega)^{-1}\right\} \{x, x\},
\]
and

and

\begin{equation}
\alpha^{spin}_{L,1}(\omega) = - \frac{ge\mu_b}{2\pi |\Lambda_L|} \int_{\Lambda_L} dx \left\{ \text{tr} \int_{\Gamma_\omega} dz f_{FD}(z) \right. \\
\left. \cdot \left\{ [P_1(0)(H_L(0) - z)^{-1}\sigma_3(H_L(0) - z)^{-1}P_2(0)H_L(0)] P_1(0)(H_L(0) - z - \omega)^{-1} \\
+ [P_1(0)(H_L(0) - z)^{-1}P_2(0)H_L(0)] P_1(0)(H_L(0) - z + \omega)^{-1}P_2(0)H_L(0)] P_1(0)(H_L(0) - z)^{-1} \\
+ [P_1(0)(H_L(0) - z + \omega)^{-1}P_2(0)H_L(0)] P_1(0)(H_L(0) - z)^{-1}\sigma_3(H_L(0)) \right\} (x, x).
\end{equation}

\section{The periodic case}

Now consider the case when $V$ is periodic. In this case, after taking the thermodynamic limit one can replace (see (3.8)) $\frac{1}{|\Omega|} \int_{\Omega} \frac{1}{|\Omega|} \int_{\Omega}$ and rewrite (5.10)-(5.12) as integrals over the Brillouin zone

\begin{equation}
\alpha^{orbit,1}_{\infty,1}(\omega) = \frac{i}{4m\pi|\Omega|} \int_{\Omega^*} dk \int_{\Omega} dx \left\{ \text{tr} \int_{\Gamma_\omega} dz f_{FD}(z) \right. \\
\left. \cdot \sum_{\alpha=1}^{2} (p_{\alpha} + k_{\alpha})(h(k) - z)^{-1}(p_{\alpha} + k_{\alpha})(h(k) - z - \omega)^{-1} \\
+ \sum_{\alpha=1}^{2} (p_{\alpha} + k_{\alpha})(h(k) - z)^{-1}(p_{\alpha} + k_{\alpha})(h(k) - z + \omega)^{-1} \\
- \sum_{\alpha=1}^{2} (p_{\alpha} + k_{\alpha})(h(k) - z)^{-1}P_{\alpha}(0)(h(k) - z)^{-1} \right\} (x, x),
\end{equation}
\[ a_{\text{orbit}, 2}^\omega = \frac{i}{4\pi m^2|\Omega|} \int_{\Omega^*} d\mathbf{k} \int_{\Omega} d\mathbf{x} \left\{ \text{tr} \int_{\Omega} dz f_{FD}(z) \right\} \]

\[ \cdot \left\{ -(p_1 + k_1)(h(k) - z)^{-1}(p_1 + k_1)(h(k) - z)^{-1} \right\} \]

\[ + (p_2 + k_2)(h(k) - z)^{-1}(p_2 + k_2)(h(k) - z - \omega)^{-1} \]

\[ + (p_1 + k_1)(h(k) - z)^{-1}(p_2 + k_2)(h(k) - z - \omega)^{-1} \]

\[ - (p_1 + k_1)(h(k) - z + \omega)^{-1}(p_1 + k_1)(h(k) - z + \omega)^{-1} \]

\[ + (p_2 + k_2)(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z + \omega)^{-1} \]

\[ - (p_1 + k_1)(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z + \omega)^{-1} \]

\[ + (p_1 + k_1)(h(k) - z + \omega)^{-1}(p_1 + k_1)(h(k) - z + \omega)^{-1} \]

\[ - (p_2 + k_2)(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z + \omega)^{-1} \]

\[ + (p_1 + k_1)(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z + \omega)^{-1} \]

\[ - (p_1 + k_1)(h(k) - z + \omega)^{-1}(p_1 + k_1)(h(k) - z + \omega)^{-1} \]

\[ + (p_2 + k_2)(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z + \omega)^{-1} \]

\[ + (p_1 + k_1)(h(k) - z + \omega)^{-1}(p_1 + k_1)(h(k) - z + \omega)^{-1} \}

\[ (x, x) \]

and

\[ a_{\text{spin}}^\omega = -\frac{g \mu_B}{2e\pi|\Omega|} \int_{\Omega^*} d\mathbf{k} \int_{\Omega} d\mathbf{x} \left\{ \text{tr} \int_{\Omega} dz f_{FD}(z) \right\} \]

\[ \cdot \left\{ [(p_1 + k_1)(h(k) - z)^{-1}\sigma_3(h(k) - z)^{-1}((p_2 + k_2)(h(k) - z - \omega)^{-1}] \right\} \]

\[ + [(p_1 + k_1)(h(k) - z)^{-1}(p_2 + k_2)(h(k) - z - \omega)^{-1}\sigma_3(h(k) - z - \omega)^{-1}] \]

\[ + [(p_1 + k_1)(h(k) - z + \omega)^{-1}\sigma_3(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z)^{-1}] \]

\[ + [(p_1 + k_1)(h(k) - z + \omega)^{-1}(p_2 + k_2)(h(k) - z)^{-1}\sigma_3(h(k) - z)^{-1}] \}

\[ (x, x) \].

Finally, for the convenience of the reader only interested in applying the theory to the case when one assumes that the Bloch bands and functions are known (as for example from Kohn-Luttinger type models), we write (6.1)-(6.3) in terms of Bloch functions and energies. The important thing here is that no derivatives with respect to the quasimomentum appear. With the usual notation (here \( \langle, \rangle \) denotes the scalar product over the spin variables):

\[ \hat{\pi}_{ij}(\alpha, \mathbf{k}) = \int_{\Omega} \langle u_i(x, \mathbf{k}), (p_\alpha + k_\alpha)u_j(x, \mathbf{k}) \rangle d\mathbf{x} \].
and after some rearrangements, the terms coming from the orbital magnetism are:

\[ a_{\infty,1}^{\text{orbit.1}}(\omega) = \frac{1}{2m \omega (2\pi)^2} \sum_{\alpha=1}^{2} \int_{\Omega^*} d\mathbf{k} \left\{ \sum_{j \geq 1} |\hat{\pi}_{j\alpha}(\alpha, \mathbf{k})|^2 f_{FD}(\lambda_{j}(\mathbf{k})) \right\} \]

\[ -\omega^2 \sum_{j \neq \ell} (\hat{\pi}_{j\alpha}(\alpha, \mathbf{k})^2 f_{FD}(\lambda_{j}(\mathbf{k})) - f_{FD}(\lambda_{\ell}(\mathbf{k}))) \]

\[ (\lambda_{j}(\mathbf{k}) - \lambda_{\ell}(\mathbf{k}))^2 - \omega^2 \]

\[ \lambda_{j}(\mathbf{k}) - \lambda_{\ell}(\mathbf{k}) \]

\[ (6.5) \]

\[ a_{\infty,1}^{\text{orbit.2}}(\omega) = \frac{1}{2m^2 (2\pi)^3} \int_{\Omega^*} d\mathbf{k} \sum_{n_1,n_2,n_3,n_4 \geq 1} \frac{1}{2\pi i} \int_{\Gamma_\omega} d\omega F D \]

\[ \pi_{n_1n_2n_3n_4}(1, \mathbf{k}) \pi_{n_1n_2}(1, \mathbf{k}) \pi_{n_3n_4}(2, \mathbf{k}) \pi_{n_2n_4}(2, \mathbf{k}) \]

\[ \left\{ \begin{array}{l}
(z - \lambda_{n_1}(\mathbf{k}))(z - \lambda_{n_3}(\mathbf{k}))(z + \omega - \lambda_{n_4}(\mathbf{k}))
\hat{\pi}_{n_4n_1}(1, \mathbf{k}) \pi_{n_1n_2}(1, \mathbf{k}) \pi_{n_3n_4}(2, \mathbf{k})
\pi_{n_2n_4}(2, \mathbf{k})
\end{array} \right\} \]

\[ \left\{ \begin{array}{l}
(z - \lambda_{n_1}(\mathbf{k}))(z - \lambda_{n_3}(\mathbf{k}))(z + \omega - \lambda_{n_4}(\mathbf{k}))
\hat{\pi}_{n_4n_1}(1, \mathbf{k}) \pi_{n_1n_2}(1, \mathbf{k}) \pi_{n_3n_4}(2, \mathbf{k})
\pi_{n_2n_4}(2, \mathbf{k})
\end{array} \right\} \]

\[ (6.6) \]

As for the spin contribution, with the notation

\[ \hat{s}_{ij}(\mathbf{k}) := \int_{\Omega} (u_i(x, \mathbf{k}), \sigma_j u_j(x, \mathbf{k})) dx, \]

\[ (6.7) \]
one has:

\[
\mathcal{a}^{\text{spin}}_{\infty, 1}(\omega) = -\frac{ge\mu_B}{(2\pi)^4 e} \int_{\Omega^*} d\mathbf{k} \sum_{n_1,n_2,n_3 \geq 1} \frac{1}{2\pi i} \int_{\Gamma_\omega} dz f_{FD}(z) \tag{6.8}
\]

\[
\left\{ \hat{\pi}_{n_1 n_2}(1, k) \delta_{n_2 n_3} (k) \hat{\pi}_{n_3 n_1}(2, k) \right. \\
\left. \frac{1}{(\lambda_{n_2}(k) - z)(\lambda_{n_1}(k) - z)(\lambda_{n_1}(k) - z - \omega)} \right.
\]

\[
+ \frac{\hat{\pi}_{n_1 n_2}(1, k) \delta_{n_2 n_3} (k) \hat{\pi}_{n_3 n_1}(2, k)}{\lambda_{n_1}(k) - z} \right.
\]

\[
+ \frac{\hat{\pi}_{n_1 n_2}(1, k) \delta_{n_2 n_3} (k) \hat{\pi}_{n_3 n_1}(2, k)}{\lambda_{n_1}(k) - z + \omega} \right.
\]

\[
\left. + \frac{\hat{\pi}_{n_1 n_2}(1, k) \delta_{n_2 n_3} (k) \hat{\pi}_{n_3 n_1}(2, k)}{\lambda_{n_1}(k) - z + \omega} \right. \}
\]

7 Conclusions

We presented in the present paper a method which shed new light on the quantum dynamics/optical response in bulk media in the presence of a constant magnetic field. We applied the gauge invariant magnetic perturbation theory and gave a clear and very general way of dealing with long range magnetic perturbations.

Equations (5.9)-(5.12) and (6.4)-(6.8) contain our main result concerning the Verdet constant and the Faraday effect: it gives the linear term in \( B \) of the transverse conductivity in terms of the zero magnetic field Green function. They open the way of using the recently developed Green function techniques for the calculation of optical and magneto-optical properties of solids, to the case when an external magnetic field is present. Our method can be applied to ordered, as well as to random systems (with the appropriate average over configurations).

Of course, in the last case one has to assume ergodicity properties in order to insure convergence of results in the thermodynamic limit. Layers or other geometries can also be considered.

There are many subtle and difficult mathematical questions left aside in this paper, as those related to the thermodynamic limit, the convergence of infinite series over Bloch bands, the low frequency limit and the connection with the integer quantum Hall effect. Another open problem is to consider self-interacting electrons and investigate excitonic effects on the Faraday effect. These questions will be addressed elsewhere.

Our results are not only theoretical. In a future publication we will use the residue theorem in equations (6.4)-(6.8) to calculate the Verdet constant for various finite band models, and compare our results with the existing experimental data. Moreover, our results will be shown to imply those of Roth [1] and Nedoluha [14].
8 Acknowledgments

This paper has been written at the Department of Mathematical Sciences, Aalborg University. G.N. kindly thanks the Department for invitation and financial support.

H.C. acknowledges support from the Statens Naturvidenskabelige Forskningsråd grant *Topics in Rigorous Mathematical Physics*, and partial support through the European Union’s IHP network Analysis & Quantum HPRN-CT-2002-00277.

References


