Rigorous Aspects of

Orbital Magnetism in Graphene-like Materials

Speciale i fysik

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RESUMÉ

Vi udvikler i denne prœsentation en teori for off-diagonal elementet af $2D$ konduktivitetstensoren $\overleftrightarrow{\sigma}$ for en todimensionel krystal, påtrykt et statisk, homogent magnetisk felt. Vi bruger en diskret model, med en Harper-type Hamiltonoperator og Peierls substitution. Vi viser at σ_{21} har en asymtotisk ekspansion i den magnetiske feltstyrke b, samt at $\sigma_{12}(b=0)$ er nul, og finder en formel for den første afledte $\sigma'_{12}(b=0)$. Denne koefficient spiller en vigtig rolle i teorien om Faraday ratation.

De anvendte matematiske metoder er: Spektral teori for Harper-type operatorer, Combes-Thomas lokalisering , magnetisk pertubationsteori og Bloch-Floquet teori.

ABSTRACT

In this presentation we develop a theory for calculating the off-diagonal tensor element of the $2D$ conductivity tensor $\overleftrightarrow{\sigma}$, for a two dimensional crystal immersed in a constant homogenous magnetic field, using a Harper-type Hamiltonian and Peierls substituion and a discrete model of the crystal. Ve show that σ_{21} has an asymptotic expansion in the magnetic field strength b, that $\sigma_{12}(b=0)$ is zeroand develop a formula for the first derivative $\sigma'_{12}(b=0)$. This coefficient plays a major role in the theory concerning the Faraday rotation effect.

The main mathematical tolls used here is spectral theory for Harper-type operators, Combes-Thomas localization, Magnetic pertubation theory and Bloch-Floquet theory.

Preface

This thesis was written in the period february 1st to june 1st, 2011, at Aalborg University. This paper is the result of a 5 year study in Physics and Mathematics.

This presentation requires some basic knowledge of quantum mechanics, real and complex analysis, and operator theory (bounded operators on Hilbert space).

I would like to thank my main supervisor Horia Cornean for his support.

Aalborg, june 1st, 2011.

til Lars Brynildsen.

CONTENTS

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INTRODUCTION

1.1 PHYSICAL ASPECTS OF FARADAY ROTATION

We set the stage by a physical discussion about Faraday rotation. This section is not "rigorous", in a mathematical sense.

Graphene in a magnetic field

Graphene is a two-dimensional allotrope of carbon, with the carbon atoms organized in a "honeycomb" crystal, fig. 1.1. Imagine the following idealization of a experiment: Con-

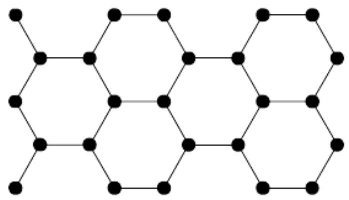

Figure 1.1: a "honeycomb" pattern

sider a single layer of graphene, placed in a constant magnetic field ("the system"). Let this layer be subject to a monocromatic (plane-wave) light-beam of known polarization. We would like to be able to make a quantum mechanical prediction, of how the electrons of the graphene layer respond to the applied electro-magnetic fields.

Faraday rotation

Faraday rotation is a dispersion effect. It describes the rotation of the polarization of radiation passing through a substance in the direction of an applied magnetic field. As in the article by Jian-Ping Peng et.al. [3], we calculate the Faraday rotation, physically a three-dimensional effect, in a quasi-two-dimensional electron system in a magnetic field B applied perpendicular to the layer. The electrons are confined within a slab of thickness d and move freely along the xy plane. Physically the Faraday rotation arises from the difference in the propagation of the two types of circular polarizations into which the plane polarized beam may be resolved. The Faraday rotation ϑ is defined as

$$\vartheta = \frac{\omega d(\eta_- - \eta_+)}{2c},$$

where η_- and η_+ are the indices of refraction of right and left circularly polarized radiation of frequency ω. Expressions for $\eta_\pm$ can be obtained from Maxwell's equations

$$\boldsymbol{\nabla} \times \boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{B}}{\partial t}, \quad \boldsymbol{\nabla} \times \boldsymbol{H} = \frac{4\pi}{c}\boldsymbol{J} + \frac{1}{c}\frac{\partial \boldsymbol{D}}{\partial t}$$

which, combined with the constitutive equations

$$\boldsymbol{J} = \overleftrightarrow{\sigma}\boldsymbol{E}, \qquad \boldsymbol{B} = \mu\boldsymbol{H}, \qquad \boldsymbol{D} = \varepsilon\boldsymbol{E},$$

give

$$\boldsymbol{\nabla}(\boldsymbol{\nabla} \times \boldsymbol{E}) - \boldsymbol{\nabla}^2\boldsymbol{E} = -\left(\frac{4\pi\mu}{c^2}\right)\overleftrightarrow{\sigma}\frac{\partial \boldsymbol{E}}{\partial t} - \left(\frac{\mu\varepsilon}{c^2}\right)\frac{\partial^2 \boldsymbol{E}}{\partial t^2}.$$

For the Faraday effect one takes the propagation along the applies dc magnetic field. Assuming a plane-wave solution of the form

$$\boldsymbol{E} = \boldsymbol{E}_0 e^{i(\omega t - Kz)}$$

leads to

$$K^2\boldsymbol{E}_0 = \mu\varepsilon(\omega/c)^2\left[\overleftrightarrow{\mathbb{1}} - (4\pi i/\omega\varepsilon)\overleftrightarrow{\sigma}\right]\boldsymbol{E}_0$$

where $\overleftrightarrow{\mathbb{1}}$ is a unit tensor. Assuming a circularly polarized wave $\boldsymbol{E}_0 = \boldsymbol{E}_{0x} \pm i\boldsymbol{E}_{0y}$, then

$$K_\pm^2 = \mu\varepsilon(\omega/c)^2\left[1 - (4\pi i/\omega\varepsilon)\sigma_\pm^{(3D)}\right].$$

Where $\sigma_\pm^{(3D)} = \sigma_{xx}^{(3D)} \pm i\sigma_{xy}^{(3D)}$. The complex index of refraction $(\eta - i\kappa)$ is then obtained from

$$(\eta_\pm - i\kappa_\pm)^2 = \mu\varepsilon\left[1 - (4\pi i/\omega\varepsilon)\sigma_\pm^{(3D)}\right]. \tag{1.1}$$

The diagonal 3D conductivity σ_{zz} makes no contribution to the Faraday rotation. The form of $\sigma_{12}^{(2D)}$ is

$$\sigma^{(2D)} = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ -\sigma_{12} & \sigma_{22} \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{yy} \end{bmatrix}$$

Considering the finite thickness d of the layer, the three-dimensional conductivity tensor is related to the two-dimensional conductivity tensor by the following expression

$$\sigma^{(3D)} = \sigma^{(2D)}/d$$

Isolating $\eta_\pm$ in formula (1.1), we have

$$\mathrm{Re}\left[(\eta_\pm - i\kappa_\pm)^2\right] = \mu\varepsilon\left(1 \pm \frac{4\pi}{\omega\varepsilon}\sigma_{xy}^{(3D)}\right), \qquad \mathrm{Im}\left[(\eta_\pm - i\kappa_\pm)^2\right] = -\mu\varepsilon\frac{4\pi}{\omega\varepsilon}\sigma_{xx}^{(3D)}.$$

We are looking for

$$\eta_\pm = \sqrt{\mu\varepsilon}\mathrm{Re}\left[\frac{\eta_\pm - i\kappa_\pm}{\sqrt{\mu\varepsilon}}\right].$$

Physically, $\eta_\pm$ should be non-negative, so we choose the solution,

$$\frac{\eta_\pm}{\sqrt{\mu\varepsilon}} = \left[\left(1 \pm \frac{4\pi}{\omega\varepsilon}\sigma_{12}^{(2D)}\right)^2 + \left(\frac{4\pi}{\omega\varepsilon}\sigma_{11}^{(2D)}\right)^2\right]^{\frac{1}{4}} \cos\left(\frac{1}{2}\arctan\left[\frac{\sigma_{11}^{(2D)}}{\left(\frac{\omega\varepsilon}{4\pi} \pm \sigma_{12}^{(2D)}\right)}\right]\right).$$

Considering σ_{11} and $\sigma_{12}^{(2D)}$ as variables u and v, respectively, $\eta_\pm$ is thus, up to a constant, given by the function

$$\frac{\eta_\pm}{\sqrt{\mu\varepsilon}} = f(u,v) = \left[\left(1 \pm \frac{4\pi}{\omega\varepsilon}u\right)^2 + \left(\frac{4\pi}{\omega\varepsilon}v\right)^2\right]^{\frac{1}{4}} \cos\left(\frac{1}{2}\arctan\left[\frac{v}{\left(\frac{\omega\varepsilon}{4\pi} \pm u\right)}\right]\right).$$

We will show how one can find the asymptotic expansion of $\sigma_{12}^{(2D)}(b)$, in powers of the magnetic field strength b and in particular we will show that in the small b limit, $\sigma_{12}(b)$ can be written

$$\sigma_{12}^{(2D)}(b) = b\sigma_{12}^{(1)} + \mathcal{O}(b^2),$$

using a method that could also be used to find the expansion of $\sigma_{11}^{(2D)}(b)$

$$\sigma_{11}^{(2D)}(b) = \sigma_{11}^{(0)} + b\sigma_{11}^{(1)} + \mathcal{O}(b^2)$$

In this presentation we a interested in how ϑ, and therefore $(\eta_- - \eta_+) \propto [f(-u,v) - f(u,v)]$, varies with the first power of b, so considering the expansion of $f(u,v)$ in powers of u we have

$$f(-u,v) - f(u,v) = \underbrace{\left[2\frac{\partial f}{\partial u}(0,v_0)\right]u}_{\text{linear in b}} + \underbrace{\mathcal{O}(u^2)}_{\propto b^2}$$

where v_0 denotes $\sigma_{xx}(b=0)$. We can omit all but the constant $\sigma_{11}^{(0)}$ term in $\sigma_{11}^{(2D)}(b)$. ϑ is proportional with

$$b\left(\frac{\mathrm{d}}{\mathrm{d}b}\sigma_{12}^{(2D)}\right)(0).$$

The question of calculating the faraday rotation is therefore a question of differentiating the off-diagonal conductivity $\sigma_{12}^{(2D)}$.

1.2 Setup

One-electron approximation

We work in a one-electron setup, neglecting electron-electron interactions.

The crystal

We settle for a simpler model than graphene. Consider a 2 - dimensional crystal, with the nuclei fixed at their equilibrium positions

$$\Lambda = \{\boldsymbol{x} \in \mathbb{R}^2 \ : \ \text{there is a nucleous at position } \boldsymbol{x}\}.$$

A point in Λ is denoted a *site*. The crystal is assumed invariant under translations that transforms functions defined on $\mathbb{R}^2$ according to the rule

$$(\mathcal{T}_\gamma f)(\boldsymbol{r}) = f(\boldsymbol{r} - m\boldsymbol{a}_1 - n\boldsymbol{a}_2), \qquad \gamma = m\boldsymbol{a}_1 + n\boldsymbol{a}_2,$$

where m and n are integers, and the basis vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ generate the *Bravais Lattice*, Γ:

$$\Gamma = \{\gamma \in \mathbb{R}^2 \ : \ \gamma = m\boldsymbol{a}_1 + n\boldsymbol{a}_2\}.$$

(The two vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ should not be linearly dependent.) The points of Λ are generated by appending one *unit cell* to each point of Γ (making a choice of origo). I denote the (finite) set of vectors that constitutes the unit cell by Ω:

$$\Omega = \{\underline{\boldsymbol{x}}_n\}_{n=1}^{|\Omega|}$$

The choice of Bravais lattice and unit cell should lead to the unique decomposition of all site position vectors,

$$\boldsymbol{x} = \gamma + \underline{\boldsymbol{x}}, \quad \gamma \in \Gamma, \quad \underline{\boldsymbol{x}} \in \Omega,$$

for all $\boldsymbol{x} \in \Lambda$.

When used as a summation index or site label, we will not use the bold notation $\boldsymbol{x}, \gamma$ and $\underline{\boldsymbol{x}}$, but simply use x, γ and $\underline{x}$. That is, $|x\rangle$ denotes a localized state at position $\boldsymbol{x}$, and the sum $\sum_{\gamma\in\Gamma}|\gamma - \boldsymbol{y}|$ is a sum over all position vectors in Γ. Sometimes I will write $\sum_\gamma$ for $\sum_{\gamma\in M}$, when it is clear from the context, which set, M, γ is to be summed over.

Reciprocal lattice

Define the *dual basis* $\{\boldsymbol{b}_1, \boldsymbol{b}_2\}$ by the relations

$$\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij},$$

where δ_{ij} is the Kronecker delta. The *reciprocal lattice*, Γ^*, is the set of all vectors $\gamma^* \in \mathbb{R}^2$ such that

$$\gamma^* = m\boldsymbol{b}_1 + n\boldsymbol{b}_2, \qquad m, n \in \mathbb{Z}$$

The definition of the reciprocal lattice has the consequence that

$$\gamma^* \cdot \gamma = n2\pi, \quad \text{for some } n \in \mathbb{Z},$$

for all vectors γ in the Bravais lattice and for all vectors γ^* in the reciprocal lattice.

We denote by Ω^* the basic periodic cell for the dual basis :

$$\Omega^* = \left\{ t_1\boldsymbol{b}_1 + t_2\boldsymbol{b}_2 \ : \ -\frac{1}{2} \leq t_i < \frac{1}{2}. \right\}$$

The unit cell

We restrict ourselves to a unit cell with two sites, one at $\underline{x} = (0,0)$ and one at $\underline{x} = (\frac{a_1}{2}, 0)$ (fig. 1.2).

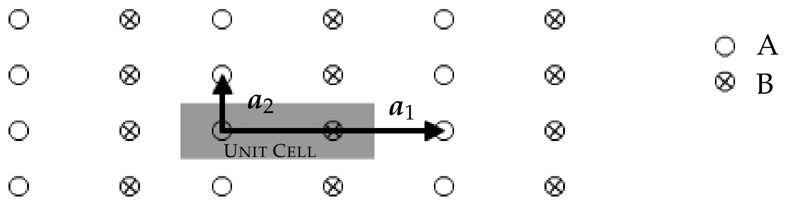

Figure 1.2: The ion-core mesh, $\Lambda = \{x\}$ ("A" *and* "B" type points), is generated by appending a basis of two sites, A and B, to the Bravais lattice, $\Gamma = \{\gamma\}$ ("A" type points), generated by the primitive vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$. We choose a simple Bravais lattice where the primitive vectors are orthogonal.

Crystal Hamiltonian, potential term

The potential term, $\mathbf{V}_0$ of the crystal Hamiltonian, $\mathbf{H}_0 = \mathbf{T} + \mathbf{V}_0$ is in the model given by:

$$(\mathbf{V}_0\psi)(\gamma + \underline{x}) = \begin{cases} v\,\psi(\gamma + \underline{x}), & \underline{x} = (0,0) \\ 0, & \underline{x} = \left(\frac{a_1}{2}, 0\right) \end{cases} \tag{1.2}$$

Crystal Hamiltonian, kinetic term

We fix the kinetic term kernel $t_0(x, y)$ ("hopping matrix elements") of the Hamiltonian as:

$$t_0(\boldsymbol{x}, \boldsymbol{y}) = t_0(x_1, y_1)^{(1)}\delta_{x_2,y_2} + t_0(x_2, y_2)^{(2)}\delta_{x_1,y_1}, \tag{1.3}$$

for all sites $\boldsymbol{x} = (x_1, x_2)$ and $\boldsymbol{y} = (y_1, y_2)$ in Λ. This models a crystal with no oblique interactions. We consider a nearest-neighbour model, where

$$t_0(x_1, y_1)^{(1)} = 0, \text{ unless } y_1 = x_1 \pm \frac{a_1}{2},$$
$$t_0(x_2, y_2)^{(2)} = 0, \text{ unless } y_2 = x_2 \pm a_2,$$

and we fix the magnitude of the non-zero hopping elements to 1, so the crystal Hamiltonian has the kernel:

$$h_0(\boldsymbol{x}, \boldsymbol{y}) = \delta_{x_1, y_1 \pm a_1/2}\delta_{x_2,y_2} + \delta_{x_2,y_2 \pm a_2}\delta_{x_1,y_1} + v(\underline{x}_1)\delta_{\boldsymbol{x},\boldsymbol{y}}, \tag{1.4}$$

Finite, but large crystal

Define a central region of the crystal by

$$\Lambda_N := \{(\gamma + \underline{x}) \in \Lambda \ : \ \gamma = m\boldsymbol{a}_1 + n\boldsymbol{a}_2, \ |m| \le N, |n| \le N\}.$$

This central region is a region of $|\Lambda_{\rm N}| = (2N+1)^2$ unit cells, and $(2N+1)^2 \cdot |\Omega|$ sites. The *characteristic function*, χ_{Λ_N}, of Λ_N, is a multiplicative operator defined by:

$$\left(\chi_{\Lambda_N}\boldsymbol{\psi}\right)(\boldsymbol{x}) = \chi_{\Lambda_N}(\boldsymbol{x})\psi(\boldsymbol{x}),$$
$$\text{where} \quad \chi_{\Lambda_N}(\boldsymbol{x}) = \begin{cases} 1 & , \boldsymbol{x} \in \Lambda_N, \\ 0 & , \boldsymbol{x} \notin \Lambda_N. \end{cases}$$

The *support* of $\boldsymbol{\psi} \in \ell^2(\Lambda)$, denoted supp$\{\psi\}$, is the collection of all points $\boldsymbol{x} \in \Lambda$, that satisfies $\psi(\boldsymbol{x}) \neq 0$. We will from here on work with the Hamilton operator, subject to *Dirichlet boundary conditions* (DBC) in Λ_N:

$$\mathbf{H}_{0,\rm N} = \chi_{\Lambda_N}\mathbf{H}_0\,\chi_{\Lambda_N}, \tag{1.5}$$

where $\mathbf{H}_0$ is an operator defined on $\ell^2(\Lambda)$. $\mathbf{H}_{0,\rm N}$ is a $(2N+1)^2|\Omega| \times (2N+1)^2|\Omega|$ matrix, so there exists a one-to-one relation between (linear) $\chi_{\Lambda_N}\mathbf{A}\,\chi_{\Lambda_N}$ operators on $\ell^2(\Lambda)$, and $(2N+1)^2|\Omega| \times (2N+1)^2|\Omega|$ matrices. The restricted operator $\mathbf{H}_{0,\rm N}$ approximates $\mathbf{H}_0$ in the sense

$$\mathbf{H}_0|\psi\rangle = \chi_{\Lambda_N}\mathbf{H}_0\,\chi_{\Lambda_N}|\psi\rangle, \qquad * \tag{1.6}$$

for $|\psi\rangle$ where both supp$\{\psi\}$ *and* supp$\{\mathbf{H}_0\psi\}$ is fully enclosed in Λ_N.

A consequence of the tight binding model is, that functions $\boldsymbol{\psi}$ with supp$\{\mathbf{H}_0\psi\} \nsubseteq \Lambda_N$ but supp$\{\psi\} \subset \Lambda_N$ can only be functions $\psi(\boldsymbol{x})$ with non-zero values near the edge of Λ_N. Conversely, the transformed vector $\mathbf{H}_0\boldsymbol{\psi}$ is not different from the vector $\mathbf{H}_{0,\rm N}\boldsymbol{\psi}$ for wavefunctions $\boldsymbol{\psi}$ with their support localized in the "inner part" [1] of the central region, that is for $\boldsymbol{\psi}$ with the support "situated far enough from" the edge of Λ_N, this line of thought will be formalized and expanded later , as a key part of the proof of the large N limit.

We use as a notation for an operator $\mathbf{O}$ with the DBC the subscript N, $\mathbf{O}_{\rm N}$

Operators with the subscript "N" are from here on always subject to DBC.

Peierls substitution

We include a static magnetic field into the model, it is thought of as having always existed (before the light pertubation was turned on). This is done by the use of *Peierls substitution*. In the Peierls substitution, the Hamiltonian matrix element in a constant magnetic field can be obtained through multiplication of the crystal Hamiltonian matrix element h_0 by a phase factor [6],

$$h_{\rm b}(\boldsymbol{x}, \boldsymbol{y}) = e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}h_0(\boldsymbol{x}, \boldsymbol{y}).$$

[1] How close to the edge this "inner" part can come, is of course linked to the number of "neighbours" of a given site one allow to have non-zero hopping matrix elements in to the model. A second-nearest tb. model will have a smaller inner part than a nearest-neighbour tb. model, for a fixed N.

The magnetic field is assumed perpendicular to the crystal, directed in the $z+$ direction, having constant magnitude $b,$. The phase factor is given by the flux of a $+z$ directed field of strength unity through a triangle defined by origo, the site $\boldsymbol{x}$ and the site $\boldsymbol{y}$[2]. We set

$$\varphi(\boldsymbol{x},\boldsymbol{y}) \quad := \quad \frac{1}{2}(y_1x_2 - x_1y_2). \tag{1.7}$$

With a slight abuse of notation (using 3D cross-product), $\varphi(\boldsymbol{x},\boldsymbol{y})$ given by formula (1.7) can be calculated by:

$$\varphi(\boldsymbol{x},\boldsymbol{y}) \quad = \quad \frac{1}{2}\left[(\boldsymbol{y}\times\boldsymbol{x})\right]_z,$$

where in this 3D mindset, $\boldsymbol{x}\to(x_1,x_2,0)$, $\boldsymbol{y}\to(y_1,y_2,0)$ and $[\boldsymbol{v}]_z$ denotes the z-component of the 3D vector $\boldsymbol{v}$. Note that $\varphi(\boldsymbol{x},\boldsymbol{y})$ is not bound by a constant multiplying $\|\boldsymbol{x}-\boldsymbol{y}\|$! but we can use the estimate

$$|\varphi(\boldsymbol{x},\boldsymbol{y})| \leq \min\{\|x\|,\|\boldsymbol{y}\|\}\|\boldsymbol{x}-\boldsymbol{y}\|.$$

Note also that φ is antisymmetric, that is

$$\varphi(\boldsymbol{x},\boldsymbol{y}) = -\varphi(\boldsymbol{y},\boldsymbol{x}).$$

We denote by $\mathrm{fl}(\boldsymbol{x},\boldsymbol{x}',\boldsymbol{x}'')$ the magnetic flux of a field of unity field-strength through the triangle defined by origo, the site $\boldsymbol{x}-\boldsymbol{x}'$ and the site $\boldsymbol{x}'-\boldsymbol{x}''$. We will need the equality, where $\boldsymbol{x},\boldsymbol{x}'$ and $\boldsymbol{y}'$ are vectors in the xy-plane extended of $\mathbb{R}^3$,

$$\frac{1}{2}(\boldsymbol{x}'\times\boldsymbol{x}) + \frac{1}{2}(\boldsymbol{x}''\times\boldsymbol{x}') = \frac{1}{2}(\boldsymbol{x}''\times\boldsymbol{x}) + \frac{1}{2}\left[(\boldsymbol{x}'-\boldsymbol{x}'')\times(\boldsymbol{x}-\boldsymbol{x}')\right],$$

This gives

$$\varphi(\boldsymbol{x},\boldsymbol{x}') + \varphi(\boldsymbol{x}',\boldsymbol{x}'') = \varphi(\boldsymbol{x},\boldsymbol{x}'') + \mathrm{fl}(\boldsymbol{x},\boldsymbol{x}',\boldsymbol{x}''),$$

with the definition

$$\mathrm{fl}(\boldsymbol{x},\boldsymbol{x}',\boldsymbol{x}'') = \frac{1}{2}\left[(\boldsymbol{x}'-\boldsymbol{x}'')\times(\boldsymbol{x}-\boldsymbol{x}')\right]_z.$$

The fact that $\varphi(\boldsymbol{x},\boldsymbol{x}) = 0$ means that we only need to consider the effect of the phase factor on the kinetic term of the Hamiltonian, since the potential term has the factor $\delta(\boldsymbol{x},\boldsymbol{y})$ in the kernel:

$$\begin{aligned} & e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}\left(\delta_{\boldsymbol{x}_1,\boldsymbol{y}_1\pm a_1/2}\delta_{x_2,y_2} + \delta_{\boldsymbol{x}_2,\boldsymbol{y}_2\pm a_2}\delta_{x_1,y_1} + v(\underline{y}_1)\delta_{\underline{\boldsymbol{x}},\underline{\boldsymbol{y}}}\right) \\ & = e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}\left(\delta_{\boldsymbol{x}_1,\boldsymbol{y}_1\pm a_1/2}\delta_{x_2,y_2} + \delta_{\boldsymbol{x}_2,\boldsymbol{y}_2\pm a_2}\delta_{x_1,y_1}\right) + v(\underline{y}_1)\delta_{\underline{\boldsymbol{x}},\underline{\boldsymbol{y}}}, \end{aligned}$$

that is

$$\mathbf{H}_\mathrm{b} = \mathbf{T}_\mathrm{b} + \mathbf{V}_0,$$

with the "magnetic" kinetic operator defined as the operator having the kernel

$$t_\mathrm{b} := e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}\left(\delta_{\boldsymbol{x}_1,\boldsymbol{y}_1\pm a_1/2}\delta_{x_2,y_2} + \delta_{\boldsymbol{x}_2,\boldsymbol{y}_2\pm a_2}\delta_{x_1,y_1}\right).$$

[2]See R. Saito et al. section 6.2, expecially around formula (6.14).

Units

To simplify the notation we work in a system of units, where

$$\boxed{\hbar = 2m_{electron} = e = 1}$$

Here $\hbar$ is Plancks reduced constant and e denotes the charge of an proton.

Position operator

We define the position operators $\mathbf{X}_1$ and $\mathbf{X}_2$, by how they transform the basis elements $\delta_{\boldsymbol{x}}, \boldsymbol{x} \in \Lambda$,

$$\mathbf{X}_1 \delta_{\boldsymbol{x}} := x_1 \delta_{\boldsymbol{x}}, \quad \forall \boldsymbol{x} \in \Lambda,$$
$$\mathbf{X}_2 \delta_{\boldsymbol{x}} := x_2 \delta_{\boldsymbol{x}}, \quad \forall \boldsymbol{x} \in \Lambda,$$

(remember $\boldsymbol{x} = (x_1, x_2)$). For a general $\boldsymbol{\psi}$ in $\ell^2(\Lambda)$, and fixed $\boldsymbol{x} \in \Lambda$, we have

$$(\mathbf{X}_1 \boldsymbol{\psi})(\boldsymbol{x}) = \sum_{y \in \Lambda} X_1(\boldsymbol{x}, \boldsymbol{y}) \psi(\boldsymbol{y}) = x_1 \psi(\boldsymbol{x}),$$

so the kernel of $\mathbf{X}_\nu$, in the $\{\delta_{\boldsymbol{x}}\}$ representation, must be $\mathbf{X}_\nu(x, y) = \delta_{\boldsymbol{x},\boldsymbol{y}} x_\nu$ for $\nu \in \{1, 2\}$. Since these operators do nothing else than pick up the spatial label of the basis states, we could denote it the *label operator*, but we will use it as the representation of the position operator in the $\{\delta_{\boldsymbol{x}}\}$ basis. Note that the position operator is not bounded in the operatornorm, and that even though $\boldsymbol{\psi} \in \ell^2(\Lambda)$ it is not always true that $\mathbf{X}_\nu \boldsymbol{\psi} \in \ell^2(\Lambda)$. It holds, though, that $\mathbf{X}_{\nu,\mathrm{N}} \boldsymbol{\psi} \in \ell^2(\Lambda)$ for $\mathbf{X}_\nu \boldsymbol{\psi} \in \ell^2(\Lambda)$.

The field of the light beam

We introduce the light-beam incident on the crystal as a monochromatic, plane-wave EM-field, with the electric field parallel with the x-axis

$$\boldsymbol{E}(t) = (E_x, E_y) := (Ee^{i\omega t}, 0), \qquad E \geq 0,$$

with *a negative imaginary part* of the frequency; $\mathrm{Im}\omega = -\eta < 0$.

Note on notation: I write cartesian vectors component-wise the same way as I write points in the plane; $\boldsymbol{v} = (v_x, v_y)$, but nonetheless a vector (v_x, v_y) is to be thought of as a column vector when multiplying matrices.

$$(v_x, v_y) \to \begin{bmatrix} v_x \\ v_y \end{bmatrix}.$$

We treat the light beam as an external time-dependent potential term $\mathbf{V}_\mathrm{E}(t)$. The Hamilton operator is now given by

$$\mathbf{H}_\mathrm{E}(t) = \mathbf{H}_\mathrm{b} + \mathbf{V}_\mathrm{E}(t). \tag{1.8}$$

The potential operator representing the light beam, as introduced above, can be calculated by use of the first component position operator,

$$\mathbf{V}_\mathrm{E}(t) = Ee^{i\omega t} \mathbf{X}_1. \tag{1.9}$$

Dynamic equation for the density operator

We denote by μ the chemical potential, and $\beta := \frac{1}{k_B \tau}$ is the inverse temperature, so the Fermi-Dirac distribution can be written

$$f_{\mathrm{FD}}(z) = \frac{1}{e^{\beta(z-\mu)} + 1}.$$

We set as a condition for the system, that the density operator in the limit $t \to -\infty$ is given by the Fermi-Dirac distribution function :

$$\varrho_{\mathrm{N}}(t \to -\infty) = \varrho_{0,\mathrm{N}} = f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{b,N}}).$$

An example: if $\{|\psi_j\rangle\}$ is a basis of energy-eigenvectors for the self-adjoint matrix $\mathbf{H}_{\mathrm{b},N}$, we have $\mathbf{H}_{\mathrm{b},N}|\psi_j\rangle = \lambda_j|\psi_j\rangle$. In this case for the infinite past, the state of system should be defined by the density operator:

$$\sum_j f_{\mathrm{FD}}(\lambda_j)|\psi_j\rangle\langle\psi_j|,$$

where $\{|\psi_j\rangle\}$ is an energy eigenvector basis for wavefunctions on the central region Λ_N of the site-mesh.

We will sometimes just use "density" for "density operator". To find the density at an arbitrary time t, we need to solve the dynamic (Liouville) equation for $\varrho_{\mathrm{E,N}}(t)$. This is:

$$\begin{cases} i\dot{\varrho}_{\mathrm{E,N}}(t) & = [\mathbf{H}_{\mathrm{E,N}} \,, \varrho_{\mathrm{E,N}}(t)], \\ \varrho_{\mathrm{E,N}}(t \to -\infty) & = f_{\mathrm{D}}(\mathbf{H}_{\mathrm{b,N}}). \end{cases} \tag{1.10}$$

Current density

The current operator is defined:

$$\mathbf{j}_{\nu,\mathrm{b,N}} := i[\mathbf{H}_{\mathrm{b,N}} \,, \mathbf{X}_{\nu,\mathrm{N}}] \qquad \nu = 1,2$$

with (DBC), and

$$\mathbf{j}_{\nu,\mathrm{b}} := i[\mathbf{H}_{\mathrm{b}} \,, \mathbf{X}_{\nu}] \qquad \nu = 1,2$$

on the full site-mesh. The expectation value, over the central region, of the current density in the y-direction, $\langle\, \mathbf{J}_{2,\mathrm{E,N}}(E)\,\rangle := J_{2,\mathrm{E,N}}(E)$, at $t = 0$, is given by the trace of the operator product of $\boldsymbol{\rho}_{\mathrm{E,N}}(0)$ and $\mathbf{J}_{2,\mathrm{E,N}}(0)$, where $\mathbf{J}_{2,\mathrm{E,N}} = |\Lambda_N|^{-1}\mathbf{j}_{2,\mathrm{E,N}}$:

$$J_{2,\mathrm{E,N}}(E) = \frac{1}{|\Lambda_N|}\mathrm{Tr}_{\mathrm{N}}\{\boldsymbol{\rho}_{\mathrm{E,N}}(t=0)\mathbf{j}_{2,\mathrm{E,N}}\} \tag{1.11}$$

where $\mathrm{Tr}_{\mathrm{N}}\{\cdot\}$ is a notational shorhand for a trace over the central region Λ_N. We will see that $J_{2,\mathrm{N,E}}(E)$ has an analytic expansion in E:

$$J_{2,\mathrm{b}}(E) = J_{2,\mathrm{b}}(E=0) + E\sigma_{21} + \mathcal{O}(E^2). \tag{1.12}$$

The linear term in E, in formula (1.12), is just the off-diagonal conduction element that we seek to identify, because the light-field is polarized in the x-direction.

1.3 Main result of this thesis

We shall see that σ_{21} has the form:

$$\sigma_{21}(b,N) = \frac{1}{2\pi\omega|\Lambda_N|}\oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z)\Big(\mathrm{Tr}_{\mathrm{N}}\Big\{(\mathbf{H}_{\mathrm{N,b}} - z + \omega)^{-1}\,\mathbf{j}_{1,\mathrm{b,N}}(\mathbf{H}_{\mathrm{N,b}} - z)^{-1}\mathbf{j}_{2,\mathrm{b,N}}\Big\} + \mathrm{Tr}_{\mathrm{N}}\Big\{(\mathbf{H}_{\mathrm{N,b}} - z)^{-1}\mathbf{j}_{1,\mathrm{b,N}}\,(\mathbf{H}_{\mathrm{N,b}} - z - \omega)^{-1}\,\mathbf{j}_{2,\mathrm{b,N}}\Big\}\Big), \tag{1.13}$$

see equation (2.25) and figure (1.3) for details and definitions.

Define the operators in $\ell^2(\Lambda)$:

$$\mathbf{D}_{\mathrm{b},+}(z) := (\mathbf{H}_{\mathrm{b}} - z + \omega)^{-1}\,\mathbf{j}_{1,\mathrm{b}}(\mathbf{H}_{\mathrm{b}} - z)^{-1}\mathbf{j}_{2,\mathrm{b}}$$

$$\mathbf{D}_{\mathrm{b},-}(z) := (\mathbf{H}_{\mathrm{b}} - z)^{-1}\mathbf{j}_{1,\mathrm{b}}\,(\mathbf{H}_{\mathrm{b}} - z - \omega)^{-1}\,\mathbf{j}_{2,\mathrm{b}},$$

where $\mathbf{j}_{\nu,\mathrm{b}} := i[\mathbf{H}_{\mathrm{b}}, \mathbf{X}_\nu]$, $\nu = 1,2$. We are now ready to state the main result of this paper.

Theorem 1.1 (Main Result). *The following results hold true:*

1.
$$\begin{aligned}\sigma_{21}(b) &:= \lim_{N\to\infty}\sigma_{21}(b,N)\\ &= \frac{1}{2|\Omega|\pi\omega}\oint_{\mathscr{C}}\mathrm{d}z\, f_{\mathrm{FD}}(z)\sum_{\underline{x}\in\Omega}\left(\mathbf{D}_{\mathrm{b},+}(\underline{x},\underline{x};z,b) + \mathbf{D}_{\mathrm{b},-}(\underline{x},\underline{x};z,b)\right),\end{aligned} \tag{1.14}$$

   where the smooth path $\mathscr{C}$ enclose, but has no points in common with, the (real, bounded) spectrum of $\mathbf{H}_b$, and $\mathscr{C}$ is chosen such that ω lies outside *$\mathscr{C}$. $\mathscr{C}$ must furthermore be chosen so "close" to the real line, that $f_{\mathrm{FD}}(z)$ has no singularities inside $\mathscr{C}$, see fig. 1.3.*

2. *The function $\sigma_{21}(\cdot)$ is smooth and has an asymptotic expansion in b around* 0*, in particular, $\sigma_{21}(0) = 0$. All the derivatives of σ_{21} can be written only in terms of the fiber operators associated to Bloch-decomposition. The Faraday rotation ϑ is proportional with $\sigma'_{21}(0)$, which is given by formula* (3.19).

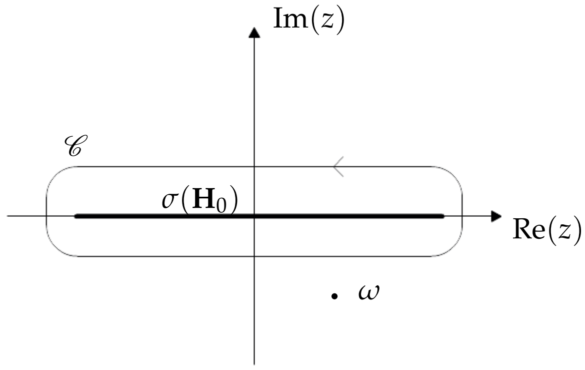

Figure 1.3: The path $\mathscr{C}$ should enclose $\sigma(\mathbf{H}_{\mathrm{b}})$, and ω should be outside $\mathscr{C}$.

2

PROOF OF THEOREM 1.1(1)

2.1 SIMPLE COMBES-THOMAS THEOREM

In this section we discuss general operators defined on $\ell^2(\Lambda)$. It should be understood that the results 2.1, 2.2, 2.3, 2.4, 2.6 and 2.5 also hold if Λ is replaced with Λ_N, uniformly in N.

Exponentially almost diagonal operators

Definition 2.1 (Schur-Holmgreen bound)**.** For a linear operator $\mathbf{A}$ with the kernel $a(\boldsymbol{x}, \boldsymbol{x}')$, $\boldsymbol{x}, \boldsymbol{x}' \in \Lambda$, we define the *Schur-Holmgreen bound*, $\|\mathbf{A}\|_1$ of $\mathbf{A}$ by:

$$\|\mathbf{A}\|_1 := \max\left\{\sup_{\boldsymbol{x}\in\Lambda}\sum_{\boldsymbol{x}'\in\Lambda}|a(\boldsymbol{x},\boldsymbol{x}')|, \sup_{\boldsymbol{x}'\in\Lambda}\sum_{\boldsymbol{x}\in\Lambda}|a(\boldsymbol{x},\boldsymbol{x}')|\right\} \tag{2.1}$$

If an operator has $\|\mathbf{A}\|_1 < \infty$ it is said to be *Schur-Holmgreen bounded*.

Lemma 2.2. *If $\|\mathbf{A}\|_1 < \infty$, then $\|\mathbf{A}\| \leq \|\mathbf{A}\|_1$, where $\|\mathbf{A}\|$ is the usual operator norm.*

$$\|\mathbf{A}\| \leq \left(\sup_{\boldsymbol{x}\in\Lambda}\sum_{\boldsymbol{x}'\in\Lambda}|a(\boldsymbol{x},\boldsymbol{x}')|\right)^{1/2}\left(\sup_{\boldsymbol{x}'\in\Lambda}\sum_{\boldsymbol{x}\in\Lambda}|a(\boldsymbol{x},\boldsymbol{x}')|\right)^{1/2} \leq \|\mathbf{A}\|_1 \tag{2.2}$$

Proof. Let $\boldsymbol{\psi} \in \ell^2(\Lambda)$, with $\|\boldsymbol{\psi}\| = 1$, assume that ψ has compact support. Let $\{\delta_{\boldsymbol{x}}\}$ be an orthonormal basis for $\ell^2(\Lambda)$. Consider

$$\begin{aligned}
|(\mathbf{A}\boldsymbol{\psi})(\boldsymbol{x})| \leq \\
\sum_{\boldsymbol{y}}|a(\boldsymbol{x},\boldsymbol{y})\psi(\boldsymbol{y})| \\
&\leq \sum_{\boldsymbol{y}\in\Lambda}(|a(\boldsymbol{x},\boldsymbol{y})|)^{1/2}(|a(\boldsymbol{x},\boldsymbol{y})|)^{1/2}|\psi(\boldsymbol{y})| \\
&\leq \left(\sum_{\boldsymbol{y}\in\Lambda}|a(\boldsymbol{x},\boldsymbol{y})|\right)^{1/2}\left(\sum_{\boldsymbol{y}\in\Lambda}|a(\boldsymbol{x},\boldsymbol{y})||\psi(\boldsymbol{y})|^2\right)^{1/2},
\end{aligned}$$

it must holde that

$$\begin{aligned}\|\mathbf{A}\boldsymbol{\psi}\|^2 &\le \left(\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{y}}|a(\boldsymbol{x}',\boldsymbol{y})|\right)\sum_{\boldsymbol{x}}\left(\sum_{\boldsymbol{x}''}|a(\boldsymbol{x},\boldsymbol{x}'')|\ |\psi(\boldsymbol{y})|^2\right)\\ &\le \left(\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{y}}|a(\boldsymbol{x}',\boldsymbol{y})|\right)\left(\sup_{\boldsymbol{y}}\sum_{\boldsymbol{x}}|a(\boldsymbol{x},\boldsymbol{y})|\right)\underbrace{\sum_{\boldsymbol{x}''}|\psi(\boldsymbol{y})|^2}_{=1},\end{aligned}$$

which shows (2.2). This result can be extended to all $\boldsymbol{\psi} \in \ell^2(\Lambda)$. □

Definition 2.3 (Exponentially Almost Diagonal Operator)**.** Let $\mathscr{H}$ be $\ell^2(\Lambda)$. We say that an operator $\mathbf{A} : \mathscr{H} \to \mathscr{H}$ is *exponentially almost diagonal*, if there exists constants C_1, C_2, both strictly positive, so that the kernel of $\mathbf{A}$ satisfies

$$|a(\boldsymbol{x},\boldsymbol{y})| \le C_1 e^{-C_2\|\boldsymbol{x}-\boldsymbol{y}\|} \tag{2.3}$$

for all $\boldsymbol{x}, \boldsymbol{y}$ in Λ.

Theorem 2.4. *An exponentially almost diagonal operator is Schur-Holmgreen bounded.*

Proof. Consider an exponentially almost diagonal operator $\mathbf{A}$. For a real number x, the geometric series $\sum_{k=1}^{\infty} x^k$ converges iff $|x| < 1$, so the series $\sum_{k=1}^{\infty} e^{-ck}$ converge iff c>0. For a exponentially almost diagonal operator, positivity of the norm shows that the sums (2.1) converge iff $C_2 > 0$, which is always true for an exponentially almost diagonal operator. □

CT-property

We now show a property for exponentially almost diagonal operators, which is a simple version of Combes-Thomas theorem [4]. We start with a prepatory lemma:

Lemma 2.5. *Let $H \subset \rho(\mathbf{A})$ be a compact set, and suppose $\sigma(A)$ is bounded, then the distance between H and $\sigma(\mathbf{A})$, defined by*

$$\operatorname{dist}(H, \sigma(\mathbf{A}) := \inf_{z\in H}\{\operatorname{dist}(z, \sigma(\mathbf{A})\,)\}\,,$$

is actually a minimum, and strictly larger than zero.

Proof. H and $\sigma(\mathbf{A})$ are disjoint sets, so by positivity of the absolute value function, for all $z \in H$ and $s \in \sigma(\mathbf{A})$ we must have

$$|z - s| > 0. \tag{2.4}$$

The distance function $|\cdot - \cdot| : \mathbb{C} \times \mathbb{C} \to \mathbb{R}$,

$$|z - s| \qquad z, s \in \mathbb{C},$$

is a continous mapping. Since $\sigma(\mathbf{A})$ is closed and bounded, and thus compact, so $H \times \sigma(\mathbf{A})$ is a compact subset of $\mathbb{C}^2$ and by the extreme-value theorem, the value

$$\inf\{\|z - s\| : z \in H, s \in \sigma(\mathbf{A})\}$$

must be attained for at least one pair $(z_0, s_0) \in H \times \sigma(\mathbf{A})$, so the infimum is actually an minimum, and by (2.4) strictly larger than zero. □

Theorem 2.6 (CT-property). *Let z be an complex number in the resolvent set $\rho(\mathbf{A})$ of an self-adjoint exponentially almost diagonal operator $\mathbf{A}$ operating on the Hilbert Space $\mathscr{H} = \ell^2(\Lambda)$ for some lattice Λ. Let constants C_1 and C_2 be defined as in definition* (2.3).

Then the resolvent, $(\mathbf{A} - z)^{-1}$ is also exponentially almost diagonal. That is, there exists two positive constants, C_3 and C_4 so that the kernel of $(\mathbf{A} - z)^{-1}$ fullfills

$$|(\mathbf{A} - z)^{-1}(\boldsymbol{x}, \boldsymbol{y})| \leq C_3 e^{-C_4\|\boldsymbol{x}-\boldsymbol{y}\|}.$$

If z is restricted to belong to a closed subset $H \subset \rho(\mathbf{A})$, then we have the bounds on C_3 and C_4:

$$\begin{aligned} C_3 &\leq 2 \sup_{z \in H} \left\{ \frac{1}{\operatorname{dist}(H, \sigma(\mathbf{A}))} \right\} \\ C_4 &\leq \min\left\{ \frac{\operatorname{dist}(H, \sigma(\mathbf{A}))}{2\tilde{C}}, \frac{C_2}{4} \right\}, \\ \tilde{C} &:= \max\{a_1, a_2\} 16\, C_1 \sum_{\boldsymbol{x} \in \Lambda} e^{-\frac{C_2}{2}\|\boldsymbol{x}\|}, \end{aligned}$$

where a_1 and a_2 are the length of the orthogonal vectors generating the Bravais lattice.

Proof. For $\alpha > 0$, and an arbitrarily fixed lattice point $\boldsymbol{x}_0 \in \Lambda$, define the operator $\mathbf{A}_\alpha : \mathscr{H} \to \mathscr{H}$ by

$$\begin{aligned} \mathbf{A}_\alpha &:= e^{\alpha\|\cdot - \boldsymbol{x}_0\|} \mathbf{A} e^{-\alpha\|\cdot - \boldsymbol{x}_0\|} \\ (\mathbf{A}_\alpha \psi)(\boldsymbol{x}) &= e^{\alpha\|\boldsymbol{x} - \boldsymbol{x}_0\|} \sum_{\boldsymbol{y} \in \Lambda} a(\boldsymbol{x}, \boldsymbol{y}) e^{-\alpha|\boldsymbol{y} - \boldsymbol{x}_0|} \psi(\boldsymbol{y}) \end{aligned}$$

, where $e^{\alpha|\cdot - \boldsymbol{x}_0|}$ and $e^{-\alpha|\cdot - \boldsymbol{x}_0|}$ are multiplicative operators, i.e. $(e^{\alpha|\cdot - \boldsymbol{x}_0|}\psi)(\boldsymbol{x}) = e^{\alpha|\boldsymbol{x} - \boldsymbol{x}_0|}\psi(\boldsymbol{x})$, for all $\boldsymbol{x} \in \Lambda$. Silimarly for $e^{-\alpha|\cdot - \boldsymbol{x}_0|}$.

If α is small enough, $\mathbf{A}_\alpha$ is bounded, since

$$\begin{aligned} |a_\alpha(\boldsymbol{x}, \boldsymbol{y})| &= \left|e^{\alpha\|\boldsymbol{x} - \boldsymbol{x}_0\|} a(\boldsymbol{x}, \boldsymbol{y}) e^{-\alpha\|\boldsymbol{y} - \boldsymbol{x}_0\|}\right| = \left|e^{\alpha\|\boldsymbol{x} - \boldsymbol{y} + \boldsymbol{y} - \boldsymbol{x}_0\|} a(\boldsymbol{x}, \boldsymbol{y}) e^{-\alpha\|\boldsymbol{y} - \boldsymbol{x}_0\|}\right| \\ &\leq \left|a(\boldsymbol{x}, \boldsymbol{y}) e^{\alpha\|\boldsymbol{x} - \boldsymbol{y}\|}\right| \leq \left|C_1 e^{-(C_2 - \alpha)\|\boldsymbol{x} - \boldsymbol{y}\|}\right|, \end{aligned}$$

where we have used the triangle inequality in the last inequality. This shows that, as long as $C_2 - \alpha$ is positive, $\mathbf{A}_\alpha$ is exponentially almost diagonal, and therefore bounded.

We will now show that if α is small enough, $\mathbf{A}_\alpha - z$ is invertible. Using a geometric series argument, like in the proof of theorem 17.2 in Peter D. Lax's book [2], we see that

$$(\mathbf{A}_\alpha - z) = (\mathbb{1} - (\mathbf{A} - \mathbf{A}_\alpha)(\mathbf{A} - z)^{-1})(\mathbf{A} - z)$$

is invertible if $\|(\mathbf{A}-\mathbf{A}_\alpha)(\mathbf{A}-z)^{-1}\| \leq \|(\mathbf{A}-\mathbf{A}_\alpha)\|\|(\mathbf{A}-z)^{-1}\| < 1$. For a fixed z this can be achieved if

$$\|\mathbf{A}-\mathbf{A}_\alpha\| \xrightarrow{\alpha \to 0} 0. \tag{2.5}$$

This is in fact true, which we can see by evaluating the Schur-Holmgreen norm of $\mathbf{A}_\alpha - \mathbf{A}$:

$$\begin{aligned}
\|\mathbf{A}_\alpha - \mathbf{A}\|_1 &= \sup_{\boldsymbol{x}} \sum_{\boldsymbol{y}} \left| e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|} a(\boldsymbol{x},\boldsymbol{y}) e^{-\alpha\|\boldsymbol{y}-\boldsymbol{x}_0\|} - a(\boldsymbol{x},\boldsymbol{y}) \right| \\
&= \sup_{\boldsymbol{x}} \sum_{\boldsymbol{y}} |a(\boldsymbol{x},\boldsymbol{y})| \left(e^{\alpha(\|\boldsymbol{x}-\boldsymbol{x}_0\|-\|\boldsymbol{y}-\boldsymbol{x}_0\|)} - 1 \right) \\
&\leq \sup_{\boldsymbol{x}} \sum_{\boldsymbol{y}} |a(\boldsymbol{x},\boldsymbol{y})| \left(e^{\alpha\|\boldsymbol{x}-\boldsymbol{y}\|} - 1 \right) \\
&\leq \sup_{\boldsymbol{x}} \sum_{\boldsymbol{y}} C_1 e^{-C_2\|\boldsymbol{x}-\boldsymbol{y}\|} \alpha \|\boldsymbol{x}-\boldsymbol{y}\| e^{\alpha\|\boldsymbol{x}-\boldsymbol{y}\|}.,
\end{aligned} \tag{2.6}$$

where we in have used that $e^x - 1 - e^x x \leq 0$ for $x \in [0,\infty[$ (it is true in $x = 0$, and $e^x - 1 - e^x x$ is a decreasing function of x on $[0,\infty[$). Using an inequality of the type $\sum_{n\geq 0} e^{-2n} n^N \leq \sum_{n \geq 0} e^{-n} N!$, we can recast inequality (2.6) in the form

$$\|\mathbf{A}_\alpha - \mathbf{A}\|_1 \leq \alpha \tilde{C}_1 \sup_{\boldsymbol{x}} \sum_{\boldsymbol{y}} e^{(\alpha - \frac{C_2}{2})\|\boldsymbol{x}-\boldsymbol{y}\|}, \quad \tilde{C}_1 := \max(a_1, a_2) \cdot 16\, C_1$$

And if $\alpha < C_2/4$ the series is convergent, and we have

$$\begin{aligned}
&\|\mathbf{A}_\alpha - \mathbf{A}\|_1 \leq \alpha \cdot \tilde{C}, \\
\tilde{C} := \sup_{\boldsymbol{x}\in\Lambda} &\sum_{\boldsymbol{y}\in\Lambda} \tilde{C}_1 e^{-\frac{C_2}{4}\|\boldsymbol{x}-\boldsymbol{y}\|} = \tilde{C}_1 \sum_{\boldsymbol{y}\in\Lambda} e^{-\frac{C_2}{4}\|\boldsymbol{y}\|}.
\end{aligned}$$

which implies (2.5), and therefore implies that $(\mathbf{A}_\alpha - z)$ is invertible. A sufficient condition for the limit (2.5), on α, is therefore

$$\alpha < \frac{C_2}{4}. \tag{2.7}$$

The equality

$$e^{-\alpha|\cdot - \boldsymbol{x}_0|}(\mathbf{A}_\alpha - z) = (\mathbf{A} - z) e^{-\alpha|\cdot - \boldsymbol{x}_0|}$$

implies that

$$(\mathbf{A} - z)^{-1} e^{-\alpha|\cdot - \boldsymbol{x}_0|} = e^{-\alpha|\cdot - \boldsymbol{x}_0|}(\mathbf{A}_\alpha - z)^{-1}.$$

This implies that for arbitrarily chosen $\boldsymbol{\phi} \in \ell^2(\Lambda)$ we have

$$(\mathbf{A} - z)^{-1} e^{-\alpha\|\cdot - \boldsymbol{x}_0\|} \boldsymbol{\phi} = e^{-\alpha\|\cdot - \boldsymbol{x}_0\|}(\mathbf{A}_\alpha - z)^{-1} \boldsymbol{\phi}, \tag{2.8}$$

and therefore we can multiply the left side of (2.8) with $e^{\alpha\|\cdot - \boldsymbol{x}_0\|}$, and still have a vector in $\ell^2(\Lambda)$. This shows the equality

$$e^{\alpha\|\cdot - \boldsymbol{x}_0\|}(\mathbf{A} - z)^{-1} e^{-\alpha\|\cdot - \boldsymbol{x}_0\|} = (\mathbf{A}_\alpha - z)^{-1}.$$

If α, for a given $z \in \rho(\mathbf{A})$, is chosen to satisfy (in addition to being less than $C_2/4$)

$$\alpha(z) \leq \frac{1}{2\tilde{C}\|(\mathbf{A}-z)^{-1}\|}, \tag{2.9}$$

so

$$\|(\mathbf{A}-\mathbf{A}_\alpha)(\mathbf{A}-z)^{-1}\| = \|\mathbf{A}-\mathbf{A}_\alpha\|\|(\mathbf{A}-z)^{-1}\| \leq \alpha(z)\tilde{C}\|(\mathbf{A}-z)^{-1}\| \leq \frac{1}{2}$$

we have

$$\begin{aligned}\left\|e^{\alpha\|\cdot-\boldsymbol{x}_0\|}(\mathbf{A}-z)^{-1}e^{-\alpha\|\cdot-\boldsymbol{x}_0\|}\right\| &= \|(\mathbf{A}_\alpha-z)^{-1}\| \\ &\leq \|(\mathbf{A}-z)^{-1}\|\frac{1}{1-\|(\mathbf{A}-\mathbf{A}_\alpha)(\mathbf{A}-z)^{-1}\|} \\ &\leq 2\|(\mathbf{A}-z)^{-1}\|,\end{aligned}$$

and therefore

$$\sup_{\boldsymbol{x}_0\in\Lambda}\left\|e^{\tilde{\alpha}\|\cdot-\boldsymbol{x}_0\|}(\mathbf{A}-z)^{-1}e^{-\tilde{\alpha}\|\cdot-\boldsymbol{x}_0\|}\right\| \leq 2\|(\mathbf{A}-z)^{-1}\| = C(z) \qquad \text{if } 0 \leq \tilde{\alpha} \leq \alpha(z).$$

We examine the kernel of $(\mathbf{A}_\alpha - z)^{-1}$:

$$\begin{aligned}\langle\delta_{\boldsymbol{x}}\,,\,(\mathbf{A}_\alpha-z)^{-1}\delta_{\boldsymbol{y}}\rangle &= \left\langle\delta_{\boldsymbol{x}}\,,\,e^{\alpha\|\cdot-\boldsymbol{x}_0\|}(\mathbf{A}-z)^{-1}e^{-\alpha\|\cdot-\boldsymbol{x}_0\|}\delta_{\boldsymbol{y}}\right\rangle \\ &= e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}(\mathbf{A}-z)^{-1}(\boldsymbol{x},\boldsymbol{y})e^{-\alpha\|\boldsymbol{y}-\boldsymbol{x}_0\|},\end{aligned}$$

where we have used the properties of the delta-function. If we choose $\boldsymbol{x}_0 = \boldsymbol{y}$ we have

$$\langle\delta_{\boldsymbol{x}}\,,\,(\mathbf{A}_\alpha-z)^{-1}\delta_{\boldsymbol{x}_0}\rangle = e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}(\mathbf{A}-z)^{-1}(\boldsymbol{x},\boldsymbol{x}_0),$$

that is, using the Cauchy-Schwartz inequality, we have the final result

$$\begin{aligned}e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}\left|\left((\mathbf{A}-z)^{-1}\right)(\boldsymbol{x},\boldsymbol{x}_0)\right| &= \langle\delta_{\boldsymbol{x}}\,,\,(\mathbf{A}_\alpha-z)^{-1}\delta_{\boldsymbol{x}_0}\rangle \\ &\leq \|\delta_{\boldsymbol{x}}\|\|(\mathbf{A}_\alpha-z)^{-1}\delta_{\boldsymbol{x}_0}\| \\ &= \|(\mathbf{A}_\alpha-z)^{-1}\| \\ &\leq C(z),\end{aligned}$$

which shows that $(\mathbf{A}-z)^{-1}$ is exponentially almost diagonal.

If we restrict z to belong to a compact subset H of $\rho(\mathbf{A})$, then because of the equality

$$\|(\mathbf{A}-z)^{-1}\| = \frac{1}{\operatorname{dist}(z,\sigma(\mathbf{A}))},$$

and lemma 2.5, we can evaluate

$$\min_{z\in H}\left\{\frac{1}{\|(\mathbf{A}-z)^{-1}\|}\right\} = \min_{z\in H}\{\operatorname{dist}(z,\sigma(\mathbf{A}))\} = \operatorname{dist}(H,\sigma(\mathbf{A})).$$

This, used on the bound (2.9), leads to the z-independent bound on α:

$$\alpha_0 \leq \frac{\operatorname{dist}(H,\sigma(\mathbf{A}))}{2\tilde{C}},$$

such that for $0 \le \alpha \le \alpha_0$, we know that

$$\begin{aligned}|(\mathbf{A}-z)^{-1}(x,y)| &\le 2\sup_{z\in H}\|(\mathbf{A}-z)^{-1}\|e^{-\alpha\|\boldsymbol{x}-\boldsymbol{y}\|}\\ &= 2\sup_{z\in H}\frac{1}{\operatorname{dist}(z,\sigma(\mathbf{A}))}e^{-\alpha\|\boldsymbol{x}-\boldsymbol{y}\|}.\end{aligned}$$

□

2.2 Magnetic pertubation

the S operator

We define the operator $\mathbf{S}_{\mathrm{b}}(z)$, for $z \in \rho(\mathbf{H}_0)$ as the operator having the matrix element

$$s_{\mathrm{b}}(x,y;z) := e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}\underbrace{\left((\mathbf{H}_0-z)^{-1}\right)(x,y)}_{s_0(x,y;z)}.$$

Now we examine the matrix element $(\mathbf{H}_{\mathrm{b}}\mathbf{S}_{\mathrm{b}})(x,x')$:

$$\begin{aligned}(\mathbf{H}_{\mathrm{b}}\mathbf{S}_{\mathrm{b}})(x,x') &= \sum_{\boldsymbol{y}\in\Lambda} h_{\mathrm{b}}(x,y)s_{\mathrm{b}}(y,x';z)\\ &= \sum_{\boldsymbol{y}} e^{ib(\varphi(\boldsymbol{x},\boldsymbol{y})+\varphi(\boldsymbol{y},\boldsymbol{x}'))}h_0(x,y)s_0(y,x';z)\\ &= e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\sum_{\boldsymbol{y}}\left(1+e^{ib\,\mathrm{fl}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{x}')}-1\right)h_0(x,y)s_0(y,x';z). \qquad (2.10)\end{aligned}$$

If we introduce the operator $\mathbf{K}_{\mathrm{b}}$ with the kernel

$$k_{\mathrm{b}}(x,x';z) := e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\sum_{\boldsymbol{y}}\left(e^{ib\,\mathrm{fl}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{x}')}-1\right)h_0(x,y)s_0(y,x';z),\rho(\mathbf{H}_{\mathrm{b}})$$

and notice that

$$e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\sum_{\boldsymbol{y}}h_0(x,y)s_0(y,x';z) = e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}(\mathbf{H}_0\mathbf{S}_0)(x,x'),$$

then (2.10) has the form

$$(\mathbf{H}_{\mathrm{b}}\mathbf{S}_{\mathrm{b}})(x,x') = e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}(\mathbf{H}_0\mathbf{S}_0)(x,x') + k_{\mathrm{b}}(x,x';z). \qquad (2.11)$$

If we examine $(\mathbf{H}_0\mathbf{S}_0)(x,x')$, we see that

$$(\mathbf{H}_0\mathbf{S}_0)(x,x') = \underbrace{((\mathbf{H}_0-z\mathbb{1})\mathbf{S}_0)(x,x')}_{\delta(\boldsymbol{x},\boldsymbol{x}')} + z\,s_0(x,x')$$

which gives that (2.11) is equivalent with

$$(\mathbf{H}_{\mathrm{b}}\mathbf{S}_{\mathrm{b}})(x,x') = e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\delta(x,x') + z\,\underbrace{e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\mathbf{S}_0(x,x')}_{s_{\mathrm{b}}(\boldsymbol{x},\boldsymbol{x}')} + k_{\mathrm{b}}(x,x'),$$

or

$$((\mathbf{H}_\mathrm{b} - z)\mathbf{S}_\mathrm{b})\,(\boldsymbol{x}, \boldsymbol{x}') = \delta(\boldsymbol{x}, \boldsymbol{x}') + k_\mathrm{b}(\boldsymbol{x}, \boldsymbol{x}'),$$

that is

$$(\mathbf{H}_\mathrm{b} - z)\mathbf{S}_\mathrm{b} = \mathbb{1} + \mathbf{K}_b. \tag{2.12}$$

Using the evaluation

$$e^{ix} - 1 = e^{i\frac{x}{2}}\left(e^{i\frac{x}{2}} - e^{-i\frac{x}{2}}\right) = 2ie^{i\frac{x}{2}}\sin(\frac{x}{2}),$$
$$|e^{ix} - 1| \leq 2|\sin(\frac{x}{2})| \leq |x|,$$

for real $x \geq 0$, we evaluate the Schur-Holmgren bound for the operator norm of $\mathbf{K}_\mathrm{b}$, consider

$$\begin{aligned}
\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}|k_\mathrm{b}(\boldsymbol{x}, \boldsymbol{x}'; z)| &\leq \sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}\sum_{\boldsymbol{y}}\left|e^{ib\,\mathrm{fl}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{x}')} - 1\right||h_0(\boldsymbol{x}, \boldsymbol{y})||s_0(\boldsymbol{y}, \boldsymbol{x}'; z)| \\
&\leq \sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}\sum_{\boldsymbol{y}} b\,\mathrm{fl}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{x}')C_1 e^{-C_2\|\boldsymbol{x}-\boldsymbol{y}\|}C_3(z)e^{-C_4(z)\|\boldsymbol{y}-\boldsymbol{x}'\|} \\
&\leq b\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}\sum_{\boldsymbol{y}}|\boldsymbol{x} - \boldsymbol{y}||\boldsymbol{y} - \boldsymbol{x}'|C_1 e^{-C_2\|\boldsymbol{x}-\boldsymbol{y}\|}C_3(z)e^{-C_4(z)\|\boldsymbol{y}-\boldsymbol{x}'\|} \\
&\leq b\,C_1C_3(z)\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}\sum_{\boldsymbol{y}}\underbrace{|\boldsymbol{x} - \boldsymbol{y}|e^{-C_2\|\boldsymbol{x}-\boldsymbol{y}\|}}_{\leq C_5 e^{-C_2/2\|\boldsymbol{x}-\boldsymbol{y}\|}}\underbrace{|\boldsymbol{y} - \boldsymbol{x}'|e^{-C_4(z)\|\boldsymbol{y}-\boldsymbol{x}'\|}}_{\leq C_6 e^{-C_4(z)/2\|\boldsymbol{y}-\boldsymbol{x}'\|}}.
\end{aligned} \tag{2.13}$$

That is, there exists a z-dependent constant, $C(z)$

$$C(z) = C_1C_3(z)C_5C_6\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}\sum_{\boldsymbol{y}} e^{-\frac{C_2}{2}\|\boldsymbol{x}-\boldsymbol{y}\| - \frac{C_4(z)}{2}\|\boldsymbol{y}-\boldsymbol{x}'\|}.$$

This constant can be chosen uniformly on compact sets $M \subset \rho(\mathbf{H}_0)$:

$$\sup_{z\in M}\left\{\sup_{\boldsymbol{x}'}\sum_{\boldsymbol{x}}|k_\mathrm{b}(\boldsymbol{x}, \boldsymbol{x}'; z)|\right\} \leq bC. \tag{2.14}$$

Similarly we can show an estimate for $\sup_{\boldsymbol{x}}\sum_{\boldsymbol{x}'}|k_\mathrm{b}(\boldsymbol{x}, \boldsymbol{x}'; z)|$, and this implies, using the Schur-Holmgreen bound, that

$$\sup_{z\in M}\{\|\mathbf{K}_\mathrm{b}(z)\|\} \leq bC. \tag{2.15}$$

Stability of $\rho(\mathbf{H})$ under Peierls substitution.

Theorem 2.7. *Let $M \subset \rho(\mathbf{H}_0)$ be compact. Then there exists $b_M > 0$, sufficiently small, such that $M \subset \rho(\mathbf{H}_\mathrm{b})$ for all $0 \leq b \leq b_M$.*

Proof. We can evaluate the norm of $\mathbf{S}_\mathrm{b}$ by using the Schur-Holmgreen norm again, equivalently to the above calculations for $\mathbf{K}_\mathrm{b}$. Doing this, we show that there exists a constant C_S only dependent on M, such that

$$\|\mathbf{S}_\mathrm{b}\| \leq \|\mathbf{S}_\mathrm{b}\|_1 \leq C_\mathrm{S}, \quad \text{for all } z \in M.$$

$\mathbf{H}_\mathrm{b}$ is a self-adjoint operator with a symmetric kernel, so the spectrum of $\mathbf{H}_\mathrm{b}$ must belong to the real line. Assume that M contains a real $\lambda \neq 0$, $\lambda \in M \cap \mathbb{R}$. Note that, because the spectrum of $\mathbf{H}_\mathrm{b}$ is real, then if $\varepsilon \neq 0$, the operator $\mathbf{H}_\mathrm{b} - (\lambda + i\varepsilon)\mathbb{1}$ is invertible.

For all $z \in [\lambda - i, \lambda + i] \subset \rho(\mathbf{H}_0)$, the estimate (2.15) holds, uniformly in $\lambda \in M$. Therefore we can choose b so small that $(\mathbb{1} + opK_\mathrm{b})$ is invertible.

Substitute $z = \lambda + i\varepsilon$ into identity (2.12), and multiply on the left by $(\mathbb{1} + \mathbf{K}_\mathrm{b})^{-1}$ and on the right by $(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}$ to obtain the formula for $(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}$:

$$\mathbf{S}_\mathrm{b}(\lambda + i\varepsilon)(\mathbb{1} + \mathbf{K}_\mathrm{b})^{-1} = (\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}$$

By the use of corollary A.4 and (2.15) we can evaluate the norm of $(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}$:

$$\begin{aligned}\left\|(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}\right\| &\leq \|\mathbf{S}_\mathrm{b}(\lambda + i\varepsilon)\| \frac{1}{1 - \|bC\|} \\ &\leq C_\mathrm{S} \frac{1}{1 - \|bC\|}\end{aligned}$$

and since M is compact then by the CT-property, $\|(\mathbf{H}_0 - \lambda - i\varepsilon)^{-1}\|$ is dominated by some M dependent constant $\varepsilon \in]0, 1]$, as long as b is small enough:

$$\left\|(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}\right\| \leq \mathrm{Cst}(M).$$

for $b < b_M$ and some M dependent number $\mathrm{Cst}(M)$. The now familiar expansion

$$(\mathbf{H}_\mathrm{b} - \lambda) = \left(\mathbb{1} + i\varepsilon(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}\right)(\mathbf{H}_b - \lambda - i\varepsilon)$$

shows that $\mathbf{H}_\mathrm{b} - \lambda$ is invertible; choose small enough ε, then $\left(\mathbb{1} + i\varepsilon(\mathbf{H}_\mathrm{b} - \lambda - i\varepsilon)^{-1}\right)$ and $\mathbf{H}_b - \lambda - i\varepsilon$ are both invertible. □

Let $z \in \rho(\mathbf{H}_\mathrm{b})$. We use the identity

$$\begin{aligned}(\mathbb{1} + \mathbf{K}_\mathrm{b})^{-1} &= \sum_{n\geq 0}(-1)^n \mathbf{K}_\mathrm{b}^n = \mathbb{1} + \sum_{n \geq 1}(-1)^n \mathbf{K}_\mathrm{b}^n \\ &= \mathbb{1} + \sum_{n\geq 0}(-1)^{n+1}\mathbf{K}_\mathrm{b}^{n+1} = \mathbb{1} - \left(\sum_{n\geq 0}(-1)^n \mathbf{K}_\mathrm{b}^n\right)\mathbf{K}_\mathrm{b} \\ &= \mathbb{1} - (\mathbb{1} + \mathbf{K}_\mathrm{b})^{-1}\mathbf{K}_\mathrm{b}\end{aligned}$$

to expand $(\mathbf{H}_\mathrm{b} - z)^{-1}$:

$$\begin{aligned}(\mathbf{H}_\mathrm{b} - z)^{-1} &= \mathbf{S}_\mathrm{b}(z)(\mathbb{1} + \mathbf{K}_\mathrm{b})^{-1} \\ &= \mathbf{S}_\mathrm{b}(z)\left(\mathbb{1} - (\mathbb{1} + \mathbf{K}_\mathrm{b})^{-1}\mathbf{K}_\mathrm{b}\right) \\ &= \mathbf{S}_\mathrm{b}(z) - (\mathbf{H}_\mathrm{b} - z)^{-1}\mathbf{K}_\mathrm{b}.\end{aligned}$$

And we can iterate this one more time to obtain

$$(\mathbf{H}_\mathrm{b} - z)^{-1} = \mathbf{S}_\mathrm{b}(z) - \mathbf{S}_\mathrm{b}(z)\mathbf{K}_\mathrm{b} + \mathcal{R}_\mathrm{b}(z), \tag{2.16}$$

with the definition

$$\mathcal{R}_{\mathrm{b}}(z) := (\mathbf{H}_{\mathrm{b}} - z)^{-1}\mathbf{K}_{\mathrm{b}}^2,$$

which we will give the name "the remainder term". We prove that the remainder term is an $\mathcal{O}(b^2)$ function, in the sense of theorem 2.8.

Theorem 2.8 (Remainder term $\mathcal{O}(b^2)$)**.** *Let $M \subset \rho(\mathbf{H}_0)$ be closed. The remainder term is exponentially almost diagonal, and there exists constants $C_5 \geq 0, C_6 > 0$, such that*

$$\sup_{z\in M}\left|\mathcal{R}_{\mathrm{b}}(\boldsymbol{x},\boldsymbol{y};z)\right| \leq b^2\, C_5 e^{-C_6\|\boldsymbol{x}-\boldsymbol{y}\|}, \quad \text{for all } z \in M.$$

Proof. For $\boldsymbol{x},\boldsymbol{y} \in \Lambda$ and $z \in M$, we have the bound

$$\sup_{z\in M}\left|(\mathbf{H}_{\mathrm{b}} - z)^{-1}(\boldsymbol{x},\boldsymbol{y})\right| \leq \tilde{C}_1 e^{-\tilde{C}_2\|\boldsymbol{x}-\boldsymbol{y}\|}.$$

so if we for a small $\alpha > 0$, an arbitrarily chosen $\boldsymbol{x}_0 \in \Lambda$ and $z \in M \subset \rho H_0$ (M closed), examine the matrix element $\langle \delta_{\boldsymbol{x}}, e^{\alpha\|\cdot-\boldsymbol{x}_0\|}\mathcal{R}_{\mathrm{b}}(z)e^{-\alpha\|\cdot-\boldsymbol{x}_0\|}\delta_{\boldsymbol{y}}\rangle$:

$$\begin{aligned}
&\langle \delta_{\boldsymbol{x}}, e^{\alpha\|\cdot-\boldsymbol{x}_0\|}\mathcal{R}_{\mathrm{b}}(z)e^{-\alpha\|\cdot-\boldsymbol{x}_0\|}\delta_{\boldsymbol{x}_0}\rangle \\
&\quad= e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}\sum_{\boldsymbol{x}',\boldsymbol{x}''}[(\mathbf{H}_{\mathrm{b}} - z)^{-1}](\boldsymbol{x},\boldsymbol{x}')[\mathbf{K}_{\mathrm{b}}(z)](\boldsymbol{x}',\boldsymbol{x}'')[\mathbf{K}_{\mathrm{b}}(z)](\boldsymbol{x}'',\boldsymbol{x}_0) \\
&\quad\leq e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}\sum_{\boldsymbol{x}',\boldsymbol{x}''}\tilde{C}_1 e^{-\tilde{C}_2\|\boldsymbol{x}-\boldsymbol{x}'\|}b\tilde{C}_3(M)e^{-\tilde{C}_4(M)\|\boldsymbol{x}'-\boldsymbol{x}''\|}b\tilde{C}_3(M)e^{-\tilde{C}_4(M)\|\boldsymbol{x}''-\boldsymbol{x}_0\|} \\
&\quad\leq e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}b^2\tilde{C}_1\tilde{C}_3(M)^2\sum_{\boldsymbol{x}'}e^{-\tilde{C}_2\|\boldsymbol{x}-\boldsymbol{x}'\|}\underbrace{\sum_{\boldsymbol{x}''}e^{-\tilde{C}_4(M)\|\boldsymbol{x}'-\boldsymbol{x}''\|}e^{-\tilde{C}_4(M)\|\boldsymbol{x}''-\boldsymbol{x}_0\|}}_{\leq\tilde{C}_5\exp\left(-\tilde{C}_4/2\,\|\boldsymbol{x}'-\boldsymbol{x}_0\|\right)} \\
&\quad\leq e^{\alpha\|\boldsymbol{x}-\boldsymbol{x}_0\|}b^2\tilde{C}_1\tilde{C}_3(M)^2\tilde{C}_5\tilde{C}_6\exp\left(-\min\left\{\frac{\tilde{C}_2}{2},\frac{\tilde{C}_4}{4}\right\}\|\boldsymbol{x}-\boldsymbol{x}_0\|\right).
\end{aligned}$$

That is, by restricting $\alpha \leq \min\left\{\frac{\tilde{C}_2}{4},\frac{\tilde{C}_4}{8}\right\}$, the kernel of the remainder term is seen to be exponentially bounded, with the evaluation

$$\left|\mathcal{R}_{\mathrm{b}}(\boldsymbol{x},\boldsymbol{x}_0;z)\right| \leq b^2\tilde{C}_7(M)e^{-\min\left\{\frac{\tilde{C}_2}{4},\frac{\tilde{C}_4}{8}\right\}\|\boldsymbol{x}-\boldsymbol{x}_0\|},$$

uniformly in $z \in M$. □

2.3 Magnetic translation

We define the magnetic translation operator as the operator that transforms $\boldsymbol{\psi} \in \ell^2(\Lambda)$ according to the rule:

$$\left(\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x}) := e^{ib\varphi(\boldsymbol{x},\gamma)}\psi(\boldsymbol{x}-\gamma), \qquad \text{for all } \gamma \in \Gamma, \boldsymbol{x} \in \Lambda.$$

The magnetic translations has some properties we prove here:

Theorem 2.9. *The Hamilton operator $\mathbf{H}_{\mathrm{b}}$ commutes with $\mathcal{T}_{\mathrm{b},\gamma}$ for all $\gamma \in \Gamma$.*

Proof. $\mathbf{H}_0$ commutes with lattice translation, by construction:

$$h_0(\boldsymbol{x}+\gamma, \boldsymbol{y}+\gamma) = h_0(\boldsymbol{x}, \boldsymbol{y}) \qquad \text{for all } \gamma \in \Gamma, \boldsymbol{x}, \boldsymbol{y} \in \Lambda,$$

Consider how $\mathcal{T}_{\mathrm{b},\gamma}\mathbf{H}_\mathrm{b}$ transforms an arbitrarily chosen $\boldsymbol{\psi} \in \ell^2(\Lambda)$:

$$\begin{aligned}
\left(\mathcal{T}_{\mathrm{b},\gamma}\mathbf{H}_\mathrm{b}\boldsymbol{\psi}\right)(\boldsymbol{x}) &= e^{ib\varphi(\boldsymbol{x},\gamma)}\left(\mathbf{H}_\mathrm{b}\boldsymbol{\psi}\right)(\boldsymbol{x}-\gamma) \\
&= e^{ib\varphi(\boldsymbol{x},\gamma)}\sum_{\boldsymbol{y}}\mathbf{H}_\mathrm{b}(\boldsymbol{x}-\gamma,\boldsymbol{y})\psi(\boldsymbol{y}) \\
&= e^{ib\varphi(\boldsymbol{x},\gamma)}\sum_{\boldsymbol{y}}e^{ib\varphi(\boldsymbol{x}-\gamma,\boldsymbol{y})}\mathbf{H}_0(\boldsymbol{x}-\gamma,\boldsymbol{y})\psi(\boldsymbol{y}) \\
&= \sum_{\boldsymbol{y}}e^{ib(\varphi(\boldsymbol{x},\gamma)+\varphi(\boldsymbol{x},\boldsymbol{y})-\varphi(\gamma,\boldsymbol{y})}\mathbf{H}_0(\gamma,\boldsymbol{y}+\gamma)\psi(\boldsymbol{y}) \\
&= \sum_{\boldsymbol{y}}e^{ib\varphi(\boldsymbol{x},\boldsymbol{y}+\gamma)}\mathbf{H}_0(\gamma,\boldsymbol{y}+\gamma)e^{ib(\varphi(\boldsymbol{y},\gamma)}\psi(\boldsymbol{y})
\end{aligned}$$

and if we change the summation index by equating $\boldsymbol{x}' = \boldsymbol{y}+\gamma$, then we have

$$\left(\mathcal{T}_{\mathrm{b},\gamma}\mathbf{H}_\mathrm{b}\boldsymbol{\psi}\right)(\boldsymbol{x}) = \sum_{\boldsymbol{x}'}e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\mathbf{H}_0(\gamma,\boldsymbol{x}')e^{ib\varphi(\boldsymbol{x}'-\gamma,\gamma)}\psi(\boldsymbol{x}'-\gamma) \tag{2.17}$$

Remembering that $\varphi(\cdot,\cdot)$ has basically the same algebraic properties as a crossproduct, it is easy to see that

$$\varphi(\boldsymbol{x}'-\gamma,\gamma) = \varphi(\boldsymbol{x}',\gamma),$$

Therefore equation (2.17) reduces to

$$\begin{aligned}
\left(\mathcal{T}_{\mathrm{b},\gamma}\mathbf{H}_\mathrm{b}\boldsymbol{\psi}\right)(\boldsymbol{x}) &= \sum_{\boldsymbol{x}'}e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}')}\mathbf{H}_0(\gamma,\boldsymbol{x}')e^{ib\varphi(\boldsymbol{x}',\gamma)}\psi(\boldsymbol{x}'-\gamma) \\
&= \sum_{\boldsymbol{x}'}h_\mathrm{b}(\boldsymbol{x},\boldsymbol{x}')\left(\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x}') \\
&= \left(\mathbf{H}_\mathrm{b}\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x}),
\end{aligned}$$

which proves the theorem. □

Lemma 2.10. *The inverse of the magnetic translation operator $\mathcal{T}_{\mathrm{b},\gamma}$ (where $\gamma \in \Gamma$) is given by $\mathcal{T}_{\mathrm{b},-\gamma}$.*

$$\mathcal{T}_{\mathrm{b},\gamma}^{-1} = \mathcal{T}_{\mathrm{b},-\gamma}$$

Proof. We prove this simply by calculating how $\mathcal{T}_{\mathrm{b},-\gamma}\mathcal{T}_{\mathrm{b},\gamma}$ transform an arbitrarily chosen $\boldsymbol{\psi} \in \ell^2(\Lambda)$, using the identity $\varphi(\boldsymbol{x},-\boldsymbol{y}) = -\varphi(\boldsymbol{x},\boldsymbol{y})$):

$$\begin{aligned}
\left(\mathcal{T}_{\mathrm{b},-\gamma}\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x}) &= e^{-ib\varphi(\boldsymbol{x},\gamma)}\left(\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x}+\gamma) \\
&= e^{-ib\varphi(\boldsymbol{x},\gamma)}e^{ib\varphi(\boldsymbol{x}+\gamma,\gamma)}\psi(\boldsymbol{x}+\gamma-\gamma) \\
&= \psi(\boldsymbol{x}).
\end{aligned}$$

This proves the lemma. □

Since $\mathbf{H}_\mathrm{b}$ commutes with magnetic translations, according to theorem 2.9, and using lemma 2.10, we have the identities:

$$\mathbf{H}_\mathrm{b} = \mathcal{T}_{\mathrm{b},\gamma}\mathbf{H}_\mathrm{b}\mathcal{T}_{\mathrm{b},-\gamma}$$

and

$$\mathbf{H}_{subb} - z = \mathcal{T}_{\mathrm{b},\gamma}(\mathbf{H}_\mathrm{b} - z)\mathcal{T}_{\mathrm{b},-\gamma}. \tag{2.18}$$

Inverting the operator (2.18), we have a result for the resolvent of $\mathbf{H}_\mathrm{b}$.

Theorem 2.11. *For $z \in \rho\mathbf{H}_\mathrm{b}$ we have*

$$(\mathbf{H}_\mathrm{b} - z)^{-1} = \mathcal{T}_{\mathrm{b},\gamma}(\mathbf{H}_\mathrm{b} - z)^{-1}\mathcal{T}_{\mathrm{b},-\gamma},$$

and therefore that the resolvent also commutes with magnetic translations.

Currentoperator commutes with magnetic translations

Consider the matrix element of the current operator

$$\begin{aligned}\mathbf{j}_{1,\mathrm{b}}(\boldsymbol{x},\boldsymbol{y}) &= ih_\mathrm{b}(\boldsymbol{x},\boldsymbol{y})(y_1 - x_1)\\ &= e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}\mathbf{j}_{1,0}(\boldsymbol{x},\boldsymbol{y}),\end{aligned}$$

where we denote

$$\mathbf{j}_{1,0}(\boldsymbol{x},\boldsymbol{y}) = ih_0(\boldsymbol{x},\boldsymbol{y})(y_1 - x_1).$$

From this we deduce, that, since $h_0(\boldsymbol{x}+\gamma,\boldsymbol{y}+\gamma) = h_0(\boldsymbol{x},\boldsymbol{y})$ (for all $\gamma \in \Gamma$), $\mathbf{j}_{1,0}$ must have the same property:

$$\mathbf{j}_{1,0}(\boldsymbol{x}+\gamma,\boldsymbol{y}+\gamma) = \mathbf{j}_{1,0}(\boldsymbol{x},\boldsymbol{y}) \quad \text{for all } \gamma \in \Gamma.$$

The current operator commutes with magnetic translations, a property we state as a lemma

Lemma 2.12. *For $\gamma \in \Gamma$ we have that*

$$\mathcal{T}_{\mathrm{b},\gamma}\mathbf{j}_{1,\mathrm{b}} = \mathbf{j}_{1,\mathrm{b}}\mathcal{T}_{\mathrm{b},\gamma}$$

Proof. The proof of this is in every way similarly to the proof of theorem 2.9, so we omit it here. □

2.4 Large N limit

We return to the off-diagonal element of the conductivity tensor, $\sigma_{21,\mathrm{N}}(t=0)$.

In the Interaction picture the y-current operator is given by:

$$\tilde{\mathbf{j}}_{2\mathrm{N}}(t) = \exp\left(it\mathbf{H}_{\mathrm{b,N}}\right)\,\mathbf{j}_{2,\mathrm{N}}\,\exp\left(-it\mathbf{H}_{\mathrm{b,N}}\right),$$

we denote other operators in the interaction picture by a "tilde", for instance $\tilde{\mathbf{j}}_{1,\mathrm{N}}$, and $\tilde{\mathbf{X}}_{\nu,\mathrm{b,N}}$, $\nu = 1, 2$. Where we must take care to be inside the (DBC) so that $\exp\left(it\mathbf{H}_{\mathrm{b,N}}\right)$ is making good sense.

In the interaction picture, an power series expansion of $\tilde{\varrho}_{\mathrm{N,E}}(t = 0)$ in powers of E can be found iteratively, (under the condition that the interaction term of the Hamiltonian is wellbehaved), since $\tilde{\varrho}_{\mathrm{N,E}}(t)$ is a solution of:

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\varrho}_{\mathrm{N,E}}(t) = -i[\tilde{\mathbf{V}}_{\mathrm{N,E}}(t), \tilde{\varrho}_{\mathrm{N,E}}(t)]$$

We can transform the differential Liouville equation for $\tilde{\varrho}_{\mathrm{N,E}}(0)$ (1.10) into an integral equation:

$$\begin{aligned}\tilde{\varrho}_{\mathrm{N,E}}(0) &= \tilde{\varrho}_{\mathrm{N,E}}(t_0) + \int_{t_0}^{0} \mathrm{d}s \frac{\mathrm{d}}{\mathrm{d}s}\tilde{\varrho}_{\mathrm{N,E}}(s)\\ &= \tilde{\varrho}_{\mathrm{N,E}}(t_0) - i\int_{t_0}^{0} \mathrm{d}s[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s), \tilde{\varrho}_{\mathrm{N,E}}(s)],\end{aligned}$$

where t_0 should thought of as a negative real number of large absolute value (we will take the limit $t_0 \to -\infty$ where we require the density operator to be $f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})$, since for all t_0 we have $\exp(i\mathbf{H}_{\mathrm{N,b}}t_0)\, f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\, \exp(-i\mathbf{H}_{\mathrm{N,b}}t_0) = f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})$). We assume a unique solution exists that can be written as power series in E. We find the term linear in E by inspecting

$$\begin{aligned}\tilde{\varrho}_{\mathrm{N,E}}(0) &= \tilde{\varrho}_{\mathrm{N,E}}(t_0) - i\int_{t_0}^{0} \mathrm{d}s_1 \left[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s_1)\,,\, \tilde{\varrho}_{\mathrm{N,E}}(t_0) - i\int_{t_0}^{s_1} \mathrm{d}s_2[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s_2), \tilde{\varrho}_{\mathrm{N,E}}(s_2)]\right],\\ &= \tilde{\varrho}_{\mathrm{N,E}}(t_0) - i\int_{t_0}^{0} \mathrm{d}s_1 \left[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s_1)\,,\, \tilde{\varrho}_{\mathrm{N,E}}(t_0)\right]\\ &\quad - \int_{t_0}^{0} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2 \left[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s_1)\,,\, [\tilde{\mathbf{V}}_{\mathrm{N,E}}(s_2), \tilde{\varrho}_{\mathrm{N,E}}(s_2)]\right]\\ &= \tilde{\varrho}_{\mathrm{N,E}}(t_0) - i\int_{t_0}^{0} \mathrm{d}s_1 \left[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s_1)\,,\, \tilde{\varrho}_{\mathrm{N,E}}(t_0)\right] + \mathcal{O}(E^2),\end{aligned}$$

and in the limit $t_0 \to -\infty$ this becomes

$$\tilde{\varrho}_{\mathrm{N,E}}(0) = f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}}) - i\int_{-\infty}^{0} \mathrm{d}s \left[\tilde{\mathbf{V}}_{\mathrm{N,E}}(s)\,,\, f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right] + \mathcal{O}(E^2)\,.$$

Therefore, in the linear response approximation we set

$$\varrho_{\mathrm{N,E,lin}}(0) = \tilde{\varrho}_{\mathrm{N,E,,lin}}(0) := f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}}) - iE\int_{-\infty}^{0} \mathrm{d}s\, e^{i\omega s} \left[\tilde{\mathbf{X}}_{1\mathrm{N,E}}(s)\,,\, f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right]\,, \qquad (2.19)$$

andwe focus our attention on calculating

$$J_{2,\mathrm{b,N,,lin}}(E, t = 0) = \mathrm{Tr}_{\mathrm{N}}\left\{\varrho_{\mathrm{N,E,,lin}}(0)\frac{\mathbf{j}_{2,\mathrm{b,N}}}{|\Lambda_N|}\right\}\,.$$

By examining formulae (1.11), (1.12) and (2.19), we can single out the conduction term, and see that

$$\sigma_{\mathrm{N},12}(t = 0) = -\frac{i}{|\Lambda_N|}\int_{-\infty}^{0} \mathrm{d}s\, e^{i\omega s}\, \mathrm{Tr}_{\mathrm{N}}\{\left[\tilde{\mathbf{X}}_{1,\mathrm{b,N}}(s)\,,\, f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right]\mathbf{j}_{2,\mathrm{b,N}}\}, \qquad (2.20)$$

where we have interchanged the order of the trace and the integral (this doesn't change the sum or integral by Fubini's theorem).

The zero-field term, $J_2(0)$ is given by:

$$\begin{aligned} J_{2,\mathrm{b,N}}(0) &\propto \mathrm{Tr_N}\{f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})[\mathbf{H}_{\mathrm{N,b}}, \mathbf{X}_{2,\mathrm{N}}]\} \\ &= \mathrm{Tr_N}\{[f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}}), \mathbf{H}_{\mathrm{N,b}}]\mathbf{X}_{2,\mathrm{N}}\} \\ &= 0, \end{aligned}$$

which makes sense; no light gives no (oblique) current.

Some commutators

With the choice of hopping integrals as described in section 1.2, the first component of the current operator $i[\mathbf{T}_{\mathrm{b,N}}\,, \mathbf{X}_{1,\mathrm{N}}]$ commutes with the second component of the position operator:

$$\begin{aligned} ([\mathbf{j}_{1,\mathrm{b,N}}, \mathbf{X}_{2,\mathrm{N}}]\psi)\,(\boldsymbol{x}) &= ([i[\mathbf{T}_{\mathrm{b,,N}}\,, \mathbf{X}_{1,\mathrm{N}}]\,, \mathbf{X}_{2,\mathrm{N}}]\,\psi)\,(\boldsymbol{x}) \\ &= ([i(\mathbf{T}_{\mathrm{b,N}}\mathbf{X}_{1,\mathrm{N}}) - i(\mathbf{X}_{1,\mathrm{N}}\mathbf{T}_{\mathrm{b,N}})\,, \mathbf{X}_{2,\mathrm{N}}]\,\psi)\,(\boldsymbol{x}) \\ &= ((i(\mathbf{T}_{\mathrm{b,N}}\mathbf{X}_{1,\mathrm{N}}\mathbf{X}_{2,\mathrm{N}}) - i(\mathbf{X}_{1,\mathrm{N}}\mathbf{T}_{\mathrm{b,N}}\mathbf{X}_{2,\mathrm{N}}) - i(\mathbf{X}_{2,\mathrm{N}}\mathbf{T}_{\mathrm{b,N}}\mathbf{X}_{1,\mathrm{N}}) + i(\mathbf{X}_{2,\mathrm{N}}\mathbf{X}_{1,\mathrm{N}}\mathbf{T}_{\mathrm{b,N}}))\,\psi)\,(\boldsymbol{x}) \\ &= i\chi_{\Lambda_N}(\boldsymbol{x})\sum_y e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}t_0(\boldsymbol{x},\boldsymbol{y})(y_1y_2 - x_1y_2 - x_2y_1 + x_2x_1)\chi_{\Lambda_N}(\boldsymbol{y})\psi(\boldsymbol{y}) \\ &= i\chi_{\Lambda_N}(\boldsymbol{x})\sum_y e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}t_0(\boldsymbol{x},\boldsymbol{y})(x_1 - y_1)(x_2 - y_2)\chi_{\Lambda_N}(\boldsymbol{y})\psi(\boldsymbol{y}) \\ &= i\sum_y \chi_{\Lambda_N}(\boldsymbol{x})e^{ib\varphi(\boldsymbol{x},\boldsymbol{y})}\left(\delta_{x_1,y_1\pm a_1/2}\delta_{x_2,y_2} + \delta_{x_2,y_2\pm a_2}\delta_{x_1,y_1}\right)(x_1 - y_1)(x_2 - y_2)\chi_{\Lambda_N}(\boldsymbol{y})\psi(\boldsymbol{y}) \\ &= 0, \qquad \text{for all } \boldsymbol{x} \in \Lambda_N. \end{aligned}$$

This also hold on the full site-mesh. Doing equivalent calculations, one can see, that $([\mathbf{j}_{1,\mathrm{b,N}}, \mathbf{X}_{2,\mathrm{N}}]\psi)\,(\boldsymbol{x}) = 0$ for all $\boldsymbol{x} \in \Lambda_N$.

Using the trace-commutator rule (A.2), we see that expression (2.20) can be re-expressed as:

$$\begin{aligned} \sigma_{21,\mathrm{N}}(t=0) &= \frac{-i}{|\Lambda_N|}\int_{-\infty}^{0} \mathrm{d}s\, e^{i\omega s}\ \mathrm{Tr_N}\left\{f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\,[\mathbf{j}_{2,\mathrm{b,N}}\,, e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{X}_{1,\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}]\right\} \\ &= \frac{-i}{|\Lambda_N|}\int_{-\infty}^{0} \mathrm{d}s\, e^{i\omega s}\ \mathrm{Tr_N}\left\{[\mathbf{j}_{2,\mathrm{b,N}}\,, e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{X}_{1,\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}]\,f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,0}})\right\} \end{aligned} \qquad (2.21)$$

Now use the identity

$$e^{i\omega s} = \frac{1}{i\omega}\frac{\mathrm{d}}{\mathrm{d}s}e^{i\omega s}$$

and the partial integration rule for a function $G(s)$

$$\int_{-\infty}^{0}\frac{\mathrm{d}}{\mathrm{d}s}\left(\frac{1}{i\omega}e^{i\omega s}\right)G(s)\mathrm{d}s = \left[\frac{1}{i\omega}e^{i\omega s}G(s)\right]_{-\infty}^{0} - \int_{-\infty}^{0}\frac{1}{i\omega}e^{i\omega}G'(s)\mathrm{d}s$$

to re-express (2.21):

$$\sigma_{21,\mathrm{N}}(t=0) = \frac{-i}{|\Lambda_N|}\left[\frac{1}{i\omega}e^{i\omega s}\,\mathrm{Tr}_{\mathrm{N}}\left\{[\mathbf{j}_{2,\mathrm{b},\mathrm{N}}, e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{X}_{1,\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}]f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right\}\right]_{-\infty}^{0} + \frac{i}{|\Lambda_N|}\int_{-\infty}^{0}\mathrm{d}s\,\frac{1}{i\omega}e^{i\omega s}\frac{\mathrm{d}}{\mathrm{d}s}\left(\mathrm{Tr}_{\mathrm{N}}\left\{[\mathbf{j}_{2,\mathrm{b},\mathrm{N}}, e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{X}_{1,\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}]f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right\}\right). \tag{2.22}$$

The first term of (2.22) is zero, because:

- The $s=0$ term; the exponential factors vanish, since $s=0$, furthermore, $\mathbf{j}_{2,\mathrm{b},\mathrm{N}}$ and $\mathbf{X}_{1,\mathrm{N}}$ commute.
- The $s\to-\infty$ term; the choice of negative imaginary part of ω ensures, that $e^{i\omega s}$ tends to zero as s tends to minus infinity and the trace is performed over a finite set of sites, so it must be bounded. $i\cdot(-i|\mathrm{Im}\omega|)\cdot t = |\mathrm{Im}\omega|t \to -\infty$ as $t\to-\infty$.

The differentiating in the second term of (2.22) is done by considering that $\mathbf{j}_{2,\mathrm{b}}$ has no explicit time dependence, noticing that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{it\mathbf{H}_{\mathrm{N,b}}}\mathbf{X}_{1,\mathrm{N}}e^{-it\mathbf{H}_{\mathrm{N,b}}}\right) = e^{it\mathbf{H}_{\mathrm{N,b}}}i(\mathbf{H}_{\mathrm{N,b}}\mathbf{X}_{1,\mathrm{N}} - \mathbf{X}_{1,\mathrm{N}}\mathbf{H}_{\mathrm{N,b}})e^{-it\mathbf{H}_{\mathrm{N,b}}} = e^{it\mathbf{H}_{\mathrm{N,b}}}i[\mathbf{H}_{\mathrm{N,b}}, \mathbf{X}_{1,\mathrm{N}}]e^{-it\mathbf{H}_{\mathrm{N,b}}} = e^{it\mathbf{H}_{\mathrm{N,b}}}\mathbf{j}_{1,\mathrm{b},\mathrm{N}}e^{-it\mathbf{H}_{\mathrm{N,b}}}$$

by the definition of $\mathbf{j}_{1,\mathrm{b}}$. We thus have

$$\sigma_{21,\mathrm{N}}(t=0) = \frac{1}{\omega|\Lambda_N|}\int_{-\infty}^{0}\mathrm{d}s\,e^{i\omega s}\;\mathrm{Tr}_{\mathrm{N}}\left\{[\mathbf{j}_{2,\mathrm{b},\mathrm{N}}\,,\,e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{j}_{1,\mathrm{b},\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}]\,f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right\} = \frac{1}{\omega|\Lambda_N|}\int_{-\infty}^{0}\mathrm{d}s\,e^{i\omega s}\;\mathrm{Tr}_{\mathrm{N}}\left\{e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{j}_{1,\mathrm{b},\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}\,[f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\,,\,\mathbf{j}_{2,\mathrm{b},\mathrm{N}}]\right\},$$

where we have used the trace-commutator rule in the last equation. The problem is therefore to evaluate

$$\sigma_{21,\mathrm{N}}(t=0) = \frac{1}{\omega|\Lambda_N|}\int_{-\infty}^{0}\left(\mathrm{Tr}_{\mathrm{N}}\left\{e^{is(\omega+\mathbf{H}_{\mathrm{N,b}})}\mathbf{j}_{1,\mathrm{b},\mathrm{N}}e^{-is\mathbf{H}_{\mathrm{N,b}}}f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\mathbf{j}_{2,\mathrm{b},\mathrm{N}}\right\} - \mathrm{Tr}_{\mathrm{N}}\left\{e^{is(\omega+\mathbf{H}_{\mathrm{N,b}})}\,\mathbf{j}_{1,\mathrm{b},\mathrm{N}}\,e^{-is\mathbf{H}_{\mathrm{N,b}}}\,\mathbf{j}_{2,\mathrm{b},\mathrm{N}}\,f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\right\}\right)\mathrm{d}s. \tag{2.23}$$

By using the trace-permutation rule on the second term, and by noticing that $f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})$ and $e^{is(\omega+\mathbf{H}_{\mathrm{N,b}})}$ commute, we have

$$\sigma_{21,\mathrm{N}}(t=0) = \frac{1}{\omega|\Lambda_N|}\int_{-\infty}^{0}\left(\mathrm{Tr}_{\mathrm{N}}\left\{e^{is\mathbf{H}_{\mathrm{N,b}})}\mathbf{j}_{1,\mathrm{b},\mathrm{N}}e^{-is(\mathbf{H}_{\mathrm{N,b}}-\omega)}f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\mathbf{j}_{2,\mathrm{b},\mathrm{N}}\right\} - Tr\left\{e^{is(\omega+\mathbf{H}_{\mathrm{N,b}})}f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})\mathbf{j}_{1,\mathrm{b},\mathrm{N}}e^{is\mathbf{H}_{\mathrm{N,b}}}\mathbf{j}_{2,\mathrm{b},\mathrm{N}})\right\}\right)\mathrm{d}s$$

We can use the Cauchy integral formula to express the operator $e^{is(\omega+\mathbf{H}_{\mathrm{N,b}})}f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})$ by a curve integral in the complex plane, involving the resolvent of $\mathbf{H}_{\mathrm{N,b}}$:

$$e^{is(\omega+\mathbf{H}_{\mathrm{N,b}})}f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}}) = \frac{i}{2\pi}\oint_{\mathscr{C}}e^{is(z+\omega)}f_{\mathrm{FD}}(z)(\mathbf{H}_{\mathrm{N,b}}-z)^{-1}dz,$$

where the path $\mathscr{C}$ enclose, but has no points in common with, the (real, bounded) spectrum, $\sigma(\mathbf{H}_{0,\mathrm{N}})$, of $\mathbf{H}_{0,\mathrm{N}}$. We claim that it is possible, given ω, β and μ, to choose such a curve such that ω lies *outside* $\mathscr{C}$, and so "close" (small imaginary parts of $z \in \mathscr{C}$) to the real line, that

$$f_{\mathrm{FD}}(z) = \frac{1}{e^{\beta(z-\mu)} + 1}$$

has no singularities inside $\mathscr{C}$. ($\mu \in \mathbb{R}, \beta \in \mathbb{R}$, if $\mathrm{Re}z = \mu$, then we can make sure that $\beta \cdot \mathrm{Im}z$ cannot atain the value 2π, i.e. choose that all $z \in \mathscr{C}$ fullfills $|\mathrm{Im}z| < \frac{\pi}{2\beta}$, also ω is assumed to have a non-zero, (negative) imaginary part.) This leads to

$$\begin{aligned}
&\boldsymbol{\sigma}_{21,\mathrm{N}}(t=0) \\
&= \frac{1}{\omega|\Lambda_N|} \int_{-\infty}^{0} \mathrm{d}s \left(\mathrm{Tr}_{\mathrm{N}} \left\{ e^{is\mathbf{H}_{\mathrm{N,b}}} \mathbf{j}_{1,\mathrm{b,N}} \underbrace{\left(\frac{i}{2\pi} \oint_{\mathscr{C}} \mathrm{d}z\, e^{-is(z-\omega)} f_{\mathrm{FD}}(z) (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \right)}_{=e^{-is(\mathbf{H}_{\mathrm{N,b}}-\omega)} f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})} \mathbf{j}_{2,\mathrm{b,N}} \right\} \right. \\
&\qquad \left. - \mathrm{Tr}_{\mathrm{N}} \left\{ \underbrace{\left(\frac{i}{2\pi} \oint_{\mathscr{C}} \mathrm{d}z\, e^{is(z+\omega)} f_{\mathrm{FD}}(z) (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \right)}_{=e^{is(\mathbf{H}_{\mathrm{N,b}}+\omega)} f_{\mathrm{FD}}(\mathbf{H}_{\mathrm{N,b}})} \mathbf{j}_{1,\mathrm{b,N}}\, e^{-is\mathbf{H}_{\mathrm{N,b}}}\, \mathbf{j}_{2,\mathrm{b,N}} \right\} \right)
\end{aligned} \tag{2.24}$$

. The two integrals, $\oint_{\mathscr{C}} \mathrm{d}z \cdots$ and $\int_{-\infty}^{0} \mathrm{d}s \cdots$ in equation (2.24) are both absolutely convergent, therefore we can exchange integration order (Fubini). Furthermore, as $e^{\pm is(z \pm \omega)}$ is nothing but a complex scalar, we can freely place this factor in the operator product,

$$\begin{aligned}
&\boldsymbol{\sigma}_{21,\mathrm{N}}(t=0) \\
&= \frac{1}{\omega|\Lambda_N|} \oint_{\mathscr{C}} \mathrm{d}z \int_{-\infty}^{0} \mathrm{d}s \left(\mathrm{Tr}_{\mathrm{N}} \left\{ e^{is(\mathbf{H}_{\mathrm{N,b}}-z+\omega)} \mathbf{j}_{1,\mathrm{b,N}} \frac{i}{2\pi} f_{\mathrm{FD}}(z) (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b,N}} \right\} \right. \\
&\qquad \left. - \mathrm{Tr}_{\mathrm{N}} \left\{ \frac{i}{2\pi} f_{\mathrm{FD}}(z) (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \mathbf{j}_{1,\mathrm{b,N}} e^{is(z+\omega-\mathbf{H}_{\mathrm{N,b}})} \mathbf{j}_{2,\mathrm{b,N}} \right\} \right).
\end{aligned}$$

We now evaluate the (time) integration:

$$\begin{aligned}
\int_{-\infty}^{0} \mathrm{d}s\, e^{is(z+\omega-\mathbf{H}_{\mathrm{N,b}})} &= \left[\left(i((z+\omega) - \mathbf{H}_{\mathrm{N,b}}) \right)^{-1} e^{is(z+\omega-\mathbf{H}_{\mathrm{N,b}})} \right]_{-\infty}^{0}, \\
&= \left(i((z+\omega) - \mathbf{H}_{\mathrm{N,b}}) \right)^{-1} \\
&= i\, \left(\mathbf{H}_{\mathrm{N,b}} - z - \omega \right)^{-1}
\end{aligned}$$

and similar for $\int_{-\infty}^{0} \frac{\mathrm{d}d}{\mathrm{d}s}\, e^{is(\mathbf{H}_{\mathrm{N,b}}-(z-\omega))} = \left(i(\mathbf{H}_{\mathrm{N,b}} - z + \omega) \right)^{-1}$. Where we note that for

$z \in \mathscr{C}$, $z \pm \omega$ cannot be in the spectrum for $\mathbf{H}_{\mathrm{N,b}}$. This lead to the formula for $\sigma_{xy}(0)$

$$\begin{aligned}
&\sigma_{21,\mathrm{N}}(t=0) = \\
&= \frac{1}{\omega|\Lambda_N|} \oint_{\mathscr{C}} \mathrm{d}z \ \Bigg(\mathrm{Tr}_{\mathrm{N}} \left\{ (-i) \left(\mathbf{H}_{\mathrm{N,b}} - z + \omega\right)^{-1} \mathbf{j}_{1,\mathrm{b,N}} \frac{i}{2\pi} f_{\mathrm{FD}}(z) (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b,N}} \right\} \\
&\qquad - \mathrm{Tr}_{\mathrm{N}} \left\{ \frac{i}{2\pi} f_{\mathrm{FD}}(z) (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \mathbf{j}_{1,\mathrm{b,N}}\, i \left(\mathbf{H}_{\mathrm{N,b}} - z - \omega\right)^{-1} \mathbf{j}_{2,\mathrm{b,N}} \right\} \Bigg) \\
&= \frac{1}{2\pi\omega|\Lambda_N|} \oint_{\mathscr{C}} \mathrm{d}z \ f_{\mathrm{FD}}(z) \Big(\mathrm{Tr}_{\mathrm{N}} \left\{ \left(\mathbf{H}_{\mathrm{N,b}} - z + \omega\right)^{-1} \mathbf{j}_{1,\mathrm{b,N}} (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b,N}} \right\} \\
&\qquad + \mathrm{Tr}_{\mathrm{N}} \left\{ (\mathbf{H}_{\mathrm{N,b}} - z)^{-1} \mathbf{j}_{1,\mathrm{b,N}} \left(\mathbf{H}_{\mathrm{N,b}} - z - \omega\right)^{-1} \mathbf{j}_{2,\mathrm{b,N}} \right\} \Big)
\end{aligned} \tag{2.25}$$

Dealing with Dirichlet

Now we would like to get rid of the Dirichlet boundary condition. Let ε be a number between 0 and 1, $0 < \varepsilon < 1$. We divide the central region, Λ_N, up into a N^ε unit cells wide rim, $\tilde{\tilde{\Lambda}}_N$,, and a core part, a square, $2(N - N^\varepsilon) + 1$, unit cells wide, figure 2.1[1].

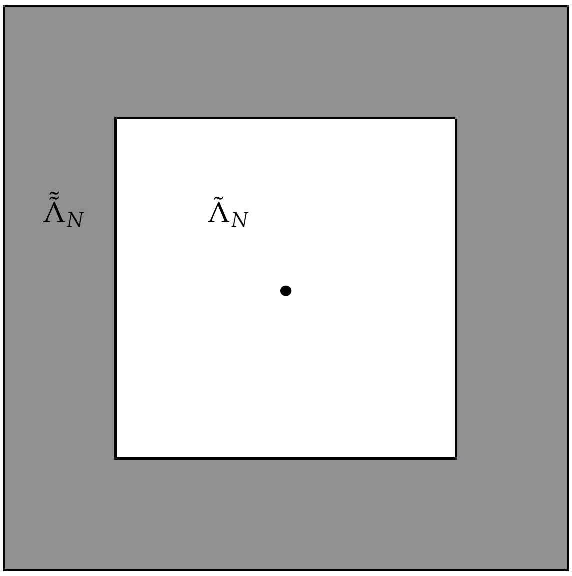

Figure 2.1: We divide the central region, Λ_N, up into a rim $\tilde{\tilde{\Lambda}}_N$, N^ε unit cells wide, and a core part $\tilde{\Lambda}_N$, $2(N - N^\varepsilon) + 1$, unit cells wide. $0 < \varepsilon < 1$

The different parts of Λ_N relate to each other by the formula:

$$\tilde{\tilde{\Lambda}}_N = \Lambda_N \setminus \tilde{\Lambda}_N.$$

The number of sites in $\tilde{\tilde{\Lambda}}_N$ is dominated by N^2,

$$\frac{|\tilde{\tilde{\Lambda}}_N|}{N^2} \to 0, \quad N \to \infty,$$

[1]Of course, it makes no sense to take a non-integer number of unit cells, so in practice, take the floor of the number N^ε. In the large N regime, which is the interesting case for this presentation, this makes no difference in the limits we are to examine.

as a consequence of the choice of ε, whereas the number of sites in $\tilde{\Lambda}_N$ converge to $4N^2$:

$$(2(N - N^{\varepsilon}) + 1)^2 = 4N^2 \left(1 - \frac{1}{N^{1-\varepsilon}} + \frac{1}{2N}\right)^2 \to 4N^2, \quad N \to \infty.$$

Some auxilliary operators

To simplify notation and maximize readability, we introduce a shorthand for the characteristic functions for Λ_N, $\tilde{\Lambda}_N$ and $\tilde{\tilde{\Lambda}}_N$:

$$\begin{aligned}\chi_{\mathrm{N}} &:= \chi_{\Lambda_N},\\ \tilde{\chi}_{\mathrm{N}} &:= \chi_{\tilde{\Lambda}_N},\\ \tilde{\tilde{\chi}}_{\mathrm{N}} &:= \chi_{\tilde{\tilde{\Lambda}}_N}.\end{aligned}$$

We now introduce a new auxilliary operator by the definition:

$$\mathbf{A}_{\mathrm{b,N}}(z) := \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \tilde{\chi}_{\mathrm{N}} + \tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}}.$$

We can express the resolvent $\left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1}$ in terms of $\left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1}$ and different characteristic functions, as a step towards taking the large N limit.

If we multiply $\mathbf{A}_{\mathrm{b,N}}(z)$ on the left by $(\mathbf{H}_{\mathrm{b,N}} - z)$, we have

$$(\mathbf{H}_{\mathrm{b,N}} - z)\, \mathbf{A}_{\mathrm{b,N}}(z) = (\mathbf{H}_{\mathrm{b,N}} - z)\, \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \tilde{\chi}_{\mathrm{N}} + (\mathbf{H}_{\mathrm{b,N}} - z)\, \tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}}. \tag{2.26}$$

Note that for large N, the nn-interaction property of $\mathbf{H}_{\mathrm{b,N}}$ implies that $(\mathbf{H}_{\mathrm{b,N}} - z)\, \tilde{\chi}_{\mathrm{N}} = (\mathbf{H}_{\mathrm{b}} - z)\, \tilde{\chi}_{\mathrm{N}}$. Therefore, if we use this in the first term of formula (2.26), and then commute $(\mathbf{H}_{\mathrm{b}} - z)$ and $\tilde{\chi}_{\mathrm{N}}$, we have:

$$(\mathbf{H}_{\mathrm{b,N}} - z)\, \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \tilde{\chi}_{\mathrm{N}} = [\mathbf{H}_{\mathrm{b}}, \tilde{\chi}_{\mathrm{N}}] \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \tilde{\chi}_{\mathrm{N}} + \tilde{\chi}_{\mathrm{N}}. \tag{2.27}$$

Similarly we commute $\mathbf{H}_{\mathrm{b,N}}$ and $\tilde{\tilde{\chi}}_{\mathrm{N}}$ in the second term of formula (2.26) to get:

$$(\mathbf{H}_{\mathrm{b,N}} - z)\, \tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}} = [\mathbf{H}_{\mathrm{b,N}}, \tilde{\tilde{\chi}}_{\mathrm{N}}] \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}} + \tilde{\tilde{\chi}}_{\mathrm{N}}.. \tag{2.28}$$

Combining, and noticing that $\tilde{\chi}_{\mathrm{N}} + \tilde{\tilde{\chi}}_{\mathrm{N}} = \chi_{\mathrm{N}}$, we have the expression for (2.26):

$$(\mathbf{H}_{\mathrm{b,N}} - z)\, \mathbf{A}_{\mathrm{b,N}}(z) = \chi_{\mathrm{N}} + [\mathbf{H}_{\mathrm{b}}, \tilde{\chi}_{\mathrm{N}}] \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \tilde{\chi}_{\mathrm{N}} + [\mathbf{H}_{\mathrm{b,N}}, \tilde{\tilde{\chi}}_{\mathrm{N}}] \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}},$$

which is equivalent with (we off course choose $z \in \rho(\mathbf{H}_{\mathrm{b}})$, so $(\mathbf{H}_{\mathrm{b,N}} - z)$ is invertible...):

$$\left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \chi_{\mathrm{N}} = \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} = \mathbf{A}_{\mathrm{b,N}}(z) - \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \mathbf{B}_{\mathrm{b,N}}(z), \tag{2.29}$$

where we have collected the terms with commutators in the definition

$$\mathbf{B}_{\mathrm{b,N}}(z) := [\mathbf{H}_{\mathrm{b}}, \tilde{\chi}_{\mathrm{N}}] \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \tilde{\chi}_{\mathrm{N}} + [\mathbf{H}_{\mathrm{b,N}}, \tilde{\tilde{\chi}}_{\mathrm{N}}] \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}}.$$

Since we in the trace in formula (2.25) we only sum over Λ_N, in this trace we omit χ_{N} on the left side of equation (2.29). If we therefore substitute

$$(\mathbf{H}_{\mathrm{b,N}} - z)^{-1} = \mathbf{A}_{\mathrm{b,N}}(z) - (\mathbf{H}_{\mathrm{b,N}} - z)^{-1}\, \mathbf{B}_{\mathrm{b,N}}(z),$$

into the formula for the off-diagonal part of the conductivity, formula (2.25), for $z = z$ and $z = z \pm \omega$, we then get a lot off different terms. We claim that only one of these terms contribute in the large N limit, that is the term:

$$\frac{1}{2\pi\omega|\Lambda_N|} \oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \Big(\mathrm{Tr}_{\mathrm{N}} \left\{ \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} \tilde{\chi}_{\mathrm{N}} \mathbf{j}_{\mathrm{N},1} \tilde{\chi}_{\mathrm{N}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \tilde{\chi}_{\mathrm{N}} \mathbf{j}_{\mathrm{N},2} \right\} \\ + \mathrm{Tr}_{\mathrm{N}} \left\{ \tilde{\chi}_{\mathrm{N}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \tilde{\chi}_{\mathrm{N}} \mathbf{j}_{\mathrm{N},1} \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z - \omega\right)^{-1} \tilde{\chi}_{\mathrm{N}} \mathbf{j}_{\mathrm{N},2} \right\} \Big).$$

The other terms all have factors of type $\tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1}$, $[\mathbf{H}_{\mathrm{b}}, \tilde{\chi}_{\mathrm{N}}]$ or $[\mathbf{H}_{\mathrm{b,N}}, \tilde{\tilde{\chi}}_{\mathrm{N}}]$. In the large N limit terms having these factors vanish, which we explain in the following.

First three kind of junk terms

The $\tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1}$ type factors:
By the trace permutation rule, it is enough to examine terms of the type

$$\frac{1}{|\Lambda_N|} \mathrm{Tr}_{\mathrm{N}} \left\{ \tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1} \cdots \right\} \propto \frac{1}{|\Lambda_N|} \sum_{x \in \tilde{\tilde{\Lambda}}_N} \{\cdots\}(\boldsymbol{x}, \boldsymbol{x}).$$

One example is

$$\frac{1}{|\Lambda_N|} \mathrm{Tr}_{\mathrm{N}} \left\{ (\mathbf{H}_{\mathrm{b,N}} - z + \omega)^{-1} \tilde{\tilde{\chi}}_{\mathrm{N}} \mathbf{j}_{1,b,\mathrm{N}} \tilde{\chi}_{\mathrm{N}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \tilde{\chi}_{\mathrm{N}} \mathbf{j}_{2,b,\mathrm{N}} \right\}. \tag{2.30}$$

By the definition of $\mathbf{j}_{1,\mathrm{b}}$, we have the kernel element for the first current factor given as $\mathbf{j}_{1,\mathrm{b}}(\boldsymbol{x}, \boldsymbol{y}) = \mathbf{H}_{\mathrm{b}}(\boldsymbol{x}, \boldsymbol{y})(y_1 - x_1))$, where the zero-field (nn) Hamiltonian, $\mathbf{H}_{\mathrm{b}}$ is known to be bounded. Similarly for $\mathbf{j}_{2,\mathrm{b}}$, $\mathbf{j}_{2,\mathrm{b}}(\boldsymbol{x}, \boldsymbol{y}) = \mathbf{H}_{\mathrm{b}}(\boldsymbol{x}, \boldsymbol{y})(y_2 - x_2))$. Now, we also know that the kernel elements of the resolvent $(\mathbf{H}_{\mathrm{b,N}} - z)^{-1}$ decays exponentially and are bounded. The sum defining the trace (2.30) is therefore absolutely bounded by the sum (by omitting some characteristic functions, we can only add to the sum of non-negative numbers.)

$$\sum_{\substack{x \in \tilde{\tilde{\Lambda}}_N \\ x''', x'', x' \in \Lambda_N}} \left| \left[(\mathbf{H}_{\mathrm{N,N}} - z + \omega)^{-1} \right] (\boldsymbol{x}, \boldsymbol{x}') \mathbf{j}_{1,\mathrm{b,N}}(\boldsymbol{x}', \boldsymbol{x}'') \left[(\mathbf{H}_{\mathrm{N}} - z)^{-1} \right] (\boldsymbol{x}'', \boldsymbol{x}''') \mathbf{j}_{2,\mathrm{b,N}}(\boldsymbol{x}''', \boldsymbol{x}) \right|$$
$$\leq \sum_{\substack{x \in \tilde{\tilde{\Lambda}}_N \\ x''', x'', x' \in \Lambda}} C_1 e^{-C_2\|\boldsymbol{x} - \boldsymbol{x}'\|} \mathbf{H}_{\mathrm{b}}(\boldsymbol{x}', \boldsymbol{x}'') |x_1'' - x_1'| C_3 e^{-C_4\|\boldsymbol{x}'' - \boldsymbol{x}'''\|} \mathbf{H}_{\mathrm{b}}(\boldsymbol{x}''', \boldsymbol{x}) |x_2 - x_2'''|.$$

For N-independent constants C_i, $i = 1, 2, 3, 4$. By using evaluations of the type

$$\mathbf{H}_{\mathrm{b}}(\boldsymbol{x}', \boldsymbol{x}'') |x_1'' - x_1'| \leq C_5 \exp(-c_6 \|\boldsymbol{x}' - \boldsymbol{x}''\|) \|\boldsymbol{x}' - \boldsymbol{x}''\|,$$

for constants C_5 and C_6, and the sum rule $\sum e^{-2Cn} n \leq \sum e^{-Cn}$, we see that all terms are exponentially located, so each sub-sub for a fixed $\boldsymbol{x} \in \tilde{\Lambda}_N$ is convergent and bounded, uniformly in N. This is supposing z and ω is chosen appropriately - according to the restrictions mentioned earlier. For each N we have finitely many sites in $\tilde{\tilde{\Lambda}}_N$ to sum over, so the sum converges, and even if the number of sites inside $\tilde{\tilde{\Lambda}}_N$ grow as $N \cdot N^{\varepsilon}$, this number is dominated by the factor $|\Lambda_N|^{-1} \propto N^{-2}$, the crucial piece of information being $\varepsilon < 1$:

$$\left|\frac{1}{|\Lambda_N|}\mathrm{Tr_N}\left\{\tilde{\tilde{\chi}}_\mathrm{N}\left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1}\cdots\right\}\right| \le \frac{1}{|\Lambda_N|}(|\tilde{\tilde{\Lambda}}_N|\cdot \mathrm{Cst.}) \to 0, \quad N \to \infty.$$

Therefore all these types of terms goes to zero in the large N limit.

The $[\mathbf{H}_\mathrm{b}, \tilde{\chi}_\mathrm{N}]$ *type factors:*
Again, we can use the trace-permutation rule and need only look at terms of the type

$$\frac{1}{|\Lambda_N|}\mathrm{Tr_N}\left\{[\mathbf{H}_\mathrm{b}, \tilde{\chi}_\mathrm{N}]\cdots\right\}.$$

We introduce another subset of the central region, a band centered on the edge of $\tilde{\Lambda}_N$ of width 10 unit cells as sketched in figure 2.2, we denote this subset $\partial\tilde{\Lambda}_N$. Now we claim

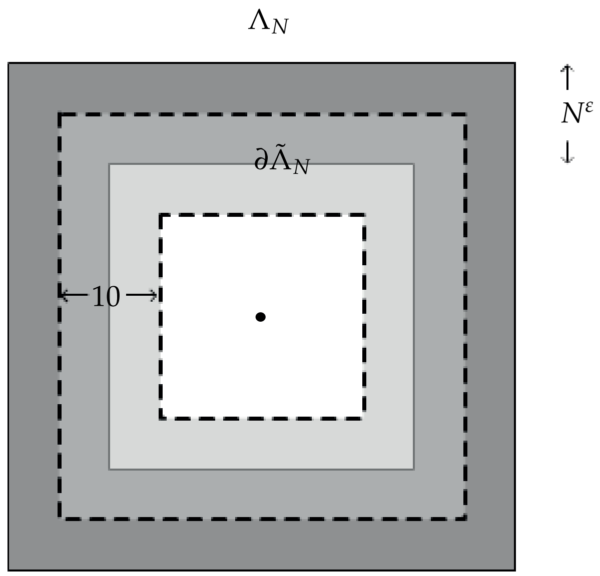

Figure 2.2: $\partial\tilde{\Lambda}_N$ is a 10 unit cell wide band centered on the edge of $\tilde{\Lambda}_N$.

that for $[\mathbf{H}_\mathrm{b}, \tilde{\chi}_\mathrm{N}]$-type factors, it suffices to sum over $\partial\tilde{\Lambda}_N$ in the trace. This is due to the equality

$$[\mathbf{H}_\mathrm{b}, \tilde{\chi}_\mathrm{N}](\boldsymbol{x}, \boldsymbol{y}) = \mathbf{H}_\mathrm{b}(\boldsymbol{x}, \boldsymbol{y})(\tilde{\chi}_\mathrm{N}(\boldsymbol{y}) - \tilde{\chi}_\mathrm{N}(\boldsymbol{x})).$$

The factor $(\tilde{\chi}_\mathrm{N}(\boldsymbol{y}) - \tilde{\chi}_\mathrm{N}(\boldsymbol{x}))$ is zero unless one of $\boldsymbol{x}$ or $\boldsymbol{y}$ falls in $\tilde{\Lambda}_N$ and the other in $\tilde{\tilde{\Lambda}}_N$. The nearest neighbour form of the Hamiltonian makes the matrix element $\mathbf{H}_\mathrm{b}(\boldsymbol{x}, \boldsymbol{y})$ be zero unless both $\|\boldsymbol{x} - \boldsymbol{y}\|$ is less than, say $2a$ (depending on the choice of hopping matrix elements in the tb-model). This proves the claim.

Again the subsum of the trace-sum for each fixed $\boldsymbol{x}$ in $\partial\tilde{\Lambda}_N$ is absolutely bounded, uniformely in N. (since we sum over kernel elements of an operator that is the product of exponentially almost diagonal operators). The number of sites in $\partial\tilde{\Lambda}_N$ grows as N whereas we divide by a factor proportional to N^2, so terms of this type must also vanish in the large N limit.

The $[\mathbf{H}_{\mathrm{b,N}}, \tilde{\tilde{\chi}}_{\mathrm{N}}]$ *type factors:*
The reason why $[\mathbf{H}_{\mathrm{b,N}}, \tilde{\tilde{\chi}}_{\mathrm{N}}]$-type factorsvanish in the large N limit is the same as for $[\mathbf{H}_{\mathrm{b}}, \tilde{\chi}_{\mathrm{N}}]$ type factors (above), only with the band $\partial\tilde{\tilde{\Lambda}}_N$ (see figure 2.3) instead of $\partial\tilde{\Lambda}_N$.

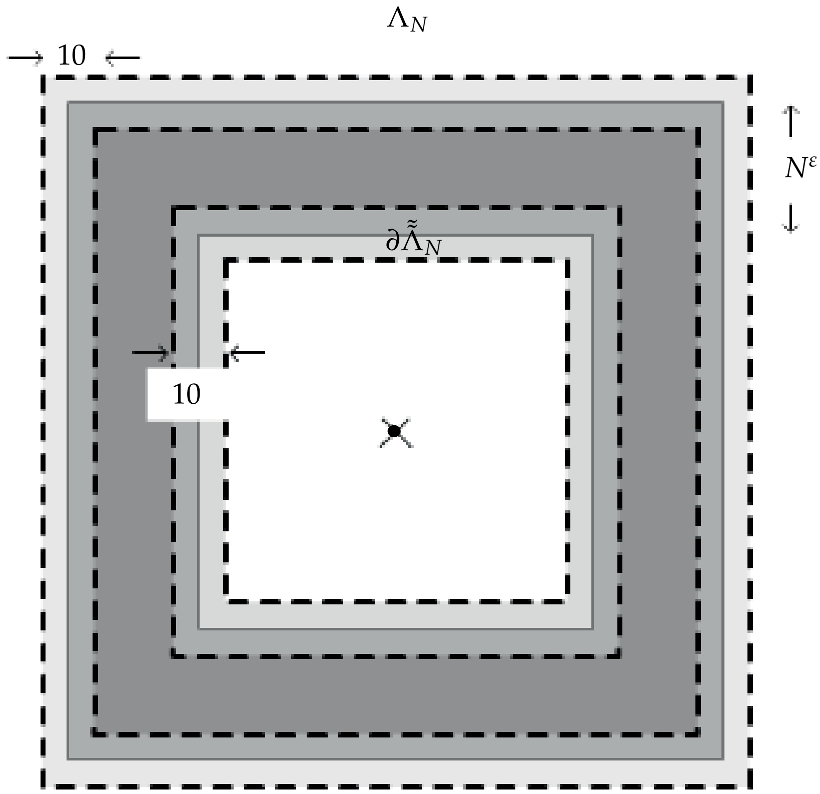

Figure 2.3: $\partial\tilde{\tilde{\Lambda}}_N$ is a 10 unit cell wide band centered on the inner and outher edges of $\tilde{\tilde{\Lambda}}_N$.

Removing more remainder terms

If a term has more than one of these first three types of "junk" terms, then it will vanish even more rapidly as N increases. We are left with one term, given by formula (2.32). We rewrite

$$\tilde{\chi}_{\mathrm{N}} = \mathbb{1} - (\mathbb{1} - \tilde{\chi}_{\mathrm{N}}),$$

and inserting this into (2.32), we have that the first trace of (2.32) is given by:

$$\frac{1}{|\Lambda_N|}\,\mathrm{Tr}\left\{\tilde{\chi}_{\mathrm{N}}\,(\mathbf{H}_{\mathrm{b}} - z + \omega)^{-1}\,\underbrace{\tilde{\chi}_{\mathrm{N}}\,\mathbf{j}_{1,\mathrm{b,N}}\,\tilde{\chi}_{\mathrm{N}}}_{=\tilde{\chi}_{\mathrm{N}}\mathbf{j}_{1,\mathrm{b}}\tilde{\chi}_{\mathrm{N}}}\,(\mathbf{H}_{\mathrm{b}} - z)^{-1}\,\underbrace{\tilde{\chi}_{\mathrm{N}}\,\mathbf{j}_{2,\mathrm{b,N}}}_{=\tilde{\chi}_{\mathrm{N}}\,\mathbf{j}_{2,\mathrm{b}}\,\tilde{\chi}_{\mathrm{N}}}\right\}$$

We notice that

$$\tilde{\chi}_{\mathrm{N}} \mathbf{j}_{1,\mathrm{b,N}} \tilde{\chi}_{\mathrm{N}} = \tilde{\chi}_{\mathrm{N}} \mathbf{j}_{1,\mathrm{b}} \tilde{\chi}_{\mathrm{N}},$$

by same arguments as above, so we consider the trace

$$\begin{aligned} \frac{1}{|\Lambda_N|} \operatorname{Tr} \Big\{ & \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} \left(\mathbb{1} - (\mathbb{1} - \tilde{\chi}_{\mathrm{N}})\right) \mathbf{j}_{1,\mathrm{b}} \times \cdots \\ & \times \left(\mathbb{1} - (\mathbb{1} - \tilde{\chi}_{\mathrm{N}})\right) \left(\mathbf{H}_{\mathrm{b}} - z\right)^{-1} \left(\mathbb{1} - (\mathbb{1} - \tilde{\chi}_{\mathrm{N}})\right) \mathbf{j}_{2,\mathrm{b}} \tilde{\chi}_{\mathrm{N}} \Big\}, \end{aligned} \tag{2.31}$$

this trace consists of the main term

$$\frac{1}{|\Lambda_N|} \operatorname{Tr} \left\{ \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} \mathbf{j}_{1,\mathrm{b}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b}} \right\},$$

and remainder terms

$$-\frac{1}{|\Lambda_N|} \operatorname{Tr} \left\{ \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} (\mathbb{1} - \tilde{\chi}_{\mathrm{N}}) \mathbf{j}_{1,\mathrm{b}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b}} \right\} + \cdots$$

All the remainder terms have at least one factor of the type

$$\mathbb{1} - \tilde{\chi}_{\mathrm{N}} = \mathbb{1} - \chi_{\mathrm{N}} + \tilde{\tilde{\chi}}_{\mathrm{N}}$$

where $\mathbb{1} - \chi_{\mathrm{N}}$ is the characteristic function of the complementary set of Λ_N. The terms arising from $\tilde{\tilde{\chi}}_{\mathrm{N}}$ part can be brought to the form

$$-\frac{1}{|\Lambda_N|} \operatorname{Tr} \left\{ \tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} \times \cdots \right\}$$

which is a $\tilde{\tilde{\chi}}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b,N}} - z\right)^{-1}$ type factor, and vanishes in the large N limit.

The term arising from the $\mathbb{1} - \chi_{\mathrm{N}}$ part also goes to zero, because resolvent kernel elements sanwiched between $\mathbb{1} - \chi_{\mathrm{N}}$ and $\tilde{\chi}_{\mathrm{N}}$ is evaluated at pairs of sitepoints seperated by at least N^{ε} unit cells, and therefore the sum terms are absolutely bounded by terms with a factor of $e^{-CN^{\varepsilon}}$ which dominates the number of sites summed over($\propto N^2$), so terms of this type also goes to zero as $N \to \infty$.

Reducing the problem to the unit cell

According to the above and formula (2.32), the only non-vanishing contribution to the off-diagonal conduction element in the large N-limit isgiven by

$$\begin{aligned} \frac{1}{2\pi\omega|\Lambda_N|} \oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \Big(& \operatorname{Tr} \left\{ \tilde{\chi}_{\mathrm{N}} \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} \mathbf{j}_{1,\mathrm{b}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b}} \tilde{\chi}_{\mathrm{N}} \right\} \\ & + \operatorname{Tr} \left\{ \tilde{\chi}_{\mathrm{N}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{1,\mathrm{b}} \left(\mathbf{H}_{\mathrm{b}} - z - \omega\right)^{-1} \mathbf{j}_{2,\mathrm{b}} \tilde{\chi}_{\mathrm{N}} \right\} \Big). \end{aligned} \tag{2.32}$$

We now introduce further notational simplifications

$$\mathbf{D}_{\mathrm{b},+}(z) := \left(\mathbf{H}_{\mathrm{b}} - z + \omega\right)^{-1} \mathbf{j}_{1,\mathrm{b}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b}} \tag{2.33a}$$

$$\mathbf{D}_{\mathrm{b},-}(z) := (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{1,\mathrm{b}} \left(\mathbf{H}_{\mathrm{b}} - z - \omega\right)^{-1} \mathbf{j}_{2,\mathrm{b}} \tag{2.33b}$$

So, using this notation, we wish to calculate the traces

$$\frac{1}{|\Lambda_N|}\sum_{\boldsymbol{x}\in\tilde{\Lambda}_N}\mathbf{D}_{\mathrm{b},+}(\boldsymbol{x},\boldsymbol{x};z)+\frac{1}{|\Lambda_N|}\sum_{\boldsymbol{x}\in\tilde{\Lambda}_N}\mathbf{D}_{\mathrm{b},-}(\boldsymbol{x},\boldsymbol{x};z) \tag{2.34}$$

By theorem and theorem, $\mathbf{D}_{\mathrm{b},\pm}(z)$ is a operator product of operators that all commute with magnetic translations, so $\mathbf{D}_{\mathrm{b},\pm}(z)$ must also commute with magnetic translations. This leads to the important lemma

Lemma 2.13. *For $\underline{x}\in\Omega$, and $\gamma\in\Gamma$, we have that*

$$\mathbf{D}_{\mathrm{b},\pm}(\underline{x}+\gamma,\underline{x}+\gamma;z)=\mathbf{D}_{\mathrm{b},\pm}(\underline{x},\underline{x};z).$$

Proof. Let γ be a fixed vector in Γ. We calculate how the operator $\mathbf{D}_{\mathrm{b},\pm}\mathcal{T}_{\mathrm{b},\gamma}$ and $\mathcal{T}_{\mathrm{b},\gamma}\mathbf{D}_{\mathrm{b},\pm}$ transforms an arbitrarily chosen vector $\boldsymbol{\psi}$ in $\ell^2(\Lambda)$ (nowing that the two calculations should be equal since $\mathbf{D}_{\mathrm{b},\pm}$ commutes with $\mathcal{T}_{\mathrm{b},\gamma}$).

$$\left(\mathbf{D}_{\mathrm{b},\pm}\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x})=\sum_{\boldsymbol{y}}\mathbf{D}_{\mathrm{b},\pm}(\boldsymbol{x},\boldsymbol{y};z)e^{ib\varphi(\boldsymbol{y},\gamma)}\psi(\boldsymbol{y}-\gamma) \tag{2.35}$$

with the definition $\boldsymbol{x}':=\boldsymbol{y}-\gamma$ this is equal to

$$\left(\mathbf{D}_{\mathrm{b},\pm}\mathcal{T}_{\mathrm{b},\gamma}\boldsymbol{\psi}\right)(\boldsymbol{x})=\sum_{\boldsymbol{x}'}\mathbf{D}_{\mathrm{b},\pm}(\boldsymbol{x},\boldsymbol{x}'+\gamma;z)e^{ib\varphi(\boldsymbol{x}'+\gamma,\gamma)}\psi(\boldsymbol{x}') \tag{2.36}$$

Calculating $\mathcal{T}_{\mathrm{b},\gamma}\mathbf{D}_{\mathrm{b},\pm}$ gives

$$\begin{aligned}\left(\mathcal{T}_{\mathrm{b},\gamma}\mathbf{D}_{\mathrm{b},\pm}\boldsymbol{\psi}\right)(\boldsymbol{x})&=e^{ib\varphi(\boldsymbol{x},\gamma)}\left(\mathbf{D}_{\mathrm{b},\pm}\boldsymbol{\psi}\right)(\boldsymbol{x}-\gamma)\\&=\sum_{\boldsymbol{x}'}e^{ib\varphi(\boldsymbol{x},\gamma)}\mathbf{D}_{\mathrm{b},\pm}(\boldsymbol{x}-\gamma,\boldsymbol{x}';z)\psi(\boldsymbol{x}')\end{aligned}$$

These equations must be true for all $\boldsymbol{\psi}$, so taking $\boldsymbol{\psi}=\delta_{\underline{x}-\gamma}$ for a fixed $\underline{x}\in\Omega$, we have

$$\mathbf{D}_{\mathrm{b},\pm}(\boldsymbol{x},\underline{x};z)e^{ib\varphi(\underline{x},\gamma)}=e^{ib\varphi(\boldsymbol{x},\gamma)}\mathbf{D}_{\mathrm{b},\pm}(\boldsymbol{x}-\gamma,\underline{x}-\gamma;z)$$

and taking $\boldsymbol{x}=\underline{x}$ we have the desired result. □

Now it is easy to see, that we only need to take the trace over the *unit cell*, in the trace (2.34):

$$\begin{aligned}&\frac{1}{|\Lambda_N|}\sum_{\boldsymbol{x}\in\tilde{\Lambda}_N}\mathbf{D}_{\mathrm{b},+}(\boldsymbol{x},\boldsymbol{x};z)+\frac{1}{|\Lambda_N|}\sum_{\boldsymbol{x}\in\tilde{\Lambda}_N}\mathbf{D}_{\mathrm{b},-}(\boldsymbol{x},\boldsymbol{x};z)\\&=\frac{\text{the number of unit cells in }\tilde{\Lambda}_N}{|\Lambda_N|}\sum_{\underline{x}\in\Omega}\left(\mathbf{D}_{\mathrm{b},+}(\underline{x},\underline{x};z)+\mathbf{D}_{\mathrm{b},-}(\underline{x},\underline{x};z)\right)\end{aligned}$$

and the fraction in this is

$$\frac{\text{the number of unit cells in }\tilde{\Lambda}_N}{|\Lambda_N|}=\frac{(2(N-N^{\varepsilon})+1)^2}{(2N+1)^2|\Omega|)}\to\frac{1}{|\Omega|},\quad N\to\infty$$

so in the large N limit the off-diagonal conduction tensor element is given by:

$$\sigma_{21}(b)=\frac{1}{2|\Omega|\pi\omega}\oint_{\mathscr{C}}\mathrm{d}z\,f_{\mathrm{FD}}(z)\sum_{\underline{x}\in\Omega}\left(\mathbf{D}_{\mathrm{b},+}(\underline{x},\underline{x};z,b)+\mathbf{D}_{\mathrm{b},-}(\underline{x},\underline{x};z,b)\right) \tag{2.37}$$

3

PROOF OF THEOREM 1.1(2)

3.1 K-SPACE REPRESENTATION

We assume that the crystal potential is periodic in Γ,

$$(\mathbf{V}_0\boldsymbol{\psi})(\gamma+\underline{x}) = (\mathbf{V}_0\boldsymbol{\psi})(\gamma+\boldsymbol{\beta}+\underline{x}). \qquad \text{for all } \boldsymbol{\beta}\in\Gamma.$$

We define $\mathscr{H}' := \ell^2(\Omega)$ and introduce

$$\mathscr{H}_{\mathrm{F}} := \int_{\Omega^*}^{\oplus} \mathscr{H}' \mathrm{d}^2 k.$$

The linear space $\mathscr{H}_{\mathrm{F}}$ can be shown to be a Hilbert space [5], with the inner product

$$\int_{\Omega^*} \mathrm{d}^2 k \sum_{\underline{x}\in\Omega^*} \overline{f(\underline{x},\boldsymbol{k})} g(\underline{x},\boldsymbol{k}).$$

(subscript "F" for "Floquet".)

We define the operator taking vectors $\boldsymbol{\psi}$ in $\ell^2(\Lambda)$, $\boldsymbol{\psi}$ having compact support, into $\mathscr{H}_{\mathrm{F}}$, $\mathbf{U} : \ell^2(\Lambda) \to \mathscr{H}_{\mathrm{F}}$, as the operation that satisfies

$$(\mathbf{U}\boldsymbol{\psi})(\boldsymbol{k},\underline{x}) = \frac{1}{\sqrt{|\Omega^*|}} \sum_{\gamma\in\Gamma} \exp(i\boldsymbol{k}\cdot\gamma)\psi(\underline{x}-\gamma), \quad \boldsymbol{k}\in\Omega^*, \underline{x}\in\Omega, \tag{3.1}$$

We will now show that $\ell^2(\Lambda)$ and $\mathscr{H}_{\mathrm{F}}$ are isomorphic, because $\mathbf{U}$ has an unitary extension. We denote by $\ell^2_c(\Lambda)$ the vectors $\boldsymbol{\psi}$ in $\ell^2(\Lambda)$ that has compact support.

Theorem 3.1. $\mathbf{U}$ *defined by formula* (3.1) *has an unitary extension.*

Proof. It can be shown that $\ell^2_c(\Lambda)$ is a dense subset of $\ell^2(\Lambda)$. For an arbitrarily $\boldsymbol{\psi}\in\ell^2_c(\Lambda)$, we examine $\|\mathbf{U}\boldsymbol{\psi}\|_{\mathrm{F}}$:

$$\|\mathbf{U}\boldsymbol{\psi}\|^2_{\mathrm{F}} = \int_{\boldsymbol{k}\in\Omega^*} \mathrm{d}^2 k \sum_{\underline{x}\in\Omega} \left(\frac{1}{\sqrt{|\Omega^*|}} \sum_{\gamma\in\Gamma} e^{-i\boldsymbol{k}\cdot\gamma} \overline{\psi(\underline{x}-\gamma)} \right) \left(\frac{1}{\sqrt{|\Omega^*|}} \sum_{\beta\in\Gamma} e^{i\boldsymbol{k}\cdot\boldsymbol{\beta}} \psi(\underline{x}-\gamma) \right). \tag{3.2}$$

The integral $\int_{\boldsymbol{k}\in\Omega^*} \mathrm{d}^2k\, e^{-i\boldsymbol{k}\cdot\gamma} e^{i\boldsymbol{k}\cdot\boldsymbol{\beta}}$ will give zero unless for $\gamma = \boldsymbol{\beta}$ where it gives $|\Omega^*|$, we thus have

$$\|\mathbf{U}\boldsymbol{\psi}\|_{\mathrm{F}}^2 = \sum_{\underline{x}\in\Omega}\sum_{\gamma\in\Gamma} \overline{\psi(\underline{x}-\gamma)}\psi(\underline{x}-\gamma) = \|\boldsymbol{\psi}\|^2_{\ell^2(\Lambda)},$$

Therefore $\mathbf{U}$ has a unique extension by continuity to $\ell^2(\Lambda)$, and we denote this extension also by $\mathbf{U}$.

The adjoint operator $\mathbf{U}^*$ satisfies, for $\boldsymbol{\psi} \in \ell^2(\Lambda)$ and $\boldsymbol{f} \in \mathscr{H}_{\mathrm{F}}$.

$$\langle \boldsymbol{f}\,, \mathbf{U}\boldsymbol{\psi}\rangle_{\mathrm{F}} = \langle \mathbf{U}^*\boldsymbol{f}, \boldsymbol{\psi}\rangle_{\ell^2(\Lambda)}\,. \tag{3.3}$$

Now we want a explicit formula for $\mathbf{U}^*\boldsymbol{f}$, $\boldsymbol{f}$ being sufficiently smooth and Ω^* periodic in the k variables.

If, in addition, $\boldsymbol{\psi} \in \ell^2_c(\Lambda)$, then the computation

$$\begin{aligned}
\langle \boldsymbol{f}, \mathbf{U}\boldsymbol{\psi}\rangle_{\mathrm{F}} &= \int_{\Omega^*} \mathrm{d}^2k \sum_{\underline{x}\in\Omega} \overline{f(\boldsymbol{k},\underline{x})}(\mathbf{U}\boldsymbol{\psi})(\boldsymbol{k},\underline{x}) \\
&= \int_{\Omega^*} \mathrm{d}^2k \sum_{\underline{x}\in\Omega} \overline{f(\boldsymbol{k},\underline{x})}\frac{1}{\sqrt{|\Omega^*|}} \sum_{\gamma\in\Gamma} \exp(i\boldsymbol{k}\cdot\gamma)\psi(\underline{x}-\gamma) \\
&= \sum_{\gamma\in\Gamma}\sum_{\underline{x}\in\Omega}\left(\overline{(|\Omega^*|)^{-1/2}\int_{\Omega^*} \mathrm{d}^2k\, f(\boldsymbol{k},\underline{x})\exp(-i\boldsymbol{k}\cdot\gamma)}\right)\psi(\underline{x}-\gamma)
\end{aligned}$$

and the equality (3.3), indicates that the adjoint of $\mathbf{U}$ is given by

$$(\mathbf{U}^*\boldsymbol{f})\,(\underline{x}-\gamma) = \frac{1}{\sqrt{|\Omega^*|}}\int_{\Omega^*} \mathrm{d}^2k\, f(\boldsymbol{k},\underline{x})\exp(-i\boldsymbol{k}\cdot\gamma).$$

A computation similar to formula (3.2) shows that for $\boldsymbol{\psi} \in \ell^2_c(\Lambda)$ and $\boldsymbol{\phi} \in \ell^2_c(\Lambda)$ it is true that

$$\begin{aligned}
\langle \mathbf{U}\boldsymbol{\psi}, \mathbf{U}\boldsymbol{\phi}\rangle_{\mathrm{F}} &= \langle \boldsymbol{\psi}, \mathbf{U}^*\mathbf{U}\boldsymbol{\phi}\rangle_{\ell^2(\Lambda)} \\
&= \langle \boldsymbol{\psi}, \boldsymbol{\phi}\rangle_{\ell^2(\Lambda)}.
\end{aligned}$$

We therefore have, for all $\boldsymbol{\psi}$ in $\ell^2(\Lambda)$, that

$$\langle \boldsymbol{\psi}, \mathbf{U}^*\mathbf{U}\boldsymbol{\phi} - \boldsymbol{\phi}\rangle_{\ell^2(\Lambda)} = 0,$$

which indicate that $\mathbf{U}^*\mathbf{U}\boldsymbol{\phi} = \boldsymbol{\phi}$ for all $\boldsymbol{\phi}$ in $\ell^2_c(\Lambda)$, and therefore the extensions obey

$$\mathbf{U}^*\mathbf{U} = \mathbb{1}. \qquad \text{(identity in } \ell^2(\Lambda)\text{)} \tag{3.4}$$

For $\boldsymbol{f} \in \mathscr{H}_{\mathrm{F}}$, $\boldsymbol{f}$ being sufficiently smooth and Ω^* periodic in the k variables, consider $\mathbf{U}\mathbf{U}^*\boldsymbol{f}$:

$$\begin{aligned}
(\mathbf{U}\mathbf{U}^*\boldsymbol{f})\,(\boldsymbol{k},\underline{x}) &= \frac{1}{\sqrt{|\Omega^*|}}\sum_{\gamma\in\Gamma} e^{i\boldsymbol{k}\cdot\gamma}(\mathbf{U}^*\boldsymbol{f})(\underline{x}-\gamma) \\
&= \frac{1}{\sqrt{|\Omega^*|}}\sum_{\gamma\in\Gamma} e^{i\boldsymbol{k}\cdot\gamma}\frac{1}{\sqrt{|\Omega^*|}}\int_{\Omega^*} \mathrm{d}^2k\, f(\boldsymbol{k},\underline{x})e^{-i\boldsymbol{k}\cdot\gamma},
\end{aligned}$$

which is nothing but the Fourier series decomposition of $f(\boldsymbol{k},\underline{x})$ [1] . If we require f to be sufficiently smooth, so that the Fourier inversion theorem holds, we therefore have

$$(\mathbf{U}\mathbf{U}^* \boldsymbol{f})\,(\boldsymbol{k},\underline{x}) = f(\boldsymbol{k},\underline{x}),$$

and from this it follows that

$$\mathbf{U}\mathbf{U}^* = \mathbb{1}.$$

with the restrictions mentioned above.

The functions in $\mathscr{H}_\mathrm{F}$ satisfying smoothness and Ω^* periodicity are dense in $\mathscr{H}_\mathrm{F}$.

The fact that $\mathbf{U}$ has a unitary extension on $\ell^2(\Lambda)$ and $\mathbf{U}^*$ an extension on $\mathscr{H}_\mathrm{F}$, satisfying all of the above, can then be shown using continuity arguments. □

K-space representation of operators allows us to work with finite matrices when calculating energy-levels and expectation values of observables. For instance, let $\mathbf{H} = \mathbf{T} + \mathbf{V}_0$ be an (hermitian adjoint. exponentially almost diagonal [2]) hamiltonian operator on Λ, that commutes with lattice translations T_γ, that is $\mathcal{T}_\gamma \mathbf{H} = \mathbf{H}\mathcal{T}_\gamma$. The translation operator transforms according to the rule $(T_\gamma \psi)(\boldsymbol{x}) = \psi(\boldsymbol{x}-\gamma)$. We can find the k-space representative of this operator as it must be $\mathbf{U}\mathbf{H}\mathbf{U}^* : \mathscr{H}_\mathrm{F} \to \mathscr{H}_\mathrm{F}$ [3]. We examine how this operator transforms an sufficiently smooth, Ω^*-periodic $\boldsymbol{f} \in \mathscr{H}_\mathrm{F}$

$$\begin{aligned}(\mathbf{U}\mathbf{H}\mathbf{U}^* \boldsymbol{f})\,(\boldsymbol{k},\underline{x}) &= \sum_{\gamma\in\Gamma} \frac{1}{\sqrt{|\Omega^*|}} e^{i\boldsymbol{k}\cdot\gamma}\,(\mathbf{H}\mathbf{U}^*\boldsymbol{f})\,(\underline{x}-\gamma)\\ &= \sum_{\gamma\in\Gamma} \frac{1}{\sqrt{|\Omega^*|}} e^{i\boldsymbol{k}\cdot\gamma}\,(\mathcal{T}_\gamma\mathbf{H}\mathbf{U}^*\boldsymbol{f})\,(\mathbf{0}+\underline{x})\\ &= \sum_{\gamma\in\Gamma} \frac{1}{\sqrt{|\Omega^*|}} e^{i\boldsymbol{k}\cdot\gamma}\,(\mathbf{H}\mathcal{T}_\gamma\mathbf{U}^*\boldsymbol{f})\,(\underline{x})\\ &= \sum_{\gamma\in\Gamma} \frac{1}{\sqrt{|\Omega^*|}} e^{i\boldsymbol{k}\cdot\gamma} \sum_{y\in\Lambda}\Big(\underbrace{t(\underline{x},y)(\mathbf{U}^*\boldsymbol{f})(\boldsymbol{y}-\gamma)}_{\text{kinetic term}} + \underbrace{v_0(\boldsymbol{y})(\mathbf{U}^*\boldsymbol{f})(\boldsymbol{y}-\boldsymbol{x})}_{\text{potential term}}\Big).\end{aligned}$$

Examine the kinetic term first.

$$\begin{aligned}&\sum_{\gamma\in\Gamma} \frac{1}{\sqrt{|\Omega^*|}} e^{i\boldsymbol{k}\cdot\gamma} \sum_{\beta\in\Gamma}\sum_{\underline{y}\in\Omega} t(\underline{x},\boldsymbol{\beta}+\underline{y})(\mathbf{U}^*\boldsymbol{f})(\boldsymbol{\beta}+\underline{y}-\gamma)\\ &\quad= \sum_{\beta\in\Gamma}\sum_{\underline{y}\in\Omega} t(\underline{x},\boldsymbol{\beta}+\underline{y}) \sum_{\gamma\in\Gamma} e^{i\boldsymbol{k}\cdot(\gamma+\boldsymbol{\beta}-\boldsymbol{\beta})} \frac{1}{|\Omega^*|}\int_{\Omega^*} \mathrm{d}^2k' f(\boldsymbol{k}',\underline{y}) e^{-i\boldsymbol{k}'\cdot(\gamma-\boldsymbol{\beta})}\\ &\quad= \sum_{\beta\in\Gamma}\sum_{\underline{y}\in\Omega} t(\underline{x},\boldsymbol{\beta}+\underline{y}) e^{i\boldsymbol{k}\cdot\boldsymbol{\beta}} \sum_{\gamma\in\Gamma} e^{i\boldsymbol{k}\cdot(\gamma-\boldsymbol{\beta})} \frac{1}{|\Omega^*|}\int_{\Omega^*} \mathrm{d}^2k' f(\boldsymbol{k}',\underline{y}) e^{-i\boldsymbol{k}'\cdot(\gamma-\boldsymbol{\beta})}\\ &\quad= \sum_{\underline{y}\in\Omega}\sum_{\beta\in\Gamma} t(\underline{x},\boldsymbol{\beta}+\underline{y}) e^{i\boldsymbol{k}\cdot\boldsymbol{\beta}} f(\boldsymbol{k},\underline{y}),\end{aligned} \tag{3.5}$$

[1]For $f \in \mathscr{H}_\mathrm{F}$, sufficiently smooth, and $\underline{x} \in \Omega, \boldsymbol{k} \in \Omega^*$ the fourier series of $f(\boldsymbol{k},\underline{x})$ is $f(\boldsymbol{k},\underline{x}) = \sum_{\gamma\in\Gamma} \hat{f}(\gamma,\underline{x}) \exp(i\boldsymbol{k}\cdot\gamma)$, with the Fourier coefficient, $\hat{f}(\gamma,\underline{x})$, given by $\hat{f}(\gamma,\underline{x}) = |\Omega^*|^{-1}\int_{\Omega^*} \mathrm{d}^2k\, f(\boldsymbol{k},\underline{x}) \exp(-i\boldsymbol{k}\cdot\gamma)$.

[2]We want to be able to use Fubini's theorem over and over - swapping integration and summation orders.

[3]The operators $\mathbf{U}\mathbf{H}\mathbf{U}^* : \mathscr{H}_\mathrm{F} \to \mathscr{H}_\mathrm{F}$ and $\mathbf{H}$ are said to be *unitarily equivalent* if $\mathbf{U}$ maps the domain of $\mathbf{H}$ bijectively onto the domain of $\mathbf{U}\mathbf{H}\mathbf{U}^* : \mathscr{H}_\mathrm{F} \to \mathscr{H}_\mathrm{F}$.

where we have used the Fourier expansion identity again in the last inequality. If we for each k define the $\underline{x}, \underline{y}$ matrix element, $t_{\mathrm{F}}(\boldsymbol{k}; \underline{x}, \underline{y})$, in a $|\Omega| \times |\Omega|$ matrix $t_{\mathrm{F}}(\boldsymbol{k})$, as

$$t_{\mathrm{F}}(\underline{x}, \underline{y}; \boldsymbol{k}) := \sum_{\beta \in \Gamma} t(\underline{x}, \boldsymbol{\beta} + \underline{y}) e^{i\boldsymbol{k}\cdot\boldsymbol{\beta}},$$

then identity (3.5) kan be seen as a matrix product of the $t_{\mathrm{F}}(\boldsymbol{k})$ matrix and a $|\Omega|$-tuple $(f(\boldsymbol{k}, \underline{y}_1), f(\boldsymbol{k}, \underline{y}_2), \cdots, f(\boldsymbol{k}, \underline{y}_{|\Omega|}))$:

$$\left(t_{\mathrm{F}}(\boldsymbol{k}) f(\boldsymbol{k}, \cdot)\right)(\underline{x}) = \sum_{\underline{\boldsymbol{y}} \in \Omega} t_{\mathrm{F}}(\underline{x}, \underline{y}; \boldsymbol{k}) f(\boldsymbol{k}, \underline{y}).$$

Note on notation: In order to lessen the amount of subscripts, we use the same operater name in both ℓ^2 and k-space, if there occurs a $\boldsymbol{k}$ in the variables of an kernel, for instance $a(\underline{x}, \underline{y}; \boldsymbol{k})$, then it is meant that this is a fiber in k-space, representing an operator in ℓ^2 with the kernel $a(\boldsymbol{x}, \boldsymbol{y})$.

The k-space representation potential operator, $\mathbf{V}_0$, is a little more simple to find, because of the periodicity of v_0:

$$\begin{aligned}
(\mathbf{U}\mathbf{V}_0\mathbf{U}^* \boldsymbol{f})(\boldsymbol{k}, \underline{x}) &= \sum_{\gamma \in \Gamma} e^{i\boldsymbol{k}\cdot\gamma} (\mathbf{V}_0 \mathbf{U}^* \boldsymbol{f})(\underline{x} - \gamma) \\
&= \sum_{\gamma \in \Gamma} e^{i\boldsymbol{k}\cdot\gamma} v_0(\underline{x} - \gamma)(\mathbf{U}^* \boldsymbol{f})(\underline{x} - \gamma) \\
&= \sum_{\gamma \in \Gamma} e^{i\boldsymbol{k}\cdot\gamma} v_0(\mathbf{0} + \underline{x})(\mathbf{U}^* \boldsymbol{f})(\underline{x} - \gamma) \\
&= \tilde{v}_0(\underline{x})(\mathbf{U}\mathbf{U}^* \boldsymbol{f})(\boldsymbol{k}, \underline{x}) \\
&= \tilde{v}_0(\underline{x}) f(\boldsymbol{k}, \underline{x}),
\end{aligned}$$

where $\tilde{v}_0 : \Omega \to \mathbb{C}$ is the values v_0 can take on the unit cell. The k-space representation of the potential operator is thus a k-independent multiplication operator. The full Hamilton operator for a given $\boldsymbol{k} \in \Omega^*$ (the fiber) can therefore be expressed by the kernel

$$h_{\mathrm{F}}(\underline{x}, \underline{y}; \boldsymbol{k}) := \sum_{\gamma \in \Gamma} e^{i\boldsymbol{k}\cdot\gamma} t(\underline{x} - \gamma, \underline{y}) + v_0(\underline{x}) \delta(\underline{x}, \underline{y}). \tag{3.6}$$

The common notation is

$$\mathbf{U}\mathbf{H}\mathbf{U}^* = \int_{\Omega^*}^{\oplus} h_{\mathrm{F}}(\underline{x}, \underline{y}; \boldsymbol{k}) \, \mathrm{d}\boldsymbol{k}.$$

We have used the calculation rule for the kinetic term of the Hamiltonian:

$$t(\boldsymbol{x}, \boldsymbol{y} + \gamma) = t(\boldsymbol{x} - \gamma, \boldsymbol{y}).$$

One can easily see, by inspecting formula (3.6), that the matrix $h_{\mathrm{F}}(\boldsymbol{k})$ inherits the property of being self-adjoint from the operator $\mathbf{T}$:

$$t(\underline{x} - \gamma, \underline{y}) = t(\underline{y}, \underline{x} - \gamma) \quad \Rightarrow \quad h_{\mathrm{F}}(\underline{x}, \underline{y}; \boldsymbol{k}) = h_{\mathrm{F}}(\underline{y}, \underline{x}; \boldsymbol{k}).$$

Energy bands

The spectral theorem [1] shows that for each $\boldsymbol{k}$, $h_{\mathrm{F}}(\boldsymbol{k})$ has a diagonal matrix with respect to some orthonormal basis of $\ell^2(\Omega)$ and thus have up to $|\Omega|$ distinct eigenvalues. These energy eigenvalues defines the *energy bands*. We define the eigenvalue with the lowest value to be $\varepsilon_1(\boldsymbol{k})$, the eigenvalue with the second lowest value to be $\varepsilon_2(\boldsymbol{k})$, and so on:

$$\varepsilon_1(\boldsymbol{k}) \leq \varepsilon_2(\boldsymbol{k}) \leq \cdots \leq \varepsilon_{|\Omega|}(\boldsymbol{k}).$$

The set of energies defined by

$$\{E \in \mathbb{R} : \text{ there exists a } \boldsymbol{k} \in \Omega^* \text{ such that } \varepsilon_i(\boldsymbol{k}) = E\}$$

is denoted the ith energy band for $i \in \{1, 2, \cdots, |\Omega|\}$. If the ith energy band and the union of other energy bands is disjoint, then we say that the ith energy band is non-degenerate. If this is not the case then we say that the ith energy band is degenerate.

A slight modification, more about operators periodic in Γ

Later we would like to find the k-space operator representing the discrete curret operators $\mathbf{j}_1$ and $\mathbf{j}_2$, these operators will be defined later. To this end, we modify the transform operator $\mathbf{U}$ defined by formula (3.1) slightly, introducing the new operator $\mathbf{U}_{\mathrm{F}}$:

$$\mathbf{U}_{\mathrm{F}} : \ell^2(\Lambda) \to \mathscr{H}_{\mathrm{F}}, \qquad (\mathbf{U}_{\mathrm{F}}\boldsymbol{\psi})(\boldsymbol{k}, \underline{x}) := \sum_{\gamma \in \Gamma} e^{-i\boldsymbol{k}\cdot(\underline{\boldsymbol{x}}-\gamma)} \psi(\underline{x} - \gamma), \tag{3.7}$$

for all $\boldsymbol{\psi} \in \ell_c^2(\Lambda))$. The connection betwen the vector component $(\mathbf{U}\boldsymbol{\psi})(\boldsymbol{k}, \underline{x})$ and the vector component $(\mathbf{U}_{\mathrm{F}}\boldsymbol{\psi})(\boldsymbol{k}, \underline{x})$ is thus a factor $e^{-i\boldsymbol{k}\cdot\underline{\boldsymbol{x}}}$, that is $\mathbf{U}_{\mathrm{F}}$ is the operator product of $\mathbf{U}$ and the multiplicative operator $e^{-\boldsymbol{k}\cdot(\cdot)}$. The inverse operator to $e^{-i\boldsymbol{k}\cdot(\cdot)} : \ell^2(\Omega) \to \ell^2(\Omega)$ is $e^{i\boldsymbol{k}\cdot(\cdot)}$, and the fact that this operator is unitary combined with theorem 3.1 implies that $\mathbf{U}_{\mathrm{F}}$ has an unitary extension as well.

Theorem 3.2. *The operator* $\mathbf{U}_{\mathrm{F}}$ *defined by formula* (3.7) *has an unitary extension.*

Assuming a Γ-translation invariant Hamilton operator $\mathbf{H}$. Doing calculations much alike the ones leading up to expression (3.5), it can be shown that for the transformed Hamiltonian having the definition

$$\mathbf{U}_{\mathrm{F}}\mathbf{H}_0\mathbf{U}_{\mathrm{F}}^* : \mathscr{H}_{\mathrm{F}} \to \mathscr{H}_{\mathrm{F}},$$

the fibers has the matrix element

$$\tilde{h}_0(\underline{x}, \underline{y}; \boldsymbol{k}) = \sum_{\boldsymbol{\gamma} \in \Gamma} h(\underline{x}, \underline{y} + \gamma) e^{-i\boldsymbol{k}\cdot(\underline{x} - \boldsymbol{\gamma} - \underline{y})},$$

which has the alternate form

$$\tilde{h}_0(\underline{x}, \underline{y}; \boldsymbol{k}) = \sum_{\boldsymbol{\gamma} \in \Gamma} h_0(\underline{x} + \gamma, \underline{y}) e^{-i\boldsymbol{k}\cdot(\underline{x} + \boldsymbol{\gamma} - \underline{y})}.$$

We denote the fiber matrices, in the model of this presentation being 2×2 matrices, by

$$\tilde{h}_0(\boldsymbol{k}) = \begin{bmatrix} \tilde{h}_0(\underline{\boldsymbol{x}}_1, \underline{\boldsymbol{x}}_1; \boldsymbol{k}) & \tilde{h}_0(\underline{\boldsymbol{x}}_1, \underline{\boldsymbol{x}}_2; \boldsymbol{k}) \\ \tilde{h}_0(\underline{\boldsymbol{x}}_2, \underline{\boldsymbol{x}}_1; \boldsymbol{k}) & \tilde{h}_0(\underline{\boldsymbol{x}}_2, \underline{\boldsymbol{x}}_2; \boldsymbol{k}), \end{bmatrix}$$

where $\underline{\boldsymbol{x}}_1 = (0,0)$ and $\underline{\boldsymbol{x}}_2 = (a_1/2, 0)$.

If we now differentiate the fiber with respect to the first component of $\boldsymbol{k}$, k_1, we have

$$\frac{\partial}{\partial k_1}\tilde{h}(\underline{\boldsymbol{x}}, \underline{\boldsymbol{y}}; \boldsymbol{k}) = -\sum_{\gamma\in\Gamma} e^{-i\boldsymbol{k}\cdot(\underline{\boldsymbol{x}}+\gamma-\underline{\boldsymbol{y}})}\, i(\underline{x}_1 + \gamma_1 - \underline{y}_1) h(\underline{\boldsymbol{x}} + \gamma, \underline{\boldsymbol{y}}). \tag{3.8}$$

The right side of equation (3.8) is the fiber of the transform of the operator

$$-i[\mathbf{X}_1, \mathbf{H}] = i[\mathbf{H}, \mathbf{X}_1],$$

that is the commutator of the Hamilton operator (first component) and the position operator - which is the current operator (x-direction). This shows that a way to work with current operators, is basically to shift to k-space and differentiate a (finite) matrix. We will use this technique later.

decomposition of the product of two Γ-periodic operators

Suppose we have two operators on $\ell^2(\Lambda)$, $\mathbf{A}$ and $\mathbf{B}$, both Γ-periodic, and exponentially almost diagonal. How does the product $\mathbf{AB}$ behave in the k-space representation?

We now show that there is no difference between taking the operator product in $\mathcal{L}(\ell^2(\Lambda))$ or multiplying the finite fiber-matrices representing $\mathbf{A}$ and $\mathbf{B}$ in $\mathcal{L}(\ell^2(\Omega))$. This is a huge advantage when it comes to calculating products of operators! now we can work with finite matrices!

Theorem 3.3. *For Γ-periodic, exponentially almost diagonal operators $\mathbf{A}$ and $\mathbf{B}$, it holds that*

$$(\mathbf{AB})(\underline{\boldsymbol{x}}, \underline{\boldsymbol{y}}; \boldsymbol{k}) = \sum_{\underline{\boldsymbol{x}}'\in\Omega} a(\underline{\boldsymbol{x}}, \underline{\boldsymbol{x}}'; k) b(\underline{\boldsymbol{x}}', \underline{\boldsymbol{y}}; k)$$

.

Proof. This is proven by straight calculation:

$$\begin{aligned}(\mathbf{AB})(\underline{\boldsymbol{x}}, \underline{\boldsymbol{y}}; \boldsymbol{k}) &= \sum_{\gamma\in\Gamma} e^{-\boldsymbol{k}\cdot(\underline{\boldsymbol{x}}+\gamma-\underline{\boldsymbol{y}})} (\mathbf{AB})(\underline{\boldsymbol{x}} + \gamma, \underline{\boldsymbol{y}}) \\ &= \sum_{\gamma\in\Gamma} e^{-\boldsymbol{k}\cdot(\underline{\boldsymbol{x}}+\gamma-\underline{\boldsymbol{y}})} \sum_{\boldsymbol{x}\in\Lambda} a(\underline{\boldsymbol{x}} + \gamma, \boldsymbol{x}) b(\boldsymbol{x}, \underline{\boldsymbol{y}}).\end{aligned}$$

If we in the above sum decompose the site points $\boldsymbol{x}$ into Bravais lattice vectors and unit cell vectors, $\boldsymbol{x} = \gamma + \underline{\boldsymbol{x}}'$, then we have, rearranging the order of summation a little:

$$\begin{aligned}(\mathbf{AB})(\underline{\boldsymbol{x}}, \underline{\boldsymbol{y}}; \boldsymbol{k}) &= \sum_{\underline{\boldsymbol{x}}'\in\Omega} \sum_{\gamma,\boldsymbol{\beta}\in\Gamma} e^{-1\boldsymbol{k}\cdot(\underline{\boldsymbol{x}}+\gamma-\underline{\boldsymbol{y}}+\boldsymbol{\beta}-\boldsymbol{\beta}+\underline{\boldsymbol{x}}'-\underline{\boldsymbol{x}}')} a(\underline{\boldsymbol{x}} + \gamma, \boldsymbol{\beta} + \underline{\boldsymbol{x}}') b(\boldsymbol{\beta} + \underline{\boldsymbol{x}}', \underline{\boldsymbol{y}}) \\ &= \sum_{\underline{\boldsymbol{x}}'\in\Omega} \sum_{\gamma,\boldsymbol{\beta}\in\Gamma} e^{-i\boldsymbol{k}\cdot(\underline{\boldsymbol{x}}+\gamma-\boldsymbol{\beta}-\underline{\boldsymbol{x}}')} e^{-i\boldsymbol{k}\cdot(\boldsymbol{\beta}+\underline{\boldsymbol{x}}'-\underline{\boldsymbol{y}})} a(\underline{\boldsymbol{x}} + \gamma - \boldsymbol{\beta}, \underline{\boldsymbol{x}}') b(\boldsymbol{\beta} + \underline{\boldsymbol{x}}', \underline{\boldsymbol{y}}),\end{aligned}$$

where we have used Γ-periodicity of $\mathbf{A}$ to rewrite $a(\underline{x}+\gamma, \boldsymbol{\beta}+\underline{x}') = a(\underline{x}+\gamma-\boldsymbol{\beta}, \underline{x}')$. Now in the last sum, two of the factors, $e^{-i\boldsymbol{k}\cdot(\boldsymbol{\beta}+\underline{x}'-\underline{y})}$ and $b(\boldsymbol{\beta}+\underline{x}', \underline{y})$ are independent of the sumation variable γ. Furthermore in the other two factors $e^{i\boldsymbol{k}\cdot(\underline{x}+\gamma-\boldsymbol{\beta}-\underline{x}')}$ and $a(\underline{x}+\gamma-\boldsymbol{\beta}, \underline{x}')$, γ only occur in terms of $\gamma-\boldsymbol{\beta}$, and since γ run through *all* of Γ and, we can decouple the summing over $\gamma' = \gamma - \boldsymbol{\beta}$ and $\boldsymbol{\beta}$:

$$(\mathbf{AB})(\underline{x}, \underline{y}; \boldsymbol{k}) = \sum_{\underline{x}'\in\Omega} \left(\sum_{\gamma'} e^{-i\boldsymbol{k}\cdot(\underline{x}+\gamma'-\underline{x}')} a(\underline{x}+\gamma', \underline{x}') \right) \left(\sum_{\boldsymbol{\beta}} e^{-i\boldsymbol{k}\cdot(\boldsymbol{\beta}+\underline{x}'-\underline{y})} b(\boldsymbol{\beta}+\underline{x}', \underline{y}) \right).$$

This is what we need to show the theorem. This theorem is reminiscent of how a convolution of two functions transform in to a product in k-space under the Fourier transform. □

3.2 Calculating $\sigma_{21}(0)$ in reciprocal space

the term independent of b

By setting $b = 0$, all the exponential factors in $\mathbf{D}_{\mathrm{b},\pm}(z)$ defined by formulae (2.33) vanish and by inserting $\mathbf{D}_{0,\pm}(z)$ in to (2.37), we have the part of σ_{21} independent of b:

$$\sigma_{21}(0) = \frac{1}{4\pi\omega} \oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \sum_{\underline{x}\in\Omega} \Big[(\mathbf{H}_0 - z + \omega)^{-1} \mathbf{j}_{1,0} (\mathbf{H}_0 - z)^{-1} \mathbf{j}_{2,0} + \cdots \tag{3.9}$$

$$+ (\mathbf{H}_0 - z)^{-1} \mathbf{j}_{1,0} (\mathbf{H}_0 - z - \omega)^{-1} \mathbf{j}_{2,0} \Big] (\underline{x}, \underline{x}). \tag{3.10}$$

One term in the trace sum consist of to products of four operators, each factor being periodic in the Bravais lattice Γ. The trace is therefore over operators periodic in Γ. This allows us to switch to k-space and take the trace over products of $2x2$ matrices. We use the modified Floquet transform. The resolvents like $(\mathbf{H}_{\mathrm{b}} - z)^{-1}$ are transformed into the inverse of regular 2×2 matrices:

$$\left[(\mathbf{H}_{\mathrm{b}} - z)^{-1} \right] (\boldsymbol{k}) = (\tilde{h}_0(\boldsymbol{k}) - z\mathbb{1}_2)^{-1}$$

The current operators we find simply by differentiating with respect to the proper component of $\boldsymbol{k} = (k_1, k_2)$:

$$\mathbf{j}_\nu(\underline{x}, \underline{y}; \boldsymbol{k}) = \frac{\partial}{\partial k_\nu} \tilde{h}(\underline{x}, \underline{y}; \boldsymbol{k}),$$

if we remember to use the modified Floquet transform throughout the calculations!

k-space representation of the crystal Hamiltonian

If we for a little while permit ourselves to working with column vectors, we can write a matrix element of the crystal Hamilton operator fiber in the following form, using the modified Floquet transform:

$$\tilde{h}_0(\underline{x}, \underline{y}; \boldsymbol{k}) = \sum_{\gamma\in\Gamma} \exp\left(-i \begin{bmatrix} k_1 \\ k_2 \end{bmatrix} \cdot \begin{bmatrix} \underline{x}_1 + \gamma_1 - \underline{y}_1 \\ \underline{x}_2 + \gamma_2 - \underline{y}_2 \end{bmatrix} \right) h_0 \left(\begin{bmatrix} \underline{x}_1 + \gamma_1 \\ \underline{x}_2 + \gamma_2 \end{bmatrix}, \begin{bmatrix} \underline{y}_1 \\ \underline{y}_2 \end{bmatrix} \right),$$

notice the difference between the dot-product in the exponential term, and the comma in the variable part of $h_0(\underline{x}+\gamma,\underline{y})$...

If we fix the hopping integral to having value 1 for nearest neighbours, $h_0(\boldsymbol{x},\boldsymbol{y})$ has the form:

$$h_0(\boldsymbol{x},\boldsymbol{y}) = \delta_{\boldsymbol{x}_1,\boldsymbol{y}_1\pm a_1}\delta_{\boldsymbol{x}_2,\boldsymbol{y}_2} + \delta_{\boldsymbol{x}_2,\boldsymbol{y}_2\pm a_2}\delta_{\boldsymbol{x}_1,\boldsymbol{y}_1} + v(\boldsymbol{x}_1)\delta_{\boldsymbol{x},\boldsymbol{y}}, \tag{3.11}$$

where the potential has the form

$$v(\boldsymbol{x}_1 = \gamma_1 + \underline{x}_1) = \begin{cases} v > 0 & ,\underline{x}_1 = 0, \\ 0 & ,\underline{x}_1 = \frac{a_1}{2}. \end{cases}$$

For fixed $\underline{x}$ and $\underline{y}$, both belonging to the origo unit cell Ω, evaluating the expression (3.11) involves nine non-zero terms of $h_0(\boldsymbol{x},\underline{y})$, $\boldsymbol{x}\in\Lambda$, $\underline{y}\in\Omega$:

$$h_0\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right) = v, \qquad h_0\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}\pm\frac{a_1}{2}\\0\end{bmatrix}\right) = 1,$$
$$h_0\left(\begin{bmatrix}\pm\frac{a_1}{2}\\0\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right) = 1, \qquad h_0\left(\begin{bmatrix}0\\\pm a_2\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right) = 1,$$
$$h_0\left(\begin{bmatrix}\frac{a_1}{2}\\\pm a_2\end{bmatrix},\begin{bmatrix}\pm\frac{a_1}{2}\\0\end{bmatrix}\right) = 1$$

Using the values, we calculate, for instance

$$\begin{aligned}\tilde{h}_0\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix};\begin{bmatrix}k_1\\k_2\end{bmatrix}\right) &= \sum_{\gamma\in\Gamma} e^{-i(k_1\gamma_1+k_2\gamma_2)}h_0\left(\begin{bmatrix}\gamma_1\\\gamma_2\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right)\\
&= h_0\left(\begin{bmatrix}0\\0\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right) + e^{-ik_2a_2}h_0\left(\begin{bmatrix}0\\a_2\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right) + e^{ik_2a_2}h_0\left(\begin{bmatrix}0\\-a_2\end{bmatrix},\begin{bmatrix}0\\0\end{bmatrix}\right)\\
&= v + 2\cos(k_2a_2).\end{aligned}$$

Making equivalent calculations for the other three matrix elements of $\tilde{h}_0(\boldsymbol{k})$, we have

$$\tilde{h}_0(\boldsymbol{k}) = \begin{bmatrix} 2\cos(k_2a_2)+v & ,2\cos\left(\frac{k_1a_1}{2}\right) \\ 2\cos\left(\frac{k_1a_1}{2}\right) & ,2\cos(k_2a_2) \end{bmatrix}.$$

We see that all matrix elements are *even*, periodic functions of k_ν, $\nu\in\{1,2\}$. The band structure is found easily by finding the two eigenvalues of $\tilde{h}_0(\boldsymbol{k})$:

$$\lambda_\pm(k_1,k_2) = 2\cos(k_2a_2) + \frac{v}{2} \pm \frac{1}{2}\sqrt{v^2 + 16\cos^2\left(\frac{k_1a_1}{2}\right)},$$

which we will not use much, but they convey some information about the model. Letting $\boldsymbol{k}$ vary over the first Brilluoin zone Ω^* we can find the energy bands.

We are now in a position to find the k-space fibers $j_{\nu,0}(\boldsymbol{k})$ and $s_0(z,\boldsymbol{k})$.

$$\begin{aligned} j_{1,0}(\boldsymbol{k}) &= \frac{\partial}{\partial k_1}\tilde{h}_0(\boldsymbol{k})\\
&= \begin{bmatrix} 0 & ,-a_1\sin\left(\frac{k_1a_1}{2}\right) \\ -a_1\sin\left(\frac{k_1a_1}{2}\right) & ,0 \end{bmatrix},\end{aligned}$$

$$
\begin{aligned}
j_{2,0}(\boldsymbol{k}) &= \frac{\partial}{\partial k_2}\tilde{h}_0(\boldsymbol{k}) \\
&= \begin{bmatrix} -2a_2\sin(k_2a_2) & ,0 \\ 0 & ,-2a_2\sin(k_2a_2) \end{bmatrix},
\end{aligned}
$$

$$
\begin{aligned}
s_0(z_0,\boldsymbol{k}) &= (\tilde{h}_0(\boldsymbol{k}) - z_0)^{-1}, \quad z_0 \in \rho(\mathbf{H}_0) \\
&= \frac{1}{Det(z_0,v)}\begin{bmatrix} 2\cos(k_2a_2) - z_0 & ,-2\cos\left(\frac{k_1a_1}{2}\right) \\ -2\cos\left(\frac{k_1a_1}{2}\right) & ,2\cos(k_2a_2) + v - z_0 \end{bmatrix}, \\
Det(z_0,v) &= \left(2\cos\left(k_2a_2\right) - z_0\right)\left(2\cos\left(k_2a_2\right) + v - z_0\right) - 4\cos^2\left(\frac{k_1a_1}{2}\right).
\end{aligned}
$$

Notice that the matrix elements of $j_{1,0}$ only depend on k_2 and is uneven in this variable, likevise, the matrix elements of $j_{2,0}$ only depend on k_1 and is uneven in this variable.

Constant term of σ_{21} is zero

We now return to the b-independent off-diagonal term of the conduction tensor, and consider the fiber of formula (3.10):

$$
\begin{aligned}
\sigma_{21}(0) = \frac{1}{4\pi\omega}\oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \sum_{\underline{x},\underline{x}',\underline{x}'',\underline{x}'''\in\Omega} \frac{1}{|\Omega^*|}\int_{\Omega^*} \mathrm{d}^2k \cdots \\
\Big(s_0(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}';z-\omega,k)\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{\boldsymbol{x}}',\underline{\boldsymbol{x}}'';\boldsymbol{k})s_0(\underline{\boldsymbol{x}}'',\underline{\boldsymbol{x}}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{\boldsymbol{x}}''',\underline{\boldsymbol{x}};\boldsymbol{k}) + \cdots \\
+ s_0(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}';z,\boldsymbol{k})\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{\boldsymbol{x}}',\underline{\boldsymbol{x}}'';\boldsymbol{k})s_0(\underline{\boldsymbol{x}}'',\underline{\boldsymbol{x}}''';z+\omega,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{\boldsymbol{x}}''',\underline{\boldsymbol{x}};\boldsymbol{k})\Big).
\end{aligned}
\tag{3.12}
$$

It turns out that $\sigma_{21}(0)$, given by formula (3.12) is zero. Consider the term:

$$
\int_{\Omega^*} \mathrm{d}^2k s_0(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}';z-\omega,k)\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{\boldsymbol{x}}',\underline{\boldsymbol{x}}'';\boldsymbol{k})s_0(\underline{\boldsymbol{x}}'',\underline{\boldsymbol{x}}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{\boldsymbol{x}}''',\underline{\boldsymbol{x}};\boldsymbol{k}).
$$

When integrating k_1 out, we integrate the product of three even and one uneven functions on the interval (first Brillouin zone), which amounts to integrate an uneven function over $k_1 \in [-\frac{\pi}{a_1},\frac{\pi}{a_1}]$. This must return zero. The other term in formula (3.12) is zero by the same line of reasoning.

That $\sigma_{21}(b=0)$ is zero makes perfect sense, physically.

3.3 The first derivative of $\sigma_{21}(b)$

the term linear in b

Now we seek to isolate the terms in

$$
\sigma_{21}(b) = \frac{1}{4\pi\omega}\oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \sum_{\underline{x}\in\Omega} \left[\mathbf{D}_{\mathrm{b},-} + \mathbf{D}_{\mathrm{b},+}\right](\underline{x},\underline{x}),
$$

containing b to the first power. Using the definitions of $\mathbf{D}_{\mathrm{b},\pm}$, we have

$$\sigma_{21}(b) = \frac{1}{4\pi\omega} \oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \sum_{\underline{x}\in\Omega} \Big[(\mathbf{H}_{\mathrm{b}} - z + \omega)^{-1} \mathbf{j}_{1,\mathrm{b}} (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{2,\mathrm{b}} + \cdots \\ + (\mathbf{H}_{\mathrm{b}} - z)^{-1} \mathbf{j}_{1,\mathrm{b}} (\mathbf{H}_{\mathrm{b}} - z - \omega)^{-1} \mathbf{j}_{2,\mathrm{b}} \Big] (\underline{x}, \underline{x}), \tag{3.13}$$

We have two types of factors in $\mathbf{D}_{\mathrm{b},\pm}$; resolvents like $(\mathbf{H}_{\mathrm{b}} - z)^{-1}$, and current operators $\mathbf{j}_{\nu,\mathrm{b}}$, $\nu = 1, 2$. We discard the $\mathcal{O}(b^2)$ -remainder term of equation (2.16) and subtitute

$$(\mathbf{H}_{\mathrm{b}} - z_0)^{-1} \approx \mathbf{S}_{\mathrm{b}}(z_0) - \mathbf{S}_{\mathrm{b}}(z_0)\mathbf{K}_{\mathrm{b}}(z_0). \tag{3.14}$$

into formula (3.13), isolating an expression containing the linear terms in b:

$$\sigma_{21,\mathrm{lin}}(b) = \frac{1}{4\pi\omega} \oint_{\mathscr{C}} \mathrm{d}z\, f_{\mathrm{FD}}(z) \times \cdots \\ \times \sum_{\underline{x}\in\Omega} \left[(\mathbf{S}_{\mathrm{b}}(z-\omega) - \mathbf{S}_{\mathrm{b}}(z-\omega)\mathbf{K}_{\mathrm{b}}(z-\omega))\, \mathbf{j}_{1,\mathrm{b}}\, (\mathbf{S}_{\mathrm{b}}(z) - \mathbf{S}_{\mathrm{b}}(z)\mathbf{K}_{\mathrm{b}}(z))\, \mathbf{j}_{2,\mathrm{b}} + \cdots \right. \\ \left. + \left((\mathbf{S}_{\mathrm{b}}(z) - \mathbf{S}_{\mathrm{b}}(z)\mathbf{K}_{\mathrm{b}}(z))\, \mathbf{j}_{1,\mathrm{b}}\, (\mathbf{S}_{\mathrm{b}}(z+\omega) - \mathbf{S}_{\mathrm{b}}(z+\omega)\mathbf{K}_{\mathrm{b}}(z+\omega))\, \mathbf{j}_{2,\mathrm{b}} \right] (\underline{x}, \underline{x}). \tag{3.15}$$

In order to keep track of the big picture when multiplying these operator products out, we introduce some shorthand notation:

$$\begin{aligned} \mathcal{S} &:= \mathbf{S}_{\mathrm{b}}(z), \\ \mathcal{S}_- &:= \mathbf{S}_{\mathrm{b}}(z-\omega), \\ \mathcal{S}_+ &:= \mathbf{S}_{\mathrm{b}}(z+\omega), \\ \mathcal{SK} &:= \mathbf{S}_{\mathrm{b}}(z)\mathbf{K}_{\mathrm{b}}(z), \\ \mathcal{SK}_- &:= \mathbf{S}_{\mathrm{b}}(z-\omega)\mathbf{K}_{\mathrm{b}}(z-\omega), \\ \mathcal{SK}_+ &:= \mathbf{S}_{\mathrm{b}}(z+\omega)\mathbf{K}_{\mathrm{b}}(z+\omega). \end{aligned}$$

For $\underline{x} \in \Omega$, we need focus on the matrix element, with the new shorthand, suppresing the integrals and sums a little while:

$$[\, (\mathcal{S}_- - \mathcal{SK}_-)\, \mathbf{j}_{1b}\, (\mathcal{S} - \mathcal{SK})\, \mathbf{j}_{2b} + (\mathcal{S} - \mathcal{SK})\, \mathbf{j}_{1b}\, (\mathcal{S}_+ - \mathcal{SK}_+)\, \mathbf{j}_{2b}\,]\, (\underline{x}, \underline{x}) \\ = [\, \mathcal{S}_-\mathcal{S} - \mathcal{S}_-\mathcal{SK} - \mathcal{SK}_-\mathcal{S} + \mathcal{SK}_-\mathcal{SK} + \mathcal{SS}_+ - \mathcal{SSK}_+ - \mathcal{SKS}_+ + \mathcal{SKSK}_+\,]\, (\underline{x}, \underline{x}), \tag{3.16}$$

where we have suppressed the sandwiched $\mathbf{j}_{1b}$ and the ending $\mathbf{j}_{2b}$ factor, common to all terms.

Consider the factor $\mathcal{SK} = \mathbf{S}_{\mathrm{b}}(z)\mathbf{K}_{\mathrm{b}}(z)$:

$$[\mathbf{S}_{\mathrm{b}}(z)\mathbf{K}_{\mathrm{b}}(z)]\, (\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{x}^I, \boldsymbol{x}^{II} \in \Lambda} e^{ib\varphi(\boldsymbol{x}, \boldsymbol{x}^I)} s_o(\boldsymbol{x}, \boldsymbol{x}^I; z) e^{ib\varphi(\boldsymbol{x}^I, \boldsymbol{y})} \left(e^{ib\mathrm{fl}(\boldsymbol{x}^I, \boldsymbol{x}^{II}, \boldsymbol{y})} - 1 \right) \times \cdots \\ \times h_0(\boldsymbol{x}^I, \boldsymbol{x}^{II}) s_o(\boldsymbol{x}^{II}, \boldsymbol{y}; z).$$

The fact that the summand contains the factor $\left(e^{ib\mathrm{fl}(\boldsymbol{x}^I,\boldsymbol{x}^{II},\boldsymbol{y})}-1\right)$ is crucial here, as the b-independent part of this, using the power series expansion of the exponential function, $e^x=\sum_{xn=0}^{\infty}x^n/n!=1+x+\mathcal{O}(x^2)$ is zero, and next term, linear in b is

$$\left(e^{ib\mathrm{fl}(\boldsymbol{x}^I,\boldsymbol{x}^{II},\boldsymbol{y})}-1\right)\approx ib\mathrm{fl}(\boldsymbol{x}^I,\boldsymbol{x}^{II},\boldsymbol{y}).$$

Thereby we see that all terms in (3.16) containing at least one of the factors $\mathcal{SK}$, $\mathcal{SK}_-$ or $\mathcal{SK}_+$ must vanish in the case $b=0$. Furthermore, when can discard the two terms $\mathcal{SK}_-\mathcal{SK}$ and $\mathcal{SKSK}_+$, when isolating the terms linear in b, since these contain no term of lower order than b^2. The matrix element $[\mathbf{S}_\mathrm{b}(z)\mathbf{K}_\mathrm{b}(z)]\,(\boldsymbol{x},\boldsymbol{y})$ is in the first order approximation thus given by

$$[\mathbf{S}_\mathrm{b}(z)\mathbf{K}_\mathrm{b}(z)]\,(\boldsymbol{x},\boldsymbol{y})=\sum_{\boldsymbol{x}^I,\boldsymbol{x}^{II}\in\Lambda}e^{ib\varphi(\boldsymbol{x},\boldsymbol{x}^I)}s_o(\boldsymbol{x},\boldsymbol{x}^I;z)e^{ib\varphi(\boldsymbol{x}^I,\boldsymbol{y})}ib\mathrm{fl}(\boldsymbol{x}^I,\boldsymbol{x}^{II},\boldsymbol{y})h_0(\boldsymbol{x}^I,\boldsymbol{x}^{II})s_o(\boldsymbol{x}^{II},\boldsymbol{y};z),\tag{3.17}$$

and we are down to considering 6 terms in the sum (3.16).

The $\mathcal{S}_-\mathcal{S}$ term

The matrix element of considaration here is

$$[\mathcal{S}_-\mathcal{S}]\,(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}})=[\mathbf{S}_\mathrm{b}(z-\omega)\mathbf{j}_{1,\mathrm{b}}\mathbf{S}_\mathrm{b}(z)\mathbf{j}_{2,\mathrm{b}}]\,(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}),\quad \underline{\boldsymbol{x}}\in\Omega.$$

Isolating the b-dependence into exponential factors this is equal to

$$\sum_{\boldsymbol{x}^I,\boldsymbol{x}^{II},\boldsymbol{x}^{III}}e^{ib\varphi(\underline{\boldsymbol{x}},\boldsymbol{x}^I)}s_0(\underline{\boldsymbol{x}},\boldsymbol{x}^I;z-\omega)e^{ib\varphi(\underline{\boldsymbol{x}}^I,\boldsymbol{x}^{II})}j_{1,0}(\boldsymbol{x}^I,\boldsymbol{x}^{II})e^{ib\varphi(\underline{\boldsymbol{x}}^{II},\boldsymbol{x}^{III})}s_0(\boldsymbol{x}^{II},\boldsymbol{x}^{III};z)e^{ib\varphi(\underline{\boldsymbol{x}}^{III},\underline{\boldsymbol{x}})}j_{2,0}(\boldsymbol{x}^{III},\underline{\boldsymbol{x}})$$

We collect all the exponential factors

$$e^{ib\varphi(\underline{\boldsymbol{x}},\boldsymbol{x}')}e^{ib\varphi(\boldsymbol{x}',\boldsymbol{x}'')}e^{ib\varphi(\boldsymbol{x}'',\boldsymbol{x}''')}e^{ib\varphi(\boldsymbol{x}''',\underline{\boldsymbol{x}})}=e^{ib(\mathrm{FL})},$$

with the definition

$$(\mathrm{FL})=\varphi(\underline{\boldsymbol{x}},\boldsymbol{x}')+\varphi(\boldsymbol{x}',\boldsymbol{x}'')+\varphi(\boldsymbol{x}'',\boldsymbol{x}''')+\varphi(\boldsymbol{x}''',\underline{\boldsymbol{x}}).$$

The power series expansion of $e^{ib(\mathrm{FL})}$ in powers of b is

$$e^{ib(\mathrm{FL})}=1+ib(\mathrm{FL})+\mathcal{O}(b^2).\tag{3.18}$$

It can be shown that

$$\begin{aligned}(\mathrm{FL})&=\mathrm{fl}(\underline{\boldsymbol{x}},\boldsymbol{x}',\boldsymbol{x}'')+\mathrm{fl}(\underline{\boldsymbol{x}},\boldsymbol{x}'',\boldsymbol{x}''')\\&=\frac{1}{2}\left[(x_1'-x_1'')(\underline{x}_2-x_2')-(x_2'-x_2'')(\underline{x}_1-x_1')\right]+\frac{1}{2}\left[(x_1''-x_1''')(\underline{x}_2-x_2'')-(x_2''-x_2''')(\underline{x}_1-x_1'')\right].\end{aligned}$$

Inserting this into formula (3.18) discarding all terms not linear in b we will make the substitution

$$
\begin{aligned}
e^{ib(\mathrm{FL})} \to & \frac{ib}{2}\left[(x_1' - x_1'')(\underline{x}_2 - x_2') - (x_2' - x_2'')(\underline{x}_1 - x_1')\right] + \cdots \\
& \quad + \frac{ib}{2}\left[(x_1'' - x_1''')(\underline{x}_2 - x_2'') - (x_2'' - x_2''')(\underline{x}_1 - x_1'')\right] \\
= & \frac{ib}{2}\left[(x_1' - x_1'')(\underline{x}_2 - x_2') - (x_2' - x_2'')(\underline{x}_1 - x_1')\right] + \cdots \\
+ & \frac{ib}{2}\left[(x_1'' - x_1''')(\underline{x}_2 - x_2') + (x_1'' - x_1''')(x_2' - x_2'') - (x_2'' - x_2''')(\underline{x}_1 - x_1') - (x_2'' - x_2''')(x_1' - x_1'')\right]
\end{aligned}
$$

into the formula for $[\mathcal{S}_-\mathcal{S}]\,(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}})$. (In the last sum, we make sure that only term of the type $(x_\nu^r - x_\nu^{r+1})$ occur in the expression). We have

$$
\begin{aligned}
[\mathcal{S}_-\mathcal{S}]\,(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}) = \frac{ib}{2} \sum_{\boldsymbol{x}^I,\boldsymbol{x}^{II},\boldsymbol{x}^{III}\in\Lambda} & \left[(\underline{x}_1 - x_1')s_0(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}';z-\omega)\,(x_2' - x_2'')j_{10}(\boldsymbol{x}',\boldsymbol{x}'')\,s_0(\boldsymbol{x}'',\boldsymbol{x}''';z)j_0(\boldsymbol{x}''',\underline{\boldsymbol{x}}) + \cdots \right. \\
& - (\underline{x}_2 - x_2')s_0(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}';z-\omega)\,(x_1' - x_1'')j_{10}(\boldsymbol{x}',\boldsymbol{x}'')\,s_0(\boldsymbol{x}'',\boldsymbol{x}''';z)j_0(\boldsymbol{x}''',\underline{\boldsymbol{x}}) + \cdots \\
& + (\underline{x}_2 - x_2')s_0(\underline{\boldsymbol{x}},\boldsymbol{x};z-\omega)\,j_{10}(\boldsymbol{x}',\boldsymbol{x}'')\,(x_1'' - x_1''')s_0(\boldsymbol{x}'',\boldsymbol{x}''';z)\,j_{20}(vt''',\underline{\boldsymbol{x}}) + \cdots \\
& - (\underline{x}_1 - x_1')s_0(\underline{\boldsymbol{x}},\boldsymbol{x};z-\omega)\,j_{10}(\boldsymbol{x}',\boldsymbol{x}'')\,(x_2'' - x_2''')s_0(\boldsymbol{x}'',\boldsymbol{x}''';z)\,j_{20}(vt''',\underline{\boldsymbol{x}}) + \cdots \\
& + s_0(\underline{\boldsymbol{x}},\boldsymbol{x}';z-\omega)\,(x_1' - x_1'')j_{10}(\boldsymbol{x}',\boldsymbol{x}'')\,(x_2'' - x_2''')\,s_0(\boldsymbol{x}'',\boldsymbol{x}''';z)\,j_{20}(\boldsymbol{x}''',\underline{\boldsymbol{x}}) + \cdots \\
& \left. - s_0(\underline{\boldsymbol{x}},\boldsymbol{x}';z-\omega)\,(x_2' - x_2'')j_{10}(\boldsymbol{x}',\boldsymbol{x}'')\,(x_1'' - x_1''')\,s_0(\boldsymbol{x}'',\boldsymbol{x}''';z)\,j_{20}(\boldsymbol{x}''',\underline{\boldsymbol{x}})\right].
\end{aligned}
$$

Switching to k-space, we have that multiplying an operator-kernel $a(\boldsymbol{x}^r,\boldsymbol{x}^{r+1})$ with $(x_\nu^r - x_\nu^{r+1})$ transfers into differentiating the fiber with respect to k_ν, $\nu \in \{1,2\}$.:

$$
i(x_\nu^r - x_\nu^{r+1})a(\boldsymbol{x}^r,\boldsymbol{x}^{r+1}) \quad \to \quad \frac{1}{|\Omega^*|}\int_{\Omega^*} \mathrm{d}^2k\,\frac{\partial}{\partial k_\nu}a(\boldsymbol{x}^r,\boldsymbol{x}^{r+1};\boldsymbol{k}).
$$

In k-space, we also again make the switch

$$
\sum_{\cdots\boldsymbol{x},\boldsymbol{x}'\cdots\in\Lambda}(\cdots)j_{\nu,0}(\boldsymbol{x},\boldsymbol{x}')(\cdots) \to \frac{1}{|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\,(\cdots)\frac{\partial}{\partial k_\nu}\tilde{h}_0(\underline{\boldsymbol{x}},\underline{\boldsymbol{x}}';\boldsymbol{k})(\cdots)
$$

Using this rule, we have

$$\sum_{\underline{x}\in\Omega}\left[\mathcal{S}_{-}\mathcal{S}\right](\underline{x},\underline{x}) = \frac{b}{2i|\Omega^*|}\sum_{\underline{x},\underline{x}^{I},\underline{x}^{II},\underline{x}^{III}\in\Omega}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\times\left[\frac{\partial}{\partial k_2}s_0(\underline{x},\underline{x}';z-\omega,\boldsymbol{k})\frac{\partial}{\partial k_1}\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{x}',\underline{x}'';\boldsymbol{k})s_0(\underline{x}'',\underline{x}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{x}''',\underline{x};\boldsymbol{k})+\cdots\right.$$
$$-\frac{\partial}{\partial k_1}s_0(\underline{x},\underline{x}';z-\omega,\boldsymbol{k})\underbrace{\frac{\partial}{\partial k_2}\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{x}',\underline{x}'';\boldsymbol{k})}_{=0}s_0(\underline{x}'',\underline{x}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{x}''',\underline{x};\boldsymbol{k})+\cdots$$
$$+\frac{\partial}{\partial k_2}s_0(\underline{x},\underline{x}';z-\omega,\boldsymbol{k})\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{x}',\underline{x}'';\boldsymbol{k})\frac{\partial}{\partial k_1}s_0(\underline{x}'',\underline{x}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{x}''',\underline{x};\boldsymbol{k})+\cdots$$
$$-\frac{\partial}{\partial k_1}s_0(\underline{x},\underline{x}';z-\omega,\boldsymbol{k})\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{x}',\underline{x}'';\boldsymbol{k})\frac{\partial}{\partial k_2}s_0(\underline{x}'',\underline{x}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{x}''',\underline{x};\boldsymbol{k})+\cdots$$
$$+s_0(\underline{x},\underline{x}';z-\omega,\boldsymbol{k})\underbrace{\frac{\partial}{\partial k_2}\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{x}',\underline{x}'';\boldsymbol{k})}_{=0}\frac{\partial}{\partial k_1}s_0(\underline{x}'',\underline{x}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{x}''',\underline{x};\boldsymbol{k})$$
$$\left.-s_0(\underline{x},\underline{x}';z-\omega,\boldsymbol{k})\frac{\partial}{\partial k_1}\frac{\partial}{\partial k_1}\tilde{h}_0(\underline{x}',\underline{x}'';\boldsymbol{k})\frac{\partial}{\partial k_2}s_0(\underline{x}'',\underline{x}''';z,\boldsymbol{k})\frac{\partial}{\partial k_2}\tilde{h}_0(\underline{x}''',\underline{x};\boldsymbol{k})\right],$$

where two terms vanish as a consequence of our choice of model, the mixed second derivatives of the Hamilton operator fiber $\tilde{h}_0(k)$ is the zero matrix. In this way we can calculate explicitly $\sum_{\underline{x}\in\Omega}\left[\mathcal{S}_{-}\mathcal{S}\right](\underline{x},\underline{x})$ when $z, z\pm\omega$ lies in the resolvent set of $\mathbf{H}_0$.

All terms in k-space

Using the method above, we can calculate the traces of $\mathcal{S}_{-}\mathcal{S}\mathcal{K}$, $\mathcal{S}\mathcal{K}_{-}\mathcal{S}$, $\mathcal{S}\mathcal{S}_{+}$, $\mathcal{S}\mathcal{S}\mathcal{K}_{+}$ and $\mathcal{S}\mathcal{K}\mathcal{S}_{+}$, for a given $z, z\pm\omega$ in the resolvent set of $\mathbf{H}_0$, explicitly, by simply inverting and differentiating known 2×2-matrices.

Written as matrix product in k-space, suppressing the $\boldsymbol{k}$-dependence all the terms are (also stating the $\mathcal{S}_{-}\mathcal{S}$ term in compressed notation):

$$\mathrm{tr}_\Omega\left\{\mathcal{S}_{-}\mathcal{S}\right\}:\frac{b}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\mathrm{tr}_\Omega\left\{\partial_2 s_0(z-\omega)\,\partial_1\partial_1\tilde{h}_0\,s_0(z)\,\partial_2\tilde{h}_0-s_0(z-\omega)\,\partial_1\partial_1\tilde{h}_0\,\partial_1 s_0(z)\,\partial_2\tilde{h}_0\right.$$
$$\left.+\partial_2 s_0(z-\omega)\,\partial_1\tilde{h}_0\,\partial_1 s_0(z)\,\partial_2\tilde{h}_0-\partial_1 s_0(z-\omega)\,\partial_1\tilde{h}_0\,\partial_2 s_0(z)\,\partial_2\tilde{h}_0\right\}.$$

$$\mathrm{tr}_\Omega\left\{\mathcal{S}_{-}\mathcal{S}\mathcal{K}\right\}:\frac{b}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\mathrm{tr}_\Omega\left\{s_0(z-\omega)\,\partial_1\tilde{h}_0\,s_0(z)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z)\right]\partial_2\tilde{h}_0\right\}$$

$$\mathrm{tr}_\Omega\left\{\mathcal{S}\mathcal{K}_{-}\mathcal{S}\right\}:\frac{b}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\mathrm{tr}_\Omega\left\{s_0(z-\omega)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z-\omega)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z-\omega)\right]\partial_1\tilde{h}_0\,s_0(z)\,\partial_2\tilde{h}_0\right\}$$

$$\mathrm{tr}_\Omega\left\{\mathcal{S}\mathcal{S}_+\right\}:\frac{b}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\mathrm{tr}_\Omega\left\{\partial_2 s_0(z)\,\partial_1\partial_1\tilde{h}_0\,s_0(z+\omega)\,\partial_2\tilde{h}_0-s_0(z)\,\partial_1\partial_1\tilde{h}_0\,\partial_1 s_0(z+\omega)\,\partial_2\tilde{h}_0\right.$$
$$\left.+\partial_2 s_0(z)\,\partial_1\tilde{h}_0\,\partial_1 s_0(z+\omega)\,\partial_2\tilde{h}_0-\partial_1 s_0(z)\,\partial_1\tilde{h}_0\,\partial_2 s_0(z+\omega)\,\partial_2\tilde{h}_0\right\}.$$

$$\mathrm{tr}_\Omega\left\{\mathcal{S}\mathcal{S}\mathcal{K}_+\right\}:\frac{b}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\mathrm{tr}_\Omega\left\{s_0(z)\,\partial_1\tilde{h}_0\,s_0(z+\omega)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z+\omega)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z+\omega)\right]\partial_2\tilde{h}_0\right\}$$

$$\mathrm{tr}_\Omega\left\{\mathcal{S}\mathcal{K}\mathcal{S}_+\right\}:\frac{b}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots$$
$$\mathrm{tr}_\Omega\left\{s_0(z)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z)\right]\partial_1\tilde{h}_0\,s_0(z+\omega)\,\partial_2\tilde{h}_0\right\},$$

where we can see some of the "cross product component" $f_1g_2-gf_2g_1$ structure is inherited from the definition of $\varphi(\boldsymbol{x},\boldsymbol{x}')=(1/2)(x_1x_2'-x_2x_1')$. Some terms, where the mixed second derivative of $\tilde{h}_0$ occur, has been omitted from the $\mathcal{S}_-\mathcal{S}$ and $\mathcal{S}\mathcal{S}_+$ terms, since these vanish in our nn. tb. model.

Collecting the terms

Collecting the terms, and inserting into formula (3.15), we have:

$$\begin{aligned}\sigma_{21}'(0)=\frac{1}{4\pi\omega}\oint_{\mathscr{C}}\mathrm{d}z\,f_{\mathrm{FD}}(z)\frac{1}{2i|\Omega^*|}\int_{\Omega^*}\mathrm{d}^2k\cdots\\
&\mathrm{tr}_\Omega\left\{\partial_2 s_0(z-\omega)\,\partial_1\partial_1\tilde{h}_0\,s_0(z)\,\partial_2\tilde{h}_0-s_0(z-\omega)\,\partial_1\partial_1\tilde{h}_0\,\partial_1 s_0(z)\,\partial_2\tilde{h}_0\right.\\
&+\partial_2 s_0(z-\omega)\,\partial_1\tilde{h}_0\,\partial_1 s_0(z)\,\partial_2\tilde{h}_0-\partial_1 s_0(z-\omega)\,\partial_1\tilde{h}_0\,\partial_2 s_0(z)\,\partial_2\tilde{h}_0\\
&-s_0(z-\omega)\,\partial_1\tilde{h}_0\,s_0(z)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z)\right]\partial_2\tilde{h}_0\\
&-s_0(z-\omega)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z-\omega)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z-\omega)\right]\partial_1\tilde{h}_0\,s_0(z)\,\partial_2\tilde{h}_0\\
&+\partial_2 s_0(z)\,\partial_1\partial_1\tilde{h}_0\,s_0(z+\omega)\,\partial_2\tilde{h}_0-s_0(z)\,\partial_1\partial_1\tilde{h}_0\,\partial_1 s_0(z+\omega)\,\partial_2\tilde{h}_0\\
&+\partial_2 s_0(z)\,\partial_1\tilde{h}_0\,\partial_1 s_0(z+\omega)\,\partial_2\tilde{h}_0-\partial_1 s_0(z)\,\partial_1\tilde{h}_0\,\partial_2 s_0(z+\omega)\,\partial_2\tilde{h}_0\\
&-s_0(z)\,\partial_1\tilde{h}_0\,s_0(z+\omega)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z+\omega)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z+\omega)\right]\partial_2\tilde{h}_0\\
&\left.-\,s_0(z-\omega)\,\left[\partial_2\tilde{h}_0\,\partial_1 s_0(z-\omega)\,-\partial_1\tilde{h}_0\,\partial_2 s_0(z-\omega)\right]\partial_1\tilde{h}_0\,s_0(z)\,\partial_2\tilde{h}_0\right\}.\end{aligned}\tag{3.19}$$

Which only contains known matrices and their derivatives.

4

Perspectives

The method shown in this paper is not restricted to working on the simple model. The model basically just simplifies the calculations to a minimum, while still not being totally unphysical. In this last chapter we will outline some questions arising, which could be a natural next step.

Actually calculating the first derivative of $\sigma_{12}(b)$ with a result from which the integrals can be calculated (probably using residue integral techniques for the path integral) should be a first step. Extending the model to a tight binding model encompassing real graphene ("honeycomb" lattice nn. tb. model) and comparing theoretical predictions of the Faraday rotation with experimental results the next. The simplest tight binding model for graphene that has a perpendicular choice of basic lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, would be using a unit cell with four sites, fig. 4.1.

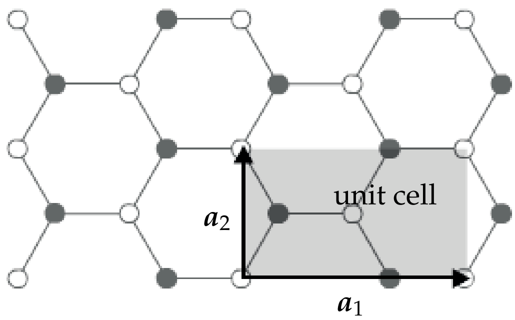

Figure 4.1: a choice of a perpendicular set of basic lattice vectors for graphene. This model has four sites per unit cell, $|\Omega| = 4$.

Higher powers

The mehod allows for computation of the second dervative of $\sigma_{12}(b)$ (relates to the "Cotton-Mouton" effect) and so on. Laborous calculations should be expected, some mean of simplifying the trace-expressions would be good.

Second quantization

It would be interesting to imcoorperate the quantized fields into the model, ideally both the light EM field aswell as the static magnetic field.

Self-consistence

Viewing the light EM field aswell as the static magnetic field as a single EM field, working with only one vector potential, and one scalar potential. This single EM field should for instance reproduce the experimental setting wherein Faraday rotation is measured.

A

APPENDICES

A.1 Selected result concerning bounded operators on a Hilbert space

Trace math

There are a few well-known tricks that we use so often, which we state here for completenes.

Theorem A.1 (Permutation rule for Trace)**.** *For operators* **A**,**B** *and* **C** *the trace is invariant under cyclic permutations:*

$$Tr\{\mathbf{ABC}\} = Tr\{\mathbf{CAB}\} \tag{A.1}$$

Theorem A.2 (Trace-Commutator Rule)**.** *For operators* **A**,**B** *and* **C**, *we have*

$$Tr\{[\mathbf{A},\mathbf{B}]\mathbf{C}\} = Tr\{\mathbf{B}[\mathbf{C},\mathbf{A}]\} \tag{A.2}$$

On resolvents

Presented here are excerpts from Peter D. Lax [2], chapter 17.

Theorem A.3. *Let $\mathcal{L}$ be a complete space of bounded linear operators on $\mathscr{H}$ (a Banach Algebra). Suppose that $\mathbf{K} \in \mathcal{L}(\mathscr{H})$ is invertible; then so are all elements of $\mathcal{L}(\mathscr{H})$ of the form $\mathbf{L} = \mathbf{K} - \mathbf{A}$, provided that*

$$\|\mathbf{A}\| < \frac{1}{\|\mathbf{K}^{-1}\|}. \tag{A.3}$$

Proof. We treat first the special case $\mathbf{K} = \mathbb{1}$; we claim that all elements of the form $\mathbb{1} - \mathbf{B}$ are invertible, provided that

$$\|\mathbf{B}\| < 1.$$

The inverse of $\mathbb{1} - \mathbf{B}$ is given by the geometric series

$$\sum_{n=0}^{\infty} \mathbf{B}^n = \mathbf{S}. \tag{A.4}$$

Since $\|B\| < 1$, the sequence of partial sums is a Cauchy sequence; since $\mathcal{L}(\mathscr{H})$ is complete, the series converges. It follows from the properties of the operator norm on infinite series that a convergent series can be multiplied termwise: multiplying (A.4) on the left by **B**, we get

$$\mathbf{BS} = \mathbf{B}\sum_{n=0}^{\infty} \mathbf{B}^n = \sum_{k=1}^{\infty} \mathbf{B}^k = \mathbf{S} - \mathbb{1},$$

from which it follows that $(\mathbb{1} - \mathbf{B})\mathbf{S} = \mathbb{1}$. Similarly, multiplying (A.4) on the right shows that $\mathbf{S}(\mathbb{1} - \mathbf{B}) = \mathbb{1}$. This shows that **S** is the inverse of $\mathbb{1} - \mathbf{B}$.

We now return to (A.3); we factor

$$\mathbf{K} - \mathbf{A} = \mathbf{K}(\mathbb{1} - \mathbf{K}^{-1}\mathbf{A}). \tag{A.5}$$

Set $\mathbf{B} = \mathbf{K}^{-1}\mathbf{A}$; by submultiplicavity, and by inequality (A.3),

$$\|\mathbf{B}\| = \|\mathbf{K}^{-1}\mathbf{A}\| = \|\mathbf{K}^{-1}\|\|\mathbf{A}\| < 1.$$

Using (A.4), we invert (A.5):

$$(\mathbf{K} - \mathbf{A})^{-1} = \left(\mathbb{1} - \mathbf{K}^{-1}\mathbf{A}\right)^{-1}\mathbf{K}^{-1} = \sum_{n=0}^{\infty}\left(\mathbf{K}^{-1}\mathbf{A}\right)^{n}\mathbf{K}^{-1}.$$

This proves that $(\mathbf{K} - \mathbf{A})$ is invertible. □

Corollary A.4. *Consider the case of the inverse to* $(\mathbb{1} - \mathbf{B})$*. The inverse exists if* $\|\mathbf{B}\| < 1$*, and we can evaluate the operator norm of* $(\mathbb{1} - \mathbf{B})^{-1}$*:*

$$\|(\mathbb{1} - \mathbf{B})^{-1}\| = \left\|\sum_{n=0}^{\infty}\mathbf{B}^{n}\right\| \leq \sum_{n=0}^{\infty}\|\mathbf{B}\|^{n} = \frac{1}{1 - \|\mathbf{B}\|}.$$

Where the last equality is the known sum of a geometric series.

Definition A.5 (Resolvent set, spectrum)**.** The *resolvent set* of $\mathbf{A}$ in $\mathscr{H}$ consists of those complex numbers λ for which $\lambda\mathbb{1} - \mathbf{A}$ is invertible. The *spectrum* of $\mathbf{A}$ consists of those λ for which $\lambda\mathbb{1} - \mathbf{A}$ is not invertible. The resolvent set of $\mathbf{A}$ is denoted $\rho(\mathbf{A})$, its spectrum by $\sigma(\mathbf{A})$.

It is an important fact, that the resolvent set for an operator $\mathbf{A}$ is an open set.

Theorem A.6 (Resolvent set open)**.** *For a bounded operator* $\mathbf{A}$*,* $\rho(\mathbf{A})$ *is open.*

Proof. Let $z_0 \in \rho(\mathbf{A})$. For an arbitrarily chosen $z \in \mathbb{C}$, the identity

$$\mathbf{A} - z = \mathbf{A} - z_0 - (z - z_0) = (\mathbb{1} - (z - z_0)(\mathbf{A} - z_0)^{-1})(\mathbf{A} - z_0)$$

show that *if* $(\mathbf{A} - z)^{-1}$ exists, it must satisfy

$$(\mathbf{A} - z)^{-1} = (\mathbf{A} - z_0)^{-1}(\mathbb{1} - (z - z_0)(\mathbf{A} - z_0)^{-1})^{-1}.$$

Denote $(z - z_0)(\mathbf{A} - z_0)^{-1}$ by $\mathbf{N}(z)$, the proof of theorem A.3 shows that if $\|\mathbf{N}(z)\| < 1$ then

$$(\mathbb{1} - (z - z_0)(\mathbf{A} - z_0)^{-1}) = (\mathbb{1} - \mathbf{N}(z))$$

is invertible. Now set $\delta = 1/\|(\mathbf{A} - z_0)^{-1}\|$, then

$$\|z - z_0\| < \delta \quad \text{implies} \quad \|\mathbf{N}(z)\| = \|z - z_0\|\|(\mathbf{A} - z_0)^{-1}\| < 1, \tag{A.6}$$

and therefore all z in the open ball $\|z - z_0\| < \delta$ must belong to $\rho(\mathbf{A})$. □

Corollary A.7. *Denote by* $\operatorname{dist}(z, \sigma(\mathbf{A}))$ *the distance between z and* $\sigma(\mathbf{A})$ *(* $\operatorname{dist}(z, \sigma(\mathbf{A}))$ *is the infimum of* $\|s - z\|$ *over all* $s \in \sigma(\mathbf{A})$ *), then the implication* (A.6) *implies that*

$$\operatorname{dist}(z, \sigma(\mathbf{A})) \geq \frac{1}{\|(\mathbf{A} - z_0)^{-1}\|}$$

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