A formula for the electrical conductivity in lattice systems

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Indice

1 Introduction

The derivation of the laws of transport phenomenon from the underlying basic laws is one of the basic problems of non equilibrium statistical mechanics. We will apply the stochastic limit approach to deduce a formula for the electrical conductivity in lattice model. Our formula has a very clear and simple physical interpretation (cf. formula (8.19) in section (8) below) and is entirely expressed in terms of the microscopic Hamiltonian model.

2 Description of the model

We will consider the following model of electronic transport in crystals (or quasi–crystals): two types of particles, say electrons and phonons, interact. Phonons push electrons and electrons jump from one site to another. The presence of an external electric field influences the rate and the direction of these jumps thus creating an electric current and we want to study the functional dependence of this current from the external electric field. In our idealized model we associate a nondegenerate electronic level to each site of a lattice L, e.g. $L = \mathbf{Z}^d$. By Pauli exclusion principle each level is either occupied by a single electron or not occupied. To each site x of the lattice L it is associated a 2–dimensional complex Hilbert space (a 2–level system) $\mathcal{H}_x \equiv C^2$. We fix an orthonormal basis

$$|0\rangle = e_0 \qquad ; \qquad e_1 = |1\rangle \tag{1}$$

of $\mathbf{C}^2$, which also fixes an identification of $\mathbf{C}^2$ with any of the spaces $\mathcal{H}_x$ and of the algebra M_2, of 2×2 complex matrices, with the algebra $\mathcal{B}_x := \mathcal{B}(\mathcal{H}_x)$ of all the linear operators on $\mathcal{H}_x$. We use the standard notations for the Pauli matrices

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad ; \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{2}$$

and for the upper and lower occupation number operators

$$\sigma_+\sigma_- = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} =: n_+ \ ; \quad \sigma_-\sigma_+ = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} =: n_- \tag{3}$$

They satisfy the anticommutation relations

$$\sigma_+\sigma_- + \sigma_-\sigma_+ = n_+ + n_- = 1 \tag{4}$$

and the orthogonality relations

$$n_+ n_- = n_- n_+ = 0 \tag{5}$$

n_+ is called the upper occupation number operator and satisfies

$$n_+|0\rangle = 0 \qquad , \qquad n_+|1\rangle = |1\rangle \tag{6}$$

where $|0\rangle$, $|1\rangle$ is the orthonormal basis (1) in $\mathbf{C}^2$. The infinite product C^*–algebra

$$\mathcal{B}_S := \otimes_{x\in L}\mathcal{B}(\mathcal{H}_x) = \otimes_{x\in L}(M_2)_x$$

has an intrinsic meaning and, if $a \in M_2$ is a 2×2 matrix and x is a site of the lattice L, we use the symbol a_x to denote the action of a on the x–th site of the lattice defined by

$$a_x := a \otimes \otimes_{x\neq y\in L} 1$$

so for example we write $\sigma_{\pm,x}, n_{\pm,x}, \dots$ and we call $n_{+,r}$ the upper occupation number operator at the r–th site of the lattice. If Λ is a finite sub–set of L, the algebra $\mathcal{B}_\Lambda := \otimes_{x\in\Lambda}(M_2)_x$ is naturally embedded into $\mathcal{B}_S$ by the prescription

$$\mathcal{B}_\Lambda \equiv \mathcal{B}_\Lambda \otimes \otimes_{x\in S\setminus\Lambda} 1$$

and it has a natural action on the Hilbert space $\mathcal{H}_\Lambda := \otimes_{x\in\Lambda}\mathcal{H}_x$. There is no intrinsic embedding of in a *infinite volume Hibert space*, but a frequently used choice is

$$\xi_\Lambda \equiv \xi_\Lambda \otimes \otimes_{x\in S\setminus\Lambda}|0\rangle_x$$

To study the electrical conductivity we model the action of the external electric field on the electrons occupying a site $r \in L$, by a shift in the the free energy of the electron system, proportional to the component of the electric field along the vector r, so that, denoting E_r the energy of an electron at site r, the system Hamiltonian will be of the form

$$H_S^{(\Lambda)} = \sum_{r\in\Lambda\subseteq L} E_r n_{+,r} = \sum_r (E_r^0 + E\cdot r) n_{+,r} \tag{7}$$

where Λ is finite sub–set of L, the E_r^0 are real numbers and $E = E(t) \in \mathbb{R}^d$ is a vector which, in general may be time dependent, for example

$$E(t) = Ee^{it\omega} \tag{8}$$

but in the present paper we shall restrict our attention to the case of a constant electric field. If $\Lambda \subseteq L$ is a finite set, the Hamiltonian $H_S^{(\Lambda)}$ has a meaning as a *bona fide* operator and the Schrödinger evolution $e^{-itH_S^{(\Lambda)}}$ exists. If Λ is an infinite set, the commutator with the Hamiltonian $[H_S^{(\Lambda)}, X]$ has a meaning for any electronic observable depending only on a finite set of points of the lattice (local observables) and the Heisenberg evolution $e^{itH_S^{(\Lambda)}}Xe^{-itH_S^{(\Lambda)}}$ always exists. We will use the notation $H_S^{(\Lambda)} =: H_S$.

The phonons are described by Boson creation and annihilation operators

$$[a_k, a^+_{k'}] = \delta(k - k') \tag{9}$$

acting in the representation space $\mathcal{F}$ whose statistics is uniquely defined by the prescriptions

$$\langle a^+_{k'} a_k \rangle = n(k)\delta(k - k') \qquad ; \qquad \langle a_k a_{k'} \rangle = 0 \tag{10}$$

where $n(k)$ is a positive function. For instance, for the grand canonical Gibbs (or equilibrium) state at inverse temperature β and chemical potential μ, is characterized by

$$n(k) = \frac{1}{e^{\beta\omega(k)-\mu} - 1} \tag{11}$$

and the Fock state by $\beta = \infty$ or $n(k) = 0$. With these notations the phonon Hamiltonian and the interaction Hamiltonian are respectively

$$H_R = \int \omega(k) a^*(k) a(k) dk \tag{12}$$

$$H_I = \sum_{r \neq s \in \Lambda \subset \mathbf{Z}^d} \sqrt{\gamma_{r,s}} (\sigma_{+r}\sigma_{-s} A(g) + \text{ h.c. }) \tag{13}$$

where $\gamma_{r,s} \geq 0$ are numbers, σ_{+r}, σ_{-s} are the Fermi creation and annihilation operators given by (2),

$$A(g) = \int \overline{g(k)} a(k) dk \tag{14}$$

and g is a momentum cut–off function related to the dispersion $\omega(k)$ by the analytical condition

$$\int_{-\infty}^{+\infty} dt \left| \int_{\mathbf{R}^d} e^{it\omega(k)} |g(k)|^2 dk \right| < \infty \tag{15}$$

Summing up: we investigate a system on a lattice L, interacting with bosonic field (phonons), whose total Hamiltonian is

$$H = H_S + H_R + \lambda H_I \tag{16}$$

where H_S, H_R, H_I are given respectively by (78), (89), (90) and λ is a coupling constant.

3 The stochastic limit of the model

The free evolution of interaction Hamiltonian (**??**) is

$$H_I(t) = e^{itH_0} H_I e^{-itH_0} = \sum_{r \neq s \in \Lambda \subset \mathbf{Z}^d} \int \overline{g(k)} dk \sigma_{+r} \sigma_{-s} a(k) e^{-it(\omega(k)+E_s-E_r)} + \text{ h.c.} \tag{17}$$

we will assume (generic case) that $\forall\, r,\ s,\ r',\ s'$

$$(r,s) \neq (r',s') \mathbf{R}ightarrow E_s - E_r \neq E_{s'} - E_{r'} \tag{18}$$

Notice that, if the E_r have the form (x.) with the E_r^o rational numbers and if the lattice is $\mathbf{Z}^d$, then assumption (x.) is equivalent to the statement that there are no rational relations among the components of the external electric field E.

In the stochastic limit different Bohr frequencies (in the generic case, different pairs of sites (r,s)) will give rise to independent Boson white noises

$$b_{r,s}(t,k) = \lim_{\lambda \to 0} \frac{1}{\lambda} e^{-i \frac{t}{\lambda^2}(\omega(k)+E_s-E_r)} a(k) \tag{19}$$

with commutator

$$[b_{r,s}(t,k), b^*_{r,s}(t',k')] = 2\pi\delta(t-t')\delta(\omega(k)+E_s-E_r)\delta(k-k') \tag{20}$$

(all the other commutators being zero) and correlation function

$$\langle b_{r,s}(t) b^+_{r,s}(t') \rangle = 2\text{Re}(g|g)_- \delta(t-t') \quad , \quad \langle b^+_{r,s}(t) b_{r,s}(t) \rangle = 2 \text{ Re } (g|g)_+ \delta(t-t') \tag{21}$$

where

$$(g|g)_- = \int |g(k)|^2 \frac{-i(n(k)+1)}{\omega(k)+E_s-E_r-i0} dk \quad , \quad (g|g)_+ = \int |g(k)|^2 \frac{-in(k))}{\omega(k)+E_s-E_r-i0} dk \tag{22}$$

To fix the ideas the density of bosons $n(k)$ will be chosen to be the equilibrium one, i.e. (x.) and the right hand side of (78) is defined by the formula

$$\int_{-\infty}^{0} e^{it\omega}dt = \frac{-i}{\omega - i0} = \pi\delta(\omega) - i \text{ P.P. } \frac{1}{\omega} \tag{23}$$

From this formula one also deduces that, since the dispersion function $\omega(k)$ is ≥ 0, only the Bohr frequencis satisfying the condition $E_r > E_s$ will give rise to non–zero master fields. We will see that this implies that only these frequencies will give contributions to the current.

The stochastic limit of the interaction Hamiltonian is the white noise Hamiltonian

$$H(t) = \sum_{r\neq s\in\Lambda\subset\mathbf{Z}^d} \sqrt{\gamma_{r,s}} \left(\int \overline{g(k)}dk\, \sigma_{+r}\sigma_{-s}b_{r,s}(t,k) + \int g(k)dk\, \sigma_{+s}\sigma_{-r}b^*_{r,s}(t,k)\right) \tag{24}$$

Introducing the notation

$$c_{r,s} := \sigma_{+r}\sigma_{-s} = c^*_{s,r} \tag{25}$$

and using the stochastic golden rule, the white noise Hamiltonian equation can be brought to normal order and becomes equivalent to the quantum stochastic differential equation

$$dU_t = \left(-i \sum_{r\neq s\in\Lambda\subset\mathbf{Z}^d} \sqrt{\gamma_{r,s}} \left(c_{r,s}dB_{r,s}(t) + c_{sr}dB^*_{r,s}(t)\right) - Gdt\right) U_t \tag{26}$$

where $dB_{r,s}(t)$ is the finite temperature Brownian motion with covariance

$$dB_{r,s}(t)dB^+_{r,s}(t) = 2 \text{ Re } (g|g)_- dt, \qquad dB^+_{r,s}(t)dB_{r,s}(t) = 2 \text{ Re } (g|g)_+ dt \tag{27}$$

The drift term has the form

$$G = \sum_{r\neq s\in\Lambda\subset\mathbf{Z}^d} \gamma_{r,s}\Big(c_{r,s}c^*_{r,s} \int |g(k)|^2 \frac{-i(n(k)+1)}{\omega(k)+E_s-E_r-i0}dk +$$

$$+c^*_{r,s}c_{r,s} \int |g(k)|^2 \frac{in(k)}{\omega(k)+E_s-E_r+i0}dk\Big) =$$

$$= \sum_{r\neq s\in\Lambda\subset\mathbf{Z}^d} \gamma_{r,s} \left(c_{r,s}c^*_{r,s}(g|g)_- + c^*_{r,s}c_{r,s}\overline{(g|g)}_+\right) \tag{28}$$

4 The Langevin equation

Now let us find the Langevin equation, i.e. the stochastic limit of the Heisenberg evolution, in interaction representation. Let X be an observable. The Langevin equation is the equation satisfied by the stochastic flow j_t, defined by:

$$j_t(X) = U_t^* X U_t \tag{29}$$

where U_t satisfies equation (**??**). To derive the Langevin equation we consider

$$dj_t(X) = j_{t+dt}(X) - j_t(X) = dU_t^* X U_t + U_t^* X dU_t + dU_t^* X dU_t \tag{30}$$

and with standard calculations, using (**??**) we arrive to the equation

$$dj_t(X) = \sum_\alpha j_t(\theta_\alpha(X)) dM^\alpha(t) = \sum_{\varepsilon=-1,1; r\neq s\in\Lambda\subset\mathbf{Z}^d} j_t(\theta_{\varepsilon,r,s}(X)) dM^{\varepsilon,r,s}(t) + j_t(\theta_0(X)) dt \tag{31}$$

where

$$dM^{-1,rs}(t) = dB_{r,s}(t), \quad \theta_{-1,j\omega}(X) = -i\sqrt{\gamma_{r,s}}[X, c_{r,s}] \tag{32}$$

$$dM^{1,rs}(t) = dB^*_{r,s}(t), \quad \theta_{1,j\omega}(X) = -i\sqrt{\gamma_{r,s}}[X, c^*_{r,s}] \tag{33}$$

and

$$\theta_0(X) = \sum_{r\neq s\in\Lambda\subset\mathbf{Z}^d} \gamma_{r,s}\Big(-i \text{ Im } (g|g)^-_{r,s}[X, c_{r,s}c^*_{r,s}] + i \text{ Im } (g|g)^+_{r,s}[X, c^*_{r,s}c_{r,s}] + \tag{34}$$

$$+2\text{Re}\,(g|g)^-_{r,s}\left(c_{r,s}Xc^*_{r,s} - \frac{1}{2}\{X, c_{r,s}c^*_{r,s}\}\right) + 2\text{Re}\,(g|g)^+_{r,s}\left(c^*_{r,s}Xc_{r,s} - \frac{1}{2}\{X, c^*_{r,s}c_{r,s}\}\right)\Big)$$

is a quantum Markovian generator. For a local observable X all the structure maps are well defined even if we take $\gamma_{r,s} = 1$, $\forall\, r, s$.

For $\gamma_{r,s}$ with a finite support the generator θ_0 grows linearly with the volume $|\Lambda|$. Let us note that we consider a generic case. Since $\theta_0(X)$ is a sum of combinations of Pauli matrices localized in finite subsets of a lattice then for $\gamma_{r,s}$ decaying sufficiently fast with $|r-s|$ (finite range interaction for instance) we can apply the Matsui approach to prove the existence of evolution for θ_0 and for corresponding extended semigroup.

5 The current vector in the linear response approximation

From our definition (**??**) of the system Hamiltonian, we see that the variation in energy due to the presence of the electric field is proportional to a vector X

$$H_S - H_S^o = E \cdot \sum_r r n_{+r} =: E \cdot X \tag{35}$$

called the *location vector* and defined by

$$X := \sum_{r \in \Lambda} r n_{+r}$$

The *electric current* vector is defined by

$$J := e \frac{d}{dt} X(t)$$

where $X(t)$ is the Heisenberg evolution of the vector X. Our goal is to study the dependence, from the external field, of the density of electric current

$$\frac{1}{|\Lambda|} \langle J_\Lambda(t) \rangle$$

where the expectation value is meant with respect to the state

$$\rho' \otimes \rho^o$$

where ρ^o is the reference state (e.g. the equilibrium state) of the field before interaction and ρ' is an arbitrary state of the system of electrons.

6 Computation of the current

According to formula (x.), to calculate the current we must evaluate the generator L on the location vector X and for this it is sufficient to know its form on the occupation numbers $n_{+,r}$. So we consider the case in which, in formula (x.6), for some $u \in \Lambda$, X has the form

$$X = n_{+,u} = \sigma_{+u} \sigma_{-u} \tag{36}$$

Then, if $r \neq u \neq s$

$$c_{r,s} n_{+,u} c^*_{r,s} = c_{r,s} c^*_{r,s} n_{+,u} = n_{+,r}(1 - n_{+,s}) n_{+,u} \tag{37}$$

If $r = u \neq s$

$$c_{r,s} n_{+,u} c^*_{us} = \sigma_{+u}\sigma_{-s}\sigma_{+u}\sigma_{-u}\sigma_{+s}\sigma_{-r} = 0 \tag{38}$$

because

$$\sigma^2_{+u} = \sigma^2_{-u} = 0 \tag{39}$$

If $s = u \neq r$

$$c_{ru} n_{+,u} \sigma^*_{ru} = \sigma_{+r}\sigma_{-u}\sigma_{+u}\sigma_{-u}\sigma_{+u}\sigma_{-r} = n_{+,r}(1 - n_{+,u})^2 \tag{40}$$

Thus in any case:

$$c_{r,s} n_{+,u} c^*_{r,s} = (1 - \delta_{u,r}) n_{+,r}(1 - n_{+,s})[(1 - \delta_{u,s}) n_{+,u} + \delta_{u,s}(1 - n_{+,u})] \tag{41}$$

Similarly, if $r \neq u \neq s$

$$c^*_{r,s} n_{+,u} c_{r,s} = n_{+,s}(1 - n_{+,r}) n_{+,u} \tag{42}$$

If $r = u \neq s$

$$\sigma_{+s}\sigma_{-u}\sigma_{+u}\sigma_{-u}\sigma_{+u}\sigma_{-s} = n_{+,s}(1 - n_{+,u})^2 \tag{43}$$

and, if $s = u \neq r$

$$\sigma_{+u}\sigma_{-s}\sigma_{+u}\sigma_{-u}\sigma_{+r}\sigma_{-u} = 0 \tag{44}$$

Notice that the case $r = u = s$ is excluded by the condition $r \neq s$. Therefore in any case

$$c^*_{r,s} n_{+,u} c_{r,s} = (1 - \delta_{u,s}) n_{+,s}(1 - n_{+,r})[(1 - \delta_{u,r}) n_{+,u} + \delta_{u,r}(1 - n_{+,u})] \tag{45}$$

Now notice that, since $r \neq s$:

$$c_{r,s} c^*_{r,s} = \sigma_{+r}\sigma_{-s}\sigma^*_{-s}\sigma^*_{+r} = \sigma_{+r}\sigma_{-r}\sigma_{-s}\sigma_{+s} = n_{+,r}(1 - n_{+,s})$$

where we have used

$$\sigma_{-s}\sigma_{+s} = 1 - \sigma_{+s}\sigma_{-s}$$

Similarly

$$c^*_{r,s} c_{r,s} = \sigma^*_{-s}\sigma^*_{+r}\sigma_{+r}\sigma_{-s} = \sigma_{+s}\sigma_{-s}\sigma_{-r}\sigma_{+r} = n_{+,s}(1 - n_{+,r})$$

Using this we see that

$$-\frac{1}{2}\left\{n_{+,u},c_{r,s}c^*_{r,s}\right\}=-n_{+,u}n_{+,r}(1-n_{+,s}) \tag{46}$$

$$-\frac{1}{2}\left\{n_{+,u},c^*_{r,s}c_{r,s}\right\}=-n_{+,u}n_{+,r}(1-n_{+,s}) \tag{47}$$

Adding (78) and (88) we find

$$\Delta^-_{r,s}(X):=c_{r,s}Xc^*_{r,s}-\frac{1}{2}\left\{X,c_{r,s}c^*_{r,s}\right\}=(1-\delta_{u,r})n_{+,r}(1-n_{+,s})[(1-\delta_{u,s})n_{+,u}+$$

$$+\delta_{u,s}(1-n_{+,u})]-n_{+,u}n_{+,r}(1-n_{+,s})=$$

$$=(1-\delta_{u,r})(1-\delta_{u,s})n_{+,r}(1-n_{+,s})n_{+,u}+(1-\delta_{u,r})n_{+,r}(1-n_{+,s})\delta_{u,s}(1-n_{+,u})-n_{+,u}n_{+,r}(1-n_{+,s})$$

Recalling that the terms $\delta_{u,r}\cdot\delta_{u,s}$ give zero contribution because $r\neq s$, we find

$$\Delta^-_{r,s}(X)=(-\delta_{u,r}-\delta_{u,s})n_{+,r}(1-n_{+,s})n_{+,u}+\delta_{u,s}n_{+,r}(1-n_{+,s})-\delta_{u,s}n_{+,r}(1-n_{+,s})n_{+,u} \tag{48}$$

The $\delta_{u,s}$–factor in the first term on the right hand side of (90) is zero and the last term is identically zero, therefore

$$\Delta^-_{r,s}(X)=\delta_{u,s}n_{+,r}(1-n_{+,s})-\delta_{u,r}n_{+,r}(1-n_{+,s})n_{+,u}=(\delta_{u,s}-\delta_{u,r})\,n_{+,r}(1-n_{+,s}) \tag{49}$$

Noticing that, (87) and (89) are obtained respectively by (78) and (88) by the substiturions

$$s\to r\to s$$

we obtain the form of the other part of the generator:

$$\Delta^+_{r,s}(X)=(\delta_{u,r}-\delta_{u,s})\,n_{+,s}(1-n_{+,r}) \tag{50}$$

Introducing the notations

$$\gamma^-_{r,s}:=\gamma_{r,s}2\ \mathrm{Re}\ (g|g)^-_{r,s}\ ;\quad \gamma^+_{r,s}:=\gamma_{r,s}2\ \mathrm{Re}\ (g|g)^+_{r,s} \tag{51}$$

we obtain the action of the full generator on $n_{+,u}$:

$$\theta_0(n_{+,u})=\sum_{r\neq s\in\Lambda}\gamma^-_{r,s}\Delta^-_{r,s}(n_{+,u})+\gamma^+_{r,s}\Delta^+_{r,s}(n_{+,u})= \tag{52}$$

$$= \sum_{r\neq s\in\Lambda} \gamma^-_{r,s} \left(\delta_{u,s} - \delta_{u,r}\right) n_{+,r}(1 - n_{+,s}) + \gamma^+_{r,s} \left(\delta_{u,r} - \delta_{u,s}\right) n_{+,s}(1 - n_{+,r}) =$$

$$= \sum_{r\in\Lambda} \gamma^-_{r,u} n_{+,r}(1-n_{+,u}) + - \sum_{s\in\Lambda} \gamma^-_{u,s} n_{+,u}(1-n_{+,s}) + \sum_{s\in\Lambda} \gamma^+_{u,s} n_{+,s}(1-n_{+,u}) + - \sum_{r\in\Lambda} \gamma^+_{r,u} n_{+,u}(1-n_{+,r}) =$$

$$= \sum_{r\in\Lambda} \gamma^-_{r,u} n_{+,r} - \sum_{r\in\Lambda} \gamma^-_{r,u} n_{+,r} n_{+,u} - \sum_{s\in\Lambda} \gamma^-_{u,s} n_{+,u} + \sum_{s\in\Lambda} \gamma^-_{u,s} n_{+,s} n_{+,u} + \sum_{s\in\Lambda} \gamma^+_{u,s} n_{+,s} - -$$

$$- \sum_{s\in\Lambda} \gamma^+_{u,s} n_{+,s} n_{+,u} - \sum_{r\in\Lambda} \gamma^+_{r,u} n_{+,u} + \sum_{r\in\Lambda} \gamma^+_{r,u} n_{+,r} n_{+,u} =$$

$$= - \sum_{r\in\Lambda} n_{+,u} \left[(\gamma^-_{u,r} + \gamma^+_{r,u}) + (\gamma^-_{u,r} - \gamma^-_{r,u} + \gamma^+_{r,u} - \gamma^+_{u,r}) n_{+,r} \right] + \sum_{r\in\Lambda} (\gamma^-_{r,u} + \gamma^+_{u,r}) n_{+,r}$$

Notice that $L(n_{+,u})$ depends only on the real part of the transport coefficient therefore the only possible origins of divergencies in the current can be the thermodynamical limit.

The calculations above are correct. Summing up:

$$\theta_0(n_{+u}) = \sum_{r,s\in\Lambda} \gamma_{rs} \left(2\mathrm{Re}\,(g|g)^-_{rs} \left(\delta_{us} - \delta_{ur}\right) n_{+r} n_{-s} + 2\mathrm{Re}\,(g|g)^+_{rs} \left(\delta_{ur} - \delta_{us}\right) n_{+s} n_{-r} \right)$$

For $\gamma_{rs} = \gamma_{sr}$ this reduces to

$$\theta_0(n_{+u}) = \sum_{r,s\in\Lambda} \gamma_{rs} \left(2\mathrm{Re}\,(g|g)^-_{rs} + 2\mathrm{Re}\,(g|g)^+_{sr} \right) \left(\delta_{us} - \delta_{ur}\right) n_{+r} n_{-s} =$$

$$= \sum_{r\in\Lambda} \gamma_{ru} \Big(\left(2\mathrm{Re}\,(g|g)^-_{ru} + 2\mathrm{Re}\,(g|g)^+_{ur} \right) n_{+r} n_{-u} - \left(2\mathrm{Re}\,(g|g)^-_{ur} + 2\mathrm{Re}\,(g|g)^+_{ru} \right) n_{+u} n_{-r} \Big)$$

7 The case of radiative dispersion

In this section we will consider the case of radiative dispersion, characterized by

$$\omega(k) = \omega_0 |k| \tag{53}$$

where ω_0 is the energy of elementary excitation.

This allows to compute explicitly the δ–functions in the generalized susceptibilities (x.). A simple variation of the arguments below yield the result in the general case. Given (1) one has

$$\gamma_{r,s}^{-} = \gamma_{r,s} G(E_r - E_s)(n(E_r - E_s) + 1) \tag{54}$$

$$\gamma_{r,s}^{+} = \gamma_{r,s} G(E_r - E_s) n(E_r - E_s) \tag{55}$$

where

$$n(\rho) := \frac{e^{-\beta\rho}}{1 - e^{-\beta\rho}} \tag{56}$$

$$G(\rho) := 2\pi\rho^{d-1} \int_{S^{(d-1)}} d\hat{k} |g(\rho\hat{k})|^2 \tag{57}$$

$$2\mathrm{Re}\,(g|g)_{rs}^{-} = \frac{2\pi}{1 - e^{-\beta(E_r - E_s) - \mu}} \int dk |g(k)|^2 \delta(\omega(k) + E_s - E_r)$$

$$2\mathrm{Re}\,(g|g)_{rs}^{+} = \frac{2\pi}{e^{\beta(E_r - E_s) + \mu} - 1} \int dk |g(k)|^2 \delta(\omega(k) + E_s - E_r)$$

Since $\omega(k) = \omega_0 |k|$ for sufficiently wide cut–offs when one can take $g(k) = 1$ we get for the integral over k and get

$$\int dk |g(k)|^2 \delta(\omega(k) + E_s - E_r) = \omega_0^{-d} \theta(E_r - E_s)(E_r - E_s)^{d-1} \text{ volume of unit sphere}$$

where $\theta(E)$ is the Heavyside function (equal to 1 for $E > 0$ and to 0 otherwise). Denoting the volume of unit sphere in d–dimensional space by V_{d-1} we get

$$2\mathrm{Re}\,(g|g)_{rs}^{-} = \frac{2\pi}{1 - e^{-\beta(E_r - E_s) - \mu}} \omega_0^{-d} \theta(E_r - E_s)(E_r - E_s)^{d-1} V_{d-1}$$

$$2\mathrm{Re}\,(g|g)_{rs}^{+} = \frac{2\pi}{e^{\beta(E_r - E_s) + \mu} - 1} \omega_0^{-d} \theta(E_r - E_s)(E_r - E_s)^{d-1} V_{d-1}$$

For a high temperature and small chemical potential limit when

$$\frac{1}{1 - e^{-\beta(E_r - E_s) - \mu}} = \frac{1}{\beta(E_r - E_s) + \mu}$$

one gets

$$2\mathrm{Re}\,(g|g)_{rs}^{-} = 2\mathrm{Re}\,(g|g)_{rs}^{+} = \frac{2\pi\omega_0^{-d}\theta(E_r - E_s)}{\beta(E_r - E_s) + \mu}(E_r - E_s)^{d-1} V_{d-1}$$

8 The linear response approximation

Using the Langevin equation (**??**) and denoting L the generator θ_o given by (**??**), the expectation value in (x.) can be computed and yields the result

$$\langle J_\Lambda(t)\rangle = tr\,(\overline{\rho}L(X_t)) \tag{58}$$

where $L = L(E)$ depends on the electric field. We will compute the current at $E = 0$ but for a state $\overline{\rho} = \rho + d\rho$ which is invariant under a generator where $L(E)$ with $E \neq 0$. For such a state the mean current at $E = 0$ is

$$\langle J_t\rangle = tr((\rho + d\rho)L(X_t)] \tag{59}$$

where X_t is the location vector, L is the generator corresponding to zero electric field, ρ is the equilibrium state in the case of zero electric field, so that

$$L^*\rho = 0 \tag{60}$$

and $\overline{\rho} = \rho + d\rho$ is the equilibrium state if the electric field is dE. Let us write

$$L(E + dE) = L + dL \tag{61}$$

Then, by assumption

$$(L^* + dL^*)(\rho + d\rho) = 0 \tag{62}$$

From (68) we know that (73) is equivalent, at first order approximation, to

$$L^*(d\rho) + dL^*(\rho) = 0 \tag{63}$$

(because $dL^*(d\rho)$ is a second order term). Thus

$$L^*(d\rho) = -dL^*(\rho) \tag{64}$$

and the formula for the current in the linear response approximation becomes

$$\langle J_t\rangle = -Tr(dL^*(\rho)X_t) = -Tr(\rho dL(X_t)) \tag{65}$$

In the appendix we will show that if, instead of using the free dynamics and the non free equilibrium state, we use the free equilibrium state and the non free dynamics, then we obtain the same result.

9 A formula for electrical conductivity

Calculating

$$\theta_0(X) = \theta_0\left(\sum_{s\in\Lambda} s n_{+s}\right)$$

and using the results of section () we get

$$\theta_0(X) = \sum_{r,s\in\Lambda} \gamma_{rs}\left(2\mathrm{Re}\,(g|g)^-_{rs} + 2\mathrm{Re}\,(g|g)^+_{sr}\right)(s-r)n_{+r}n_{-s}$$

Applying the equilibrium state of the system with

$$\langle n_{-r}\rangle = \frac{1}{1+e^{-\beta E_r-\mu}}, \qquad \langle n_{+r}\rangle = \frac{e^{-\beta E_r-\mu}}{1+e^{-\beta E_r-\mu}},$$

we get

$$\langle\theta_0(X)\rangle = \sum_{r,s\in\Lambda} \gamma_{rs}\left(2\mathrm{Re}\,(g|g)^-_{rs} + 2\mathrm{Re}\,(g|g)^+_{sr}\right)(s-r)\frac{e^{-\beta E_r-\mu}}{1+e^{-\beta E_r-\mu}}\frac{1}{1+e^{-\beta E_s-\mu}}$$

The linear responce approximation means that in the formula above we consider $(g|g)^\pm$ calculated for zero electric field and $\langle n_{\pm r}\rangle$ calculated for non–zero electric field.

Taking $E_r = E_r^{(0)} + dE\cdot r$ and using that $\langle\theta_0(X)\rangle = 0$ if both the state and the generator is taken for $dE = 0$ we get for the current

$$\langle\theta_0(X)\rangle = \langle d\theta_0(X)\rangle = \sum_{r,s\in\Lambda} \gamma_{rs}\left(d2\mathrm{Re}\,(g|g)^-_{rs} + d2\mathrm{Re}\,(g|g)^+_{sr}\right)(s-r)\frac{1}{1+e^{\beta E_r+\mu}}\frac{1}{1+e^{-\beta E_s-\mu}}$$

Using the wide cut–off approximation $|g(k)| = 1$ this is reduced to

$$\sum_{r,s\in\Lambda}\gamma_{rs}\Bigg(2\mathrm{Re}\,(g|g)^-_{rs}\left(\frac{\beta}{e^{\beta(E_r^{(0)}-E_s^{(0)})+\mu}-1} + \frac{d-1}{E_r^{(0)}-E_s^{(0)}}\right) -$$

$$-d\mathrm{Re}\,(g|g)^+_{sr}\left(\frac{\beta}{1-e^{-\beta(E_s^{(0)}-E_r^{(0)})-\mu}} + \frac{d-1}{E_s^{(0)}-E_r^{(0)}}\right)\Bigg)(r-s)\cdot dE(s-r)\frac{1}{1+e^{\beta E_r+\mu}}\frac{1}{1+e^{-\beta E_s-\mu}}$$

In the high temperature low chemical potential limit this reduces to

$$\frac{\pi}{2}\omega_0^{-d}V_{d-1}\beta^{-1}\sum_{r,s\in\Lambda}\gamma_{rs}\frac{|E_r-E_s|^{d-1}}{|E_r-E_s|+\mu/\beta}\left(\frac{1}{|E_r^{(0)}-E_s^{(0)}|+\mu/\beta} + \frac{d-1}{|E_r^{(0)}-E_s^{(0)}|}\right)(r-s)\cdot dE(s-r)$$

When $\mu = 0$ and $d = 3$ this further reduces to a very simple expression

$$6\pi^2\omega_0^{-3}\beta^{-1}\sum_{r,s\in\Lambda}\gamma_{rs}(r-s)\cdot dE(s-r)$$

We want to calculate the expression (**??**). Following (**??**) the expression of the restriction of the generator to the N_u–variables is

$$L = \sum_{\substack{r\neq s\\ E_r>E_s}}(\gamma^-_{r,s}(E)\Delta_{r,s} + \gamma^+_{r,s}(E)\Delta_{s,r}) \tag{66}$$

where the $\gamma^{\pm}_{r,s}$ are given by (**??**) and

$$\Delta_{r,s}(X) = \sum_{u\in\Lambda}\Delta_{r,s}(N_u)u = \sum_{u\in\Lambda}(-\delta_{r,u}+\delta_{s,u})n_{+,r}(1-n_{+,s})u = n_{+,r}(1-n_{+,s})(s-r) \tag{67}$$

Since the $\Delta_{s,r}$'s do not depend on the electric field, its variation will be

$$dL = \sum_{\substack{r\neq s\\ E_r>E_s}}(d\gamma^-_{r,s}(E)\Delta_{r,s} + d\gamma^+_{r,s}\Delta_{r,s}) \tag{68}$$

where

$$d\gamma^{\pm}_{r,s}(E) = \gamma^{\pm}(\{E_s + s\cdot dE_s\}) - \gamma^{\pm}(\{E_s\}) \tag{69}$$

evaluated at first order. From the expressions (**??**) for $\gamma^{\pm}_{r,s}$ we see that $\gamma^{\pm}_{r,s}$ depend only on the differences $\{E_r - E_s\}$, $(E_r > E_s)$. More explicitly:

$$d\gamma^-_{r,s} = \gamma_{r,s}G'(E_r-E_s)dE\cdot(r-s)(n(E_r-E_s)+1)+\gamma_{r,s}G(E_r-E_s)n'(E_r-E_s)dE\cdot(r-s) \tag{70}$$

$$d\gamma^+_{r,s} = \gamma_{r,s}G'(E_r-E_s)dE\cdot(r-s)n(E_r-E_s)+\gamma_{r,s}G(E_r-E_s)(E_r-E_s)dE\cdot(r-s) \tag{71}$$

So that

$$Tr(\rho\Delta_{r,s}(X)) = (s-r)Tr\rho n_{+,r}(1-n_{+,s}) \tag{72}$$

Now we know that the equilibrium state of the field is

$$\rho = \otimes_{r\in\Lambda}\frac{e^{-\beta E_r n_{+,r}-\mu}}{Tr(e^{-\beta E_r n_{+,r}-\mu})} \tag{73}$$

So that the expectation value (72) is equal to

$$Tr(\rho\Delta_{r,s}(X)) = (s-r)p_r(1)p_s(0) \tag{74}$$

where

$$p_r(1) = Tr\left(\frac{e^{-\beta E_r n_{+,r}-\mu}}{Tr(e^{-\beta})} n_{+,r}\right) = \frac{e^{-\beta E_r-\mu}}{e^{-\beta E_r-\mu}+1} \tag{75}$$

$$p_s(0) = Tr\left(\frac{e^{-\beta E_s n_{+,s}-\mu}}{Tr(e^{-\beta E_s n_{+,s}-\mu})} (1-n_{+,s})\right) = \frac{1}{e^{-\beta E_s-\mu}+1} \tag{76}$$

In conclusion

$$Tr(\rho L(X)) = \sum_{\substack{r\neq s\\ E_r>E_s}} [\gamma^-_{r,s}(s-r)p_r(1)p_s(0) + (r-s)\gamma^+_{r,s}p_s(1)p_r(0)] \tag{77}$$

Therefore the expression of its variation will be

$$Tr(\rho dL(X)) = \sum_{\substack{r\neq s\in\Lambda\\ E_r>E_s}} (r-s)[d\gamma^+_{r,s}p_s(1)p_r(0) - d\gamma^-_{r,s}p_r(1)p_s(0)] = \tag{78}$$

Remark. In (x.20), $\gamma_{r,s} = \gamma_{s,r}$ and, given the form (**??**) of $n(E)$, one has

$$(n(E_r-E_s)+1)p_r(1)p_s(0) = \frac{e^{\beta E_s+\mu}}{(1-e^{-\beta(E_r-E_s)})(1+e^{+\beta E_r+\mu})(1+e^{\beta E_s \mu})} \tag{79}$$

$$n(E_r-E_s)p_s(1)p_r(0) = \frac{e^{-\beta(E_r-E_s)}e^{\beta E_r+\mu}}{(1-e^{-\beta(E_r-E_s)})(1+e^{\beta E_r+\mu})(1+e^{\beta E_s+\mu})} \tag{80}$$

which shows that these expression are equal, i.e.

$$\gamma^-_{r,s}p_r(1)p_s(0) = \gamma^+_{r,s}p_s(1)p_r(0) \tag{81}$$

this is the *detailed balance* condition which in particular implies

$$Tr(\rho L(X)) = 0 \tag{82}$$

Similarly, denoting dL the variation of L with respect to the electric field, from (**??**), (**??**), (**??**), we have

$$Tr(\rho dL(X)) = \tag{83}$$

$$= \sum_{\substack{r\neq s\in\Lambda\\ E_r>E_s}} (r-s)[\gamma_{r,s}G'(E_r-E_s)dE\cdot(r-s)\{n(E_r-E_s)p_s(1)p_r(0) - (n(E_r-E_s)+1)p_r(1)p_s(0)\}$$

$$+\gamma_{r,s}G(E_r-E_s)dE\cdot(r-s)n'(E_r-E_s)\{p_s(1)p_r(0) - p_r(1)p_s(0)\}]$$

and the G'–term vanishes because of the identity of the expressions (**??**) and (**??**). Moreover

$$p_s(1)p_r(0) - p_r(1)p_s(0) = \frac{e^{-\beta E_s - \mu} - e^{-\beta E_r - \mu}}{(e^{-\beta E_r - \mu} + 1)(e^{-\beta E_s - \mu} + 1)} \tag{84}$$

$$n'(E) = -\beta e^{-\beta E}(1 - e^{-\beta E})^{-1} + e^{-\beta E}(-1)(1 - e^{-\beta E})^{-2}(+\beta e^{-\beta E}) = -\beta n(E)(n(E+1))$$

Therefore

$$-Tr(\rho dL(X)) =$$

$$= \sum_{\substack{r \neq s \\ E_r > E_s}} \gamma_{r,s} \beta n(E_r - E_s)(n(E_r - E_s) + 1) \frac{e^{-\beta E_s - \mu} - e^{-\beta E_r - \mu}}{(e^{-\beta E_r - \mu} + 1)(e^{-\beta E_s - \mu} + 1)} G(E_r - E_s)(r - s) dE \cdot (r - s)$$

$$=: \sum_{\substack{r \neq s \\ E_r > E_s}} \gamma_{r,s} K(r,s)(r - s) dE \cdot (r - s) \tag{85}$$

where

$$K(r,s) := \beta n(E_r - E_s)(n(E_r - E_s) + 1) \frac{e^{-\beta E_s - \mu} - e^{-\beta E_r - \mu}}{(e^{-\beta E_r - \mu} + 1)(e^{-\beta E_s - \mu} + 1)} G(E_r - E_s) \geq 0 \tag{86}$$

Now suppose that

$$\gamma_{r,s} = \gamma(r - s) \tag{87}$$

and that there is a number $d > 0$ such that

$$\gamma(x) = 0 \qquad \text{if} \qquad |x| > d \tag{88}$$

Then

$$\langle J \rangle = \sum_{\substack{s \neq r \in \Lambda \\ E_r > E_s}} \gamma(r - s) K(r,s)(r - s) dE \cdot (r - s) = \tag{89}$$

$$= \sum_{|n| \leq d} \gamma(u) u dE \cdot u \left(\sum_{\substack{r, r+u \in \Lambda \\ E_r > E_{r+u}}} K(r, r+u) \right)$$

Therefore the current density is

$$\frac{\langle J \rangle}{|\Lambda|} = \sum_{|u| \leq d} \gamma(u) u dE \cdot u \left(\frac{1}{|\Lambda|} \sum_{\substack{r, r+u \in \Lambda \\ E_r > E_{r+u}}} K(r, r+u) \right) \tag{90}$$

where K, in (52), is given by the expression (**??**). In many cases, for large Λ, the Cesaro mean in (90) does not depend on K. For example if, in , we assume that the energy levels E_r, E_r are independent, identically distributed random variables (but in fact a weak ergodicity condition would be sufficient), then we can replace the volume average in (90) by the expectation value of K:

$$\overline{K} = \mathbb{E}K(E_r, E_s) \tag{91}$$

Example: In the nearest neighbor 3–dimensional isotropic case ($\gamma(u) = \gamma$, constant and $L = \mathbf{Z}^3$, one has

$$\sum \gamma\vec{u}|\vec{u}\rangle\langle\vec{u}| = \gamma \sum_{\pm,i=1,2,3} |\pm i\rangle\langle\pm i| = 2\gamma$$

In conclusion the vector representing the density (per unit volume) of electric current is:

$$\vec{i} = \beta K \sum_{|u|\leq d} \gamma(u)(dE \cdot u)u$$

and the conductivity tensor, defined by

$$\frac{\partial\langle J_{\Lambda,i}(t)\rangle}{\partial E_j}\Big|_{t=0} =: C_{ij}(t)$$

is given, in the isotropic case, by

$$\sigma = \beta K \sum_{\vec{u}} \gamma u|\vec{u}\rangle\langle\vec{u}|$$

10 Conclusions

By applying the stochastic limit technique to a microscopic Hamiltonian model, defined by equations (**??**), (**??**), (**??**), we have deduced a stochastic Schrödinger equation (**??**) in which all the parameters defining the equation and the Brownian motions have an interpretation in terms of the microscopic Hamiltonian model. The associated Langevin equation has been deduced in section (4) and the master equation in section (5). In sections (6), (7) and (8) we have applied linear response theory to the variation of the generator of the master equation as a function of the external electric field and deduced the conductivity tensor (formula (**??**))

The equation we find belongs to the class of general equations deduced from the stochastic limit in [AcKo99a], [AcKo99b]. Shortly after R. Rebolledo and F. Fagnola, by directly postulating a quantum stochatic differential equation, constructed and studied a quantum Markov semigroup which corresponds to a natural quantum extension of the classical exclusion process. R. Rebolledo and F. Fagnola were motivated by a model of electronic transport discussed with J. Bellissard and W.von Waldenfels. Previous phenomenological models, based on classical (jump) stochastic equations, were considered by Bellissard as an improvement of previous Hamiltonian models studied by Bellisard and Schultz–Baldes in a series of a papers devoted to the problem of conductivity in a quasi–crystal.

The present paper can be considered as a deduction, from a basic Hamiltonian model of the phenomenological model considered by Rebolledo, Fagnola, Bellissard and W.von Waldenfels. In addition we compute the conductivity tensor and we prove that it is an extensive quantity.

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Added 10-8-2007 (the first time I could see the preprint below)

The reference [RFBvW00] should be complemented by the thesis of D. Spehner (of which I have no reference) and the article:

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