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LOCAL EXPECTATIONS IN TUNNELLING JUNCTION

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Abstract. We consider a quantum nano-wire in contact with two infinite reservoirs which are in thermal equilibrium at different temperatures and chemical potentials. In tight banding approximation the evolution of the system is quasi-free and for large time approaches a Non-Equilibrium Steady State (NESS) which in turn is quasi-free. This NESS is analyzed and explicit and calculable expressions for expectations of local observables is obtained.

Key words: quantum nano-wire, tunnelling, non-equilibrium steady state.

1. INTRODUCTION

In recent years there has been renewed interest in rigorous aspects of non-equilibrium quantum statistical mechanics, and a lot of significant results have been obtained in the C^*-scattering approach proposed by Ruelle in [1]. In this framework numerous examples of Non-Equilibrium Steady State (NESS) are constructed for open quantum systems (see [2, 3] for reviews of the state of art). Typically such a system is a small quantum sample $\mathcal{S}$ driven out of equilibrium by infinite reservoirs $\mathcal{R}_1$ and $\mathcal{R}_2$ which are in thermal equilibrium at different temperatures and chemical potentials. Most of the reservoir models considered in the literature are simply free quantum gases of identical particles. When confined to a finite region, the number of particles N_i, i =1, 2 in each reservoir is conserved and, according to the grand-canonical prescription, the reservoir Hamiltonians H_i are to be replaced by $H_i - \mu_i N_i$ in the Gibbs ansatz, where the multipliers μ_i are adjusted to ensure given particle densities in the reservoirs. The equilibrium states of the reservoirs in the infinite-volume limit are well-known, and turn out to be *quasi-free* states (*i.e.* states in which there are no correlations of order higher than 2) [4]. If, moreover, the perturbed (coupled) dynamics is likewise supposed quasi-free, not only the initial constrained equilibrium state of the uncoupled system, but also its time-evolution under the perturbed dynamics and hence its limit, the NESS, are quasi-free. This setting has been analyzed in a series of recent papers in the case of Fermi statistics [5–7] and Bose statistics [8, 9]. The main simplifying

feature in this case is that the problem is reduced to a scattering problem for the one-particle Hamiltonians, which is considerably simpler. However, obtaining explicit computable expressions of the different physical quantities, such as density and local-energy profiles within the system, or particle and energy currents through the sample, still remains a task to be performed, in order to obtain specific results of physical interest.

The paper is devoted to the latter task in the particular geometric setting considered in [7], which we shortly describe below.

We consider the system consisting of two particle reservoirs, $\mathcal{R}_{1,2}$, connected by a one-dimensional wire, $\mathcal{S}$. *The reservoirs* $\mathcal{R}_{1,2}$ are taken as infinitely extended lattice quantum Fermi gases. The particles in the reservoirs live, respectively, on the two infinite or half-infinite lattices,

$$\Lambda_{1,2} = \mathbb{Z}^{d_{1,2}} \quad \text{or} \quad \Lambda_{1,2} = \mathbb{Z}^{d_{1,2}-1} \times \mathbb{Z}_+, \tag{1.1}$$

where $\mathbb{Z}$ denote the set of integers and $\mathbb{Z}_+$ denote the set of strictly positive integers.

The Hilbert space of one-particle states in $\mathcal{R}_{1,2}$ is therefore

$$\mathcal{H}_i = l_2(\Lambda_i) = \left\{ f : \Lambda_i \to \mathbb{C};\ \|f\|^2 = \sum_{x\in\Lambda_i} |f(x)|^2 < \infty \right\}, \quad i = 1, 2. \tag{1.2}$$

The one particle Hamiltonian of the *reservoirs* $\mathcal{R}_{1,2}$ is the kinetic energy operator in tight binding approximation, *i.e.* is 1/2 times the lattice Laplace operator with free boundary conditions:

$$(h_i f)(x) = d\, f(x) - \frac{1}{2} \sum_{y\in\Lambda_i, |y-x|=1} f(y),\ i = 1, 2. \tag{1.3}$$

The nano-wire $\mathcal{S}$ is modeled as a free quantum Fermi gas in which particle live on the finite set of sites $\{1, 2, \ldots, n\}$ with one-particle states $\mathcal{H}_S = l_2(\Lambda_S) \equiv \mathbb{C}^n$, $\Lambda_S = \{1, 2, \ldots, n\}$ and the Hamiltonian

$$(h_0 f)_i = (1 + e_g) f_i - 1/2(f_{i-1} + f_{i+1}),\ \ i = 1, \ldots, n\ \ (f_0 = f_{n+1} = 0), \tag{1.4}$$

where the parameter e_g plays the role of an adjustable gate potential.

As consequence, the one-particle Hilbert space for the entire system, $\mathcal{R}_1 \cup \mathcal{S} \cup \mathcal{R}_2$ is

$$\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_S \oplus \mathcal{H}_2 = l_2(\Lambda),\ \text{where}\ \ \Lambda = \Lambda_1 \cup \Lambda_S \cup \Lambda_2 \tag{1.5}$$

and the evolution of the one-particle states for the uncoupled system is given by the one-particle Hamiltonian

$$h_0 = h_1 \oplus h_S \oplus h_2 \tag{1.6}$$

Let α_1 denote the site $(0,\ldots,0) \in \mathbb{Z}^{d_1}$ if $\Lambda_1 = \mathbb{Z}^{d_1}$ or $(0,\ldots,0,1) \in \mathbb{Z}^{d_1-1} \times \mathbb{Z}_+$ if $\Lambda_1 = \mathbb{Z}^{d_1-1} \times \mathbb{Z}_+$, and the similar notation α_2 in the case of Λ_2. At $t = 0$, tunneling junctions are turned on between the reservoirs and the ends of the wire through the pairs of sites $(\alpha_1, 1)$ and (α_2, n), this is given by the one-particle operator v defined by the matrix

$$v_{x,y} = \begin{cases} t, & \text{if either } \{x,y\} = \{\alpha_1, 1\} \text{ or } \{\alpha_2, n\} \\ 0, & \text{otherwise.} \end{cases} \tag{1.7}$$

Thus, the evolution of the one-particle states in the coupled system is generated by the Hamiltonian:

$$h = h_0 + v. \tag{1.8}$$

We denote a_x^* the creation operator for a Fermion at the site $x \in \Lambda$. The local observables of the system are generated by products of local operators $a^*(f) = \sum_{x\in\Lambda} f(x)a_x^*$, $a(f) = \sum_{x\in\Lambda} \overline{f}(x)a_x$, where $f \in \mathcal{H}$. The one-particle Hamiltonians h_0 and h define two Heisenberg dynamics of the local observables, which reads for the operators $a^\sharp(f)$ as

$$\begin{aligned} \alpha^t(a^\sharp(f)) &= a^\sharp(e^{ih^0 t} f), \\ \tau^t(a^\sharp(f)) &= a^\sharp(e^{iht} f). \end{aligned} \tag{1.9}$$

Also, let ϕ^θ denote the gauge automorphism group

$$\phi^\theta(a^\sharp(f)) = a^\sharp(e^{i\theta} f). \tag{1.10}$$

The states of our system are positive linear functionals ω on the algebra of local observables, of norm $\|\omega\| = \omega(1) = 1$. A state ω is gauge invariant if $\omega\left(\prod_{i=1}^n a^*(g_i)\prod_{i=1}^n a(f_i)\right) = 0$, $\forall n \neq m$. For any state ω, the formula

$$\omega(a^*(g)a(f)) = (f, \rho g) \tag{1.11}$$

defines a self-adjoint operator $0 \le \rho \le 1$ on $\mathcal{H}$, called its density operator.

Given ρ self-adjoint with $0 \le \rho \le 1$, there exists a unique quasi-free, gauge-invariant state ω with density operator ρ. The higher order expectations are expressed in this state ω by

$$\omega(a^*(g_m)\dots a^*(g_1)a(f_1)\dots a(f_n)) = \delta_{m,n}\det\{(f_i,\, \rho g_j)\}. \tag{1.12}$$

For our models of reservoirs, like for any free Fermi gas, there exist, at each values of the temperature $\beta_{1,2}^{-1}$ and chemical potentials $\mu_{1,2}$, unique equilibrium states; they are the gauge-invariant quasi-free states with density operators $f_{\beta_i,\mu_i}(h_i)$, respectively, where h_i are the one-particle Hamiltonians, and $f_{\beta,\mu}$ is the Fermi-Dirac function:

$$f_{\beta,\mu}(x) = \frac{1}{1+e^{\beta(x-\mu)}} \tag{1.13}$$

Therefore, the initial state ω^0 of our system is quasi-free and α^t-invariant (as its density operator ρ^0 commutes with h_0), and its evolution ω^t under the perturbed dynamics τ^t is likewise a quasi-free state with density operator:

$$\rho^t = [e^{-ith_0}e^{ith}]^*\rho^0 e^{-ith_0}e^{ith}; \tag{1.14}$$

indeed, using the α^0-invariance of ω^0,

$$\omega^t(a^*(g)a(f)) := \omega^0(\tau^t(a^*(g)a(f))) = \omega^0(\alpha^{-t}\circ\tau^t(a^*(g)a(f))) =$$
$$= \omega^0(a^*(e^{-ith_0}e^{ith}g)a(e^{-ith_0}e^{ith}f)) = (e^{-ith_0}e^{ith}g, \rho^0 e^{-ith_0}e^{ith}f).$$

The NESS is the large-time limit of the states ω^t. It can therefore be expressed in terms of the Möller operators of the uncoupled and coupled evolutions, *i.e.*, for f in the subspace of absolute continuity of h_0,

$$\lim_{t\to\infty} e^{-ith}e^{ith_0}f = \Omega_- f \tag{1.15}$$

and its adjoint Ω_-^*. The exact result is the following: *The NESS is the quasi-free state* ω_{stat} *with density operator*

$$\rho_{stat} = \Omega_-\rho^0\Omega_-^* + \sum_{e\in\sigma_{pp}(h)} P_e\rho^0 P_e \tag{1.16}$$

where $\sigma_{pp}(h)$ is the pure point spectrum of h and P_e is the projector on the eigenspace of eigenvalue e.

The next section is devoted to the spectral analysis of the one-particle Hamiltonian. In Sec. 3, the expression of the kernel of the Möller operators are obtained and the expectations of various physical quantities are written down.

2. ONE PARTICLE HAMILTONIAN

The spectrum and eigenvectors of the uncoupled one-particle Hamiltonian h_0 are well-known and are shortly summarized below. If $\Lambda_1 = \mathbb{Z}^{d_1}$, a complete set of generalized eigenvectors of h_1 are $\psi_1(k, \cdot) \in l_\infty(\Lambda_1)$, $k \in \mathbb{T}^{d_1}$, where the index set is the torus $\mathbb{T}^{d_1} = [0, 2\pi)^{d_1}$ and

$$\psi_1(k, x) = (2\pi)^{-d/2} \exp(ikx). \tag{2.1}$$

If $\Lambda_1 = \mathbb{Z}^{d_1-1} \times \mathbb{Z}_+$, the generalized eigenvectors of h_1 are

$$\psi_1(k, x) = 2(2\pi)^{-d/2} \exp(ik'x') \sin(k^d x^d) \tag{2.2}$$

and are indexed by $k = (k', k^{d_1}) \in \mathbb{T}^{d_1-1} \times (0, \pi)$. In both cases $\psi_1(k, \cdot)$ corresponds to the generalized eigenvalue

$$\omega(k) = 2 \sum_{\alpha=1}^{d} \sin^2(k^\alpha/2). \tag{2.3}$$

Therefore the spectrum of h_1 is absolutely continuous and coincides with the interval $[0, 2d_1]$. In fact, we define the unitary operator $u_1 : \mathcal{H}_1 \to L_2(\mathbb{T}^{d_1})$ (or $L_2(\mathbb{T}^{d_1-1} \times (0, \pi))$) by

$$(u_1\phi)(k) := \hat{\phi}(k) = \sum_{x \in \Lambda_1} \overline{\psi}_1(k, x)\phi(x); \tag{2.4}$$

then, $u_1 h_1 (u_1)^*$ is the operator of multiplication with the function $\omega(k)$ on $L_2(\mathbb{T}^{d_1})$ or $L_2(\mathbb{T}^{d_1-1} \times (0, \pi))$. Identical considerations with obvious notations are valid for one-particle Hamiltonian h_2 of second reservoir $\mathcal{R}_2$.

The eigenvalues of $h_{\mathcal{S}}$ are $\varepsilon_m = e_g + 2\sin^2(q_m/2)$; $m = 1, \ldots, n$, where $q_m = m\pi/(n+1)$, with eigenvectors $\psi^{(m)}$:

$$\psi_i^{(m)} = \sqrt{\frac{2}{n+1}} \sin(q_m i). \tag{2.5}$$

We now consider the perturbed (coupled) Hamiltonian h. As the perturbation v has finite range, general results in scattering theory (Kato-Rosenberg theorem [10]) ensure that the wave operators for the pair h, h_0 exist and are complete, therefore the absolutely continuous spectra of h and h_0 coincide, and that h has no singular continuous spectrum.

The main step in performing the spectral analysis of h, *i.e.* finding the eigenvectors for the point spectrum and generalized eigenvectors for the absolutely continuous spectrum consists in obtaining a convenient expression of its resolvent operator $R(z)=(h-z)^{-1}$.

In fact, we have to solve the equation

$$(h_0 - z + v)\psi = f, \tag{2.6}$$

for $\psi, f \in \mathcal{H} = l_2(\Lambda)$ or $\psi \in l_\infty(\Lambda)$ and $f = 0$.

Corresponding to the direct sum (1.5) we use matrix representation of vectors and operators in $\mathcal{H}$ and the equation becomes

$$\begin{aligned} &(h_1 - z)\psi_1 + t\psi_{\mathcal{S}}(1)\delta_{1,\alpha_1} = f_1 \\ &(h_{\mathcal{S}} - z)\psi_{\mathcal{S}} + t\psi_1(\alpha_1)\delta_{\mathcal{S},1} + t\psi_2(\alpha_2)\delta_{\mathcal{S},n} = f_{\mathcal{S}} \\ &(h_2 - z)\psi_2 + t\psi_{\mathcal{S}}(n)\delta_{2,\alpha_2} = f_2 \end{aligned} \tag{2.7}$$

where $\delta_{i,x}$ and $\delta_{\mathcal{S},x}$ are delta functions at point x on Λ_i, $i = 1, 2$ and on $\Lambda_{\mathcal{S}}$ respectively.

As h is selfadjoint it is sufficient to consider $\mathrm{Im} z \geq 0$. If $z \notin \sigma(h_1) \cup \sigma(h_2)$, then the resolvents $R_{1,2}(z) = (h_{1,2} - z)^{-1}$ exist, and ψ_1, ψ_2 are determined from first and third equation. The second equation becomes

$$(h_{\mathcal{S}} - z - t^2 R_1(z;\alpha_1,\alpha_1)\pi_1 - t^2 R_2(z;\alpha_2,\alpha_2)\pi_2)\psi_{\mathcal{S}} = \tilde{f}_{\mathcal{S}} \tag{2.8}$$

where

$$\tilde{f}_{\mathcal{S}} = f_{\mathcal{S}} - t(R_1(z)f_1)(\alpha_1)\delta_{\mathcal{S},1} - t(R_2(z)f_2)(\alpha_2)\delta_{\mathcal{S},n} \tag{2.9}$$

and π_1, π_n are the orthogonal projectors on $\delta_{\mathcal{S},1}$ and $\delta_{\mathcal{S},n}$ respectively. Denote $g_1(z) = R_1(z;\alpha_1,\alpha_1)$ and $g_2(z) = R_2(z;\alpha_2,\alpha_2)$. The operator

$$h_{ef}(z) = h_{\mathcal{S}} - z - t^2 g_1(z)\pi_1 - t^2 g_2(z)\pi_2 \tag{2.10}$$

acting on the finite dimensional space $\mathcal{H}_{\mathcal{S}}$ is invertible if and only if $\ker h_{ef}(z) = \{0\}$. If $\varphi \in \ker h_{ef}(z)$ we have $\mathrm{Im}(\varphi, h_{ef}(z)\varphi) = 0$, *i.e.*

$$-\mathrm{Im} z \cdot \|\varphi\|^2 - t^2(\mathrm{Im} g_1(z) \cdot \|\pi_1\varphi\|^2 + \mathrm{Im} g_2(z) \cdot \|\pi_1\varphi\|^2 = 0. \tag{2.11}$$

Due to the fact that $\mathrm{Im} g_{1,2}(z) \geq 0$ for $\mathrm{Im} z \geq 0$ and $\mathrm{Im} g_{1,2}(\lambda + i0) > 0$ for $\lambda \in \sigma(h_{1,2})$ the last equation can be fulfilled only for $z \in \mathbb{R} \setminus (\sigma(h_1) \cup \sigma(h_2))$ and we have the following result:

Proposition 1. *In the upper complex semi plan* $\mathrm{Im} z \geq 0$, *the* $\ker h_{ef}(z)$ *can be non-trivial only for z in a finite set of* $\mathbb{R} \setminus (\sigma(h_1) \cup \sigma(h_2))$. *The pure point spectrum of h is* $\sigma_{pp}(h) = \{\lambda : \lambda \in \mathbb{R},\ \ker h_{ef}(z) \neq \{0\}\}$ *and* $\sigma_{pp}(h) \cap \sigma_{ac}(h) = \varnothing$ *i.e. there are no eigenvalues in the continuous spectrum of h.*

For finding the eigenvectors and the generalized eigenvectors for the operator h we have to solve (2.7) for $f_1 = f_{\mathcal{S}} = f_2 = 0$, $\psi \in l_\infty(\Lambda)$. We start with the first equation in (2.7) . First remark that if $\lambda \in \mathbb{R} \setminus \sigma(h_1)$, then, clearly,

$$\psi_1 = -t\psi_{\mathcal{S}}(1) R_1(\lambda) \delta_{1,\alpha_1}. \tag{2.12}$$

Moreover, it can be seen that (2.12) still remains a solution if $\lambda \in \sigma(h_1)$, because the matrix elements $R_1(\lambda, x, y)$ are well defined for $x, y \in \Lambda_1$, and behave like $|x-y|^{-1/2}$ for large $|x-y|$, see [12]. However if $\lambda \in \sigma(h_1)$, the general solution is obtained by adding an arbitrary generalized eigenfunction of h_1 corresponding to eigenvalue λ, say $\phi_1(\lambda, \cdot)$. Hence, for any $\lambda \in \mathbb{R}$, we can write

$$\psi_1 = -t\psi_{\mathcal{S}}(1) R_1(\lambda) \delta_{1,\alpha_1} + \mathbf{1}_{\sigma(h_1)}(\lambda) \phi_1(\lambda, \cdot). \tag{2.13}$$

where $\mathbf{1}_A$ is characteristic function of set A.

Similarly, for any $\lambda \in \mathbb{R}$,

$$\psi_2 = -t\psi_{\mathcal{S}}(n) R_2(\lambda) \delta_{2,\alpha_2} + \mathbf{1}_{\sigma(h_2)}(\lambda) \phi_2(\lambda, \cdot). \tag{2.14}$$

Finally, from (2.8) with $f_{\mathcal{S}} = 0$,

$$\begin{aligned} \psi_{\mathcal{S}} = &-t\mathbf{1}_{\sigma(h_1)}(\lambda) \phi_1(\lambda, \alpha_1) h_{ef}^{-1}(\lambda) \delta_{\mathcal{S},1} - \\ &-t\mathbf{1}_{\sigma(h_2)}(\lambda) \phi_2(\lambda, \alpha_2) h_{ef}^{-1}(\lambda) \delta_{\mathcal{S},n} + \mathbf{1}_{\sigma_{pp}(h)} \phi_{\mathcal{S}}(\lambda, \cdot) \end{aligned} \tag{2.15}$$

where $\phi_{\mathcal{S}}(\lambda, \cdot)$ is an arbitrary element of $\ker h_{ef}(\lambda)$.

Therefore, we have proved

Proposition 2. *Suppose* $\sigma(h_1) \subset \sigma(h_2)$, *i.e.* $d_1 \leq d_2$. *For* $\lambda \in \sigma(h_1)$, *the generalized eigenfunction* $\tilde{\phi}(\lambda, \cdot) \equiv \left(\tilde{\phi}_1(\lambda, \cdot), \tilde{\phi}_{\mathcal{S}}(\lambda, \cdot), \tilde{\phi}_2(\lambda, \cdot)\right)$ *of h, which behave as the generalized eigenfunction* $\phi(\lambda, \cdot) \equiv (\phi_1(\lambda, \cdot), 0, \phi_2(\lambda, \cdot))$ *of* $h_1 + h_2$, *is*

$$\begin{aligned} \tilde{\phi}_1(\lambda, \cdot) &= R_1(\lambda) v h_{ef}^{-1} v \phi(\lambda, \cdot) + \phi_1(\lambda, \cdot) \\ \tilde{\phi}_{\mathcal{S}}(\lambda, \cdot) &= -h_{ef}^{-1} v \phi(\lambda, \cdot) \\ \tilde{\phi}_2(\lambda, \cdot) &= R_2(\lambda) v h_{ef}^{-1} v \phi(\lambda, \cdot) + \phi_2(\lambda, \cdot). \end{aligned} \tag{2.16}$$

For $\lambda \in \sigma(h_2) \setminus \sigma(h_1)$, *the same equations* (2.16) *gives the generalized eigenfunction* $\tilde{\phi}(\lambda, \cdot)$ *of h, which behave as the generalized eigenfunction* $\phi(\lambda, \cdot) \equiv (0, 0, \phi_2(\lambda, \cdot))$ *of* $h_1 + h_2$.

For $\lambda \in \sigma_{pp}(h)$ *the eingenfunction* $\tilde{\phi}(\lambda, \cdot)$ *of h corresponding to eigenfunction* $\phi_{\mathcal{S}}(\lambda, \cdot)$ *of* h_{ef} *is*

$$\begin{aligned} \tilde{\phi}_1(\lambda, \cdot) &= -R_1(\lambda) v \phi_{\mathcal{S}}(\lambda)(\cdot) \\ \tilde{\phi}_{\mathcal{S}}(\lambda, \cdot) &= \phi_{\mathcal{S}}(\lambda, \cdot) \\ \tilde{\phi}_2(\lambda, \cdot) &= -R_2(\lambda) v \phi_{\mathcal{S}}(\lambda)(\cdot). \end{aligned} \tag{2.17}$$

3. EXPECTATIONS FOR PARTICLE AND ENERGY DENSITY

We are interested to give explicit expressions for the expectations of local observables as number of particle $n_x = a_x^* a_x$ or density energy at some site $x \in \Lambda$

$$e_x = d a_x^* a_x - \frac{1}{4}\left(\sum_{y, |x-y|=1} a_x^* a_y + h.c \right), \quad d = d_1, d_2 \text{ or } 1,$$

therefore it is sufficient to have expressions for the two-point functions in the NESS:

$$\omega_{stat}(a_x^* a_y) = (\delta_y, \rho_{stat} \delta_x).) \tag{3.1}$$

In the expression Eq. (1.16) for ρ_{stat}, the second term, representing the sum over the point spectrum, can be easily calculated using the formula (2.17) for the eigenfunctions of *h*. We are thus left with the calculation of the contribution of the absolutely continuous spectrum $(\delta_y, \Omega\_\rho^0 \Omega\_^* \delta_x)$.

The generalized eigenfunctions of *h* are obtained from those of h^0, $\psi_1(k, \cdot) \oplus 0 \oplus 0$ and $0 \oplus 0 \oplus \psi_2(k, \cdot)$ using Eq. (2.16). We obtain:

$$\tilde{\psi}_1(k_1, \cdot) = \begin{cases} R_1(\omega(k_1)) v h_{ef}^{-1} v \psi_1(k_1,)(\cdot) + \psi_1(k_1 \cdot) \\ -h_{ef}^{-1} v \psi_1(k_1,)(\cdot) \\ R_2(\omega(k_1)) v h_{ef}^{-1} v \psi_1(k_1,)(\cdot) \end{cases} \tag{3.2}$$

and the analogous expression for $\tilde{\psi}_2$.

We use the expansion of δ_x over the eigenfunctions of *h*; denoting $P_{ac}(h)$ the projection onto the absolutely continuous part of *h*, we have

$$P_{ac}(h)\delta_x = \sum_{i=1}^{2} \int d^{d_i} k_i \tilde{\psi}_i(k_i,) \bar{\tilde{\psi}}_i(k_i, x) \tag{3.3}$$

As $\Omega_$sends the generalized eigenfunctions of h_0 into generalized eigenfunctions of h, we have

$$\Omega^*\_\delta_x = \sum_{i=1}^{2} \int d^{d_i} k_i \psi_i(k_i,) \bar{\tilde{\psi}}_i(k_i, x) \tag{3.4}$$

therefore

$$(\delta_y, \Omega\_\rho^0 \Omega^*\_\delta_x) = \sum_{i=1}^{2} \int d^{d_i} k_i d^{d_i} k_i' \bar{\tilde{\psi}}_i(k_i, y)(\psi_i(k_i), \rho^{0,i} \psi_i(k_i')) \bar{\tilde{\psi}}_i(k_i, x) \tag{3.5}$$

It is to be remarked that $(\psi_i(k), \rho^0 \psi_i(k)) = \delta(\omega(k) - \omega(k')) f_{\beta,\mu}(\omega(k))$, what allows to express Eq. (3.5) as one integral over energy.

Equation (3.5) together with the expressions (3.2) of the generalized eigenfunctions allow the calculation of all local physical quantities of interest.

In a subsequent publication we shall analyze the numerical results on the density and local-energy profiles through the sample corresponding to certain values of the length n of the sample, gate potential e_g and dimensions d_i of the reservoirs.

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