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Quasi-free Quantum Statistical Models for Tunnelling Junction

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1. Introduction

1.1. General frame

During the last decade considerable progress has been achieved in the statistical description of non-equilibrium thermodynamic processes. While previous work concentrated and provided a reasonable understanding of situations near thermal equilibrium, such as stability of equilibrium states (approach to equilibrium) or linear response, a consistent mathematical framework initiated by Ruelle [16], is now available for accounting for the installation, at large time, of a non-equilibrium stationary state (NESS) even when the initial state of the system is far from equilibrium (see [3] for a recent review). The typical physical situation which fits in this framework is that of several reservoirs, R_i; $i = 1, ..., r$, coupled to a finite quantum system, S (sample). One has to give account for the flow of energy and particles through the sample in the large time asymptotic regime.

The isolated sample S is a usual quantum system with Hilbert space $\mathcal{H}_S$, algebra of observables $\mathcal{A}_S$ equal to the algebra of all bounded operators on $\mathcal{H}_S$, and unitary dynamics generated by the Hamiltonian H_S. The Heisenberg picture of the evolution is the automorphism group on $\mathcal{A}_S$ defined as $\alpha_S^t(A) = \exp(\mathrm{i}tH_S)A\exp(-\mathrm{i}tH_S)$. We suppose that the sample is at time $t = 0$ in an arbitrary invariant state ω_S^0, i.e. the expectation of an observable $A \in \mathcal{A}_S$ is given by a density matrix: $\omega_S^0(A) = \mathrm{tr}(\rho_S A)$ and $[\rho_S, H_S] = 0$.

The description of the reservoirs R_i is somewhat more elaborated. A reservoir is an *infinite* quantum system, which, before the coupling to the sample is switched on, is in a certain equilibrium state. Its description in the initial state fits therefore in the well-established algebraic formalism of equilibrium quantum statistical mechanics [4]. One starts with reservoirs finitely extended in some regions Λ_i of space: the pure states are the unit vectors in a Hilbert space $\mathcal{H}_{i,\Lambda_i}$, the algebra of observables $\mathcal{A}_{i,\Lambda_i}$ consists of all bounded operators on $\mathcal{H}_{i,\Lambda_i}$ and the (Heisenberg) dynamics on $\mathcal{A}_{i,\Lambda_i}$ is generated by a self-adjoint Hamiltonian H_{i,Λ_i}, $\alpha_{i,\Lambda_i}^t(A) = \exp(\mathrm{i}tH_{i,\Lambda_i})A\exp(-\mathrm{i}tH_{i,\Lambda_i})$; at given inverse temperature β_i, the finite reservoir i has one equilibrium state $\omega_{i,\beta_i,\Lambda_i}(A) = \mathrm{tr}(A\rho_{i,\beta_i,\Lambda_i})$ given by the Gibbs ansatz for the density matrix $\rho_{i,\beta_i,\Lambda_i} = (1/Z_{i,\Lambda_i}(\beta_i))\exp(-\beta_i H_{i,\Lambda_i})$, where the statistical sum $Z_{i,\Lambda_i}(\beta_i)$ is a normalizing factor. The infinite reservoir is conceived as an idealization behaving like very large reservoirs, i.e., as a limit of the above structure: The algebra of observables $\mathcal{A}_i$ is the smallest C^*-algebra containing $\mathcal{A}_{i,\Lambda_i}$ for all finite regions Λ_i, the (strongly continuous) dynamics $\alpha_i^t(\cdot)$ on it is the strong limit (provided it exists) of the automorphism groups $\alpha^t_{i,\Lambda_i}(\cdot)$, and the equilibrium state is a limit point ω_{i,β_i} of $\omega_{i,\beta_i,\Lambda_i}$ as Λ_i increases to the infinite region L_i occupied by the reservoir R_i. The infinite reservoirs in this sense can be represented as genuine quantum systems using the so-called Gelfand-Neumark-Segal (GNS) construction. The latter consists essentially in the following: a state ω on a C^*-algebra $\mathcal{A}$ defines a sesquilinear form on it by $\langle A, B\rangle = \omega(A^*B)$; after division by the ideal $\mathcal{I}$ of all $I \in \mathcal{A}$ such that $\omega(I^*I) = 0$, $\mathcal{A}/\mathcal{I}$ becomes a pre-Hilbert space, whose completion $\mathcal{H}_\omega$ is the representation space. The representation $\pi_\omega(X)$ of an element $X \in \mathcal{A}$ is the bounded operator which sends the vector $\hat{A}$ into the vector $\widehat{XA}$; thereby, $\hat{1} =: \Omega_\omega$ is a cyclic vector for this representation, and $\omega(A) = (\Omega_\omega, \pi_\omega(A)\Omega_\omega)$. If, moreover, the state ω is invariant under the automorphism group α_t (i.e. $\omega \circ \alpha_t = \omega$), then $\pi_\omega(\alpha_t(X)) = U_\omega(-t)\pi_\omega(X)U_\omega(t)$, where $U_\omega(t) = \exp(-\mathrm{i}tH_\omega)$ is a unitary group on $\mathcal{H}_\omega$. The generator H_ω of this group, named *thermal Hamiltonian*, has Ω_ω as an eigenvector with eigenvalue 0.

To simplify the notation, we no longer mention the reference states $\omega_i^0 = \omega_{i,\beta_i}$ of the reservoirs, and simply denote $\{\mathcal{H}_i, \pi_i(\cdot), \Omega_i, H_i\}$ the GNS description for the reservoir R_i corresponding to the equilibrium state ω_i^0, i.e., respectively, the Hilbert space, the representation of the observable algebra $\mathcal{A}_i$, the cyclic vector and the thermal Hamiltonian generating the unitary implementation of the dynamical automorphism group: $\pi_i(\alpha_i^t(A)) = \exp(\mathrm{i}tH_i)A\exp(-\mathrm{i}tH_i)$. Likewise, we denote $\{\mathcal{H}_S, \pi_S(\cdot), \Omega_S, H_S\}$ the GNS representation of the sample associated to the state ω_S^0 invariant for the group α_S^t.

The composite system $S + \sum R_i$ is in turn an infinite quantum system, which is to be constructed as above from a certain reference state. The algebra of observables is taken as a C^*-tensor product of the algebras $\mathcal{A}_i$ of the reservoirs and $\mathcal{A}_S$ of the sample:

$$\mathcal{A} = \mathcal{A}_S \otimes (\otimes_i \mathcal{A}_i), \tag{1.1}$$

and the reference state is taken as the product of the initial equilibrium states ω_i^0 of the reservoirs and the α_S^t-invariant state $\omega_S^0(\cdot) = (\Omega_S, \cdot\Omega_S)$ of the sample:

$$\omega^0 = \omega_S^0 \otimes ((\otimes_i \omega_i^0). \tag{1.2}$$

On the algebra $\mathcal{A}$ one has the uncoupled dynamics described by the automorphism group $\alpha^t = \alpha_S^t \otimes ((\otimes_i \alpha_i^t)$, which leaves invariant the state ω^0: $\omega^0(\alpha^t(A)) = \omega^0(A),\ A \in \mathcal{A}$.

At time $t = 0$, a coupling between reservoirs and the sample is switched on, meaning that the dynamics of the system at positive times is given by another automorphism group of $\mathcal{A}$, τ^t. The evolved reference state will therefore change in time, and be, at time $t > 0$, the state for which the expectation of an observable equals the ω^0-expectation of the observable evolved at time t according to the new dynamics:

$$\omega^t(A) = \omega^0(\tau^t(A)) = \omega^0(\alpha^{-t} \cdot \tau^t(A)), \tag{1.3}$$

where the second equality comes from the α^t-invariance of ω^0. Suppose a stationary (τ^t-invariant) state is approached at large time. This can be expressed as the existence of the limit of $\omega^t(A)$ when $t \to +\infty$ for all $A \in \mathcal{A}$. The latter is ensured by the existence of the limits

$$\lim_{t \to +\infty} \alpha^{-t} \cdot \tau^t(A) = \Omega_+(A), \tag{1.4}$$

i.e. by the existence of the Möller endomorphisms of the two groups. In this way, the existence of (and the convergence to) a stationary state can be presented as a scattering problem for two automorphism groups on a C^*-algebra. As a rule, τ^t is constructed as a local perturbation of α^t via a strongly convergent Dyson series; more precisely, if $\lim\limits_{t\to 0} \frac{1}{t}(\alpha^t(A) - A) = \delta_0(A)$ for A in a dense subalgebra $\mathcal{D} \subset \mathcal{A}$, one supposes that there exists $V \in \mathcal{A}$, such that $\delta_V(A) := \lim\limits_{t\to 0} \frac{1}{t}(\tau^t(A) - A) = \delta_0(A) + \mathrm{i}[V, A]$ for $A \in \mathcal{D}$.

As a consequence of the choice (1.2), the composite system can be realized in the tensor product of Hilbert spaces $\mathcal{H} = \mathcal{H}_S \otimes ((\otimes_i \mathcal{H}_i)$, which carries the product representation of $\mathcal{A}$, so that $\pi(\mathcal{A})$ is the C^*-tensor product of operator algebras $\pi_S(\mathcal{A}_S) \otimes ((\otimes_i \pi_i(\mathcal{A}_i))$. Thereby, the independent (uncoupled) dynamics of the reservoirs and of the sample is implemented in $\mathcal{H}$ by the unitary group $U_0(t) = \exp(-\mathrm{i}tH_0) = \exp(-\mathrm{i}tH_S) \otimes ((\otimes_i \exp(-\mathrm{i}tH_i))$. The cyclic vector $\Omega = \Omega_S \otimes ((\otimes_i \Omega_i)$ is an eigenvector of H_0 with eigenvalue 0. Also, the locally perturbed dynamics is implemented by the unitary group $U(t) = \exp(-\mathrm{i}tH)$, where

$$H = H_0 + \pi(V). \tag{1.5}$$

In this way, the problem can be reformulated as a perturbation problem for selfadjoint operators on a Hilbert space in a setting depending on the chosen reference state.

Of course, the construction of the perturbed dynamics and the proof that the Möller endomorphisms exist are to be done for the models under consideration of reservoirs, samples and couplings between them. It happens that the program outlined before can accommodate a few reservoir models of physical interest, such as spin models or free particle models obeying Fermi statistics, and samples with finite-dimensional $\mathcal{H}_S$. One of the most restrictive assumptions is the existence of the infinite-volume dynamical group of automorphisms α^t and its assumed strong continuity. A way out to a more permissible framework for the reservoirs, R_i, is to construct as above the reference states ω_i^0 as limit points of finite-volume Gibbs states and further work within the GNS representation associated to it. In particular, a weakly continuous infinite-volume dynamics may appear as a limit of the local dynamics $\alpha^t_{\Lambda_i}(\cdot)$ viewed as automorphisms of the *weak* closures of the operator algebras $\pi_i(\mathcal{A}_i)$ representing $\mathcal{A}_i$, i.e. of the von Neumann algebras $\pi_i(\mathcal{A}_i)''$. This allows to define a representation-dependent dynamics and self-adjoint thermal Hamiltonian. Hence, the steps leading to a scattering problem in a Hilbert space are to be performed. In particular, this is the case of free-boson reservoirs, see Sec. 4. below.

1.2. Quasi-free models

In the paper we shall consider instances of concrete realizations, within a class of very simple models, of the paradigm outlined above. Essentially, we suppose that:

1. The reservoirs are free quantum identical particle systems, obeying Fermi-Dirac or Bose-Einstein statistics.

2. The perturbed (coupled) dynamics is quasi-free.

In more detail, point 1 means the following: Before taking the thermodynamic limit, i.e. when the reservoir is confined to a finite region Λ, the appropriate Fock space, which bears the Fock representation of the canonical (anti)commutation relations, can be used, whereby the number of particles $N_\Lambda = \mathrm{d}\Gamma(1)$ and Hamiltonian $H_\Lambda = d\Gamma(h^0_\Lambda)$. According to the grand-canonical prescription, H_Λ is to be replaced by $H_\Lambda - \mu N_\Lambda$ in the Gibbs ansatz for the equilibrium density matrix, where the multiplier μ is adjusted to ensure given particle density in the reservoir. In the thermodynamic limit, the C^*-algebra of observables should "contain" the local operators, i.e. functions of $a^\sharp(f)$ with f having support in some finite region. It is therefore natural to take it as the canonical (anti)commutation relations algebra, CAR($\mathcal{D}$), respectively CCR($\mathcal{D}$), over a certain subspace of the space of reservoir's one-particle states, $\mathcal{D} \subset \mathcal{H}^{(1)}$, containing at least the functions with compact support. The equilibrium states of the reservoir, i.e. the limit states of the finite-volume Gibbs states, are well-known (see e.g. [4]), and turn out to be *quasi-free* states (i.e. states in which there are no correlations of order higher than 2) over these C^*-algebras. $\mathcal{D}$ may be extended such that the limit states be defined on the corresponding C^*-algebra. In the Fermi case $\mathcal{D} = \mathcal{H}^{(1)}$. In the Bose case, however, due to the phenomenon of Bose-Einstein condensation, $\mathcal{D} \neq \mathcal{H}^{(1)}$; in the paper, in order to avoid the domain problems, we suppose also that the Bosons live on the lattice $\mathbb{Z}^d$, leaving the general case for another publication.

The point 2 means that the evolution automorphism of the C^*-algebra is given by a unitary evolution $\mathrm{e}^{-\mathrm{i}th}$ in $\mathcal{H}^{(1)}$ which leaves $\mathcal{D}$ invariant: $\tau^t(a^\sharp(f)) = a^\sharp(\mathrm{e}^{\mathrm{i}th} f)$. As a consequence, not only the initial (reference) state ω^0, but also all ω^t, $t > 0$ and the stationary state are quasi-free. Thereby, the problem is reduced to a scattering problem for the one-particle Hamiltonians, which can be explicitly solved.

In this respect, the quasi-free models are trivial, in particular they allow no interaction between particles and thus restrict consideration to simple tunneling junctions, but they turn out to be a good laboratory for conjectures concerning various phenomena and providing instances of interesting physical behavior. In particular, the coupled dynamics no longer conserves the energy and number of particles in the reservoirs, implying that, in the stationary state, there exist persistent currents of energy and particles, depending on the parameters fixing the initial equilibria of the reservoirs, and also on the geometry of the sample and its coupling to them. In this way various formulae of transport theory can be obtained beyond the linear response regime.

1.3. Summary

There is an extensive literature on quasi-free quantum systems. This work started as an attempt to systematize their application to the problems of return to equilibrium and of approach to NESS in a more abstract, comprehensive frame, as outlined in the previous subsection. In the meantime, we became aware of two recent papers with the same purpose in the Fermi case [2], [12], so we limited to the more modest aim of giving a (hopefully more friendly) presentation of their general result, of indicating its extension to the Bose case and of providing a few examples of calculation for certain interesting physical quantities.

Section 2 is concerned with the spectral and scattering problems for the one-particle Hamiltonians, as the same analysis applies to both Fermi and Bose statistics. In order to have as far as possible explicit expressions, we consider, as an application, in subsections 2.3. and 2.4. the case of two reservoirs, in which the particles live on two d-dimensional lattices, and those in the sample on a chain of $N \geq 0$ sites; thereby, the coupling is a simple tunneling involving one site of each reservoir.

Section 3 is devoted to the Fermi statistics case, which is simpler in many respects, in particular the C^*-framework is sufficient, as the infinite-volume dynamics is a strongly continuous group of automorphisms of $CAR(\mathcal{H}^{(1)})$. A comprehensive study of this case has been performed in [2], the results of which are briefly presented. We make explicit their result for the particular setting in Section 2.3. and point out a few peculiarities of the NESS, such as the resonant character of the transport and the plateau effect for the carrier density.

Section 4 is concerned with Bose reservoirs. This brings in several new phenomena and complications. First, at high density and low temperature, Bose condensation may appear, implying the spontaneous gauge-symmetry breaking, i.e. existence of several extremal equilibrium states labeled by a phase. Moreover, the infinite volume dynamics cannot be a strongly continuous group of the CCR algebra; fortunately, as quasi-free states are regular, it is continuous in the GNS representation corresponding to equilibrium states. The interesting question here is the dependence of the NESS on the particular mixtures of phases constituting the initial equilibria of the reservoirs. This may be viewed as a caricature of the Josephson tunneling of Cooper pairs between two superconductors. The approach to equilibrium in the presence of a condensate has been analyzed by Merkli [8]. The problem of approach to a NESS, left open there, was considered by us in [1], the result of which is presented in the present, slightly more general, setting.

2. Scattering for the one-particle Hamiltonians

This section is devoted to the spectral analysis of the one-particle Hamiltonian $h = h^0 + v$, where h^0 is the one-particle Hamiltonian of the decoupled system, i.e. the direct sum of the one-particle Hamiltonians $h_i\,(i = 1, ..., r)$, h_S of the isolated reservoirs and sample and v describes the tunneling between them. We make the following assumptions:

Assumption 2.1 *The one-particle Hilbert space is an orthogonal sum*

$$\mathcal{H}^{(1)} = \mathcal{H}_S^{(1)} \oplus \mathcal{H}_R^{(1)};\;\; \mathcal{H}_R^{(1)} = \oplus_{i=1}^{r} \mathcal{H}_i^{(1)},$$

with $\dim \mathcal{H}_S^{(1)} = N < \infty$. *Let* $J : \mathcal{H}_R^{(1)} \to \mathcal{H}^{(1)}$ *and* $I : \mathcal{H}_S^{(1)} \to \mathcal{H}^{(1)}$ *be the natural injections:*

$$Jf = 0 \oplus f \qquad If = f \oplus 0,$$

Assumption 2.2 *In the matrix representation associated to this decomposition, the unperturbed Hamiltonian* h_0 *is block-diagonal:*

$$h^0 = h_S \oplus h^0_{\mathrm{ac}}; \;\; h^0_{\mathrm{ac}} = \oplus_{i=1}^r h_i,$$

and the perturbation v *has the following structure: There exist maps* τ_i : $\mathcal{H}_i^{(1)} \to \mathcal{H}_S^{(1)}$, *such that*

$$v = I\tau J^* + J\tau^* I^*,$$

where

$$\tau : \mathcal{H}_R^{(1)} \to \mathcal{H}_S^{(1)}, \;\; \tau(\oplus_{i=1}^r f_i) = \sum_{i=1}^r \tau_i f_i.$$

Assumption 2.3 h_i, $i = 1, ..., r$, *have absolutely continuous spectra equal to the bounded intervals* $I_i \subset \mathbb{R}$. *Thereby, we suppose that* $\bigcup_{i=1}^r \mathrm{Int}(I_i)$ *is an interval* $(e_{\min}, e_{\max})$. *We denote* $R_i(z) = (h_i - z)^{-1}$, $(z \in \mathbb{C} \setminus I_i)$ *and* $R^0_{\mathrm{ac}} = (h_{\mathrm{ac}} - z)^{-1} = \oplus_{i=1}^r R_i(z)$. *Let* p_i, π_i *denote the right, respectively left, support of* τ_i *(i.e. the orthogonal projections onto the subspaces* $\tau_i(\mathcal{H}_i^{(1)}) \subset \mathcal{H}_S^{(1)}$, *respectively* $\tau_i^*(\mathcal{H}_S^{(1)}) \subset \mathcal{H}_i^{(1)}$*). For* **all** $x \in I_i$, *the limits*

$$\lim_{\epsilon \searrow 0} \pi_i R_i(x + \mathrm{i}\epsilon)|_{\pi_i(\mathcal{H}_i^{(1)})}$$

exist as operators in the corresponding subspaces and are continuous functions of x*; thereby, for all interior points* x *of* I_i, ,

$$\lim_{\epsilon \searrow 0} \pi_i \Im R_i(x + \mathrm{i}\epsilon)|_{\pi_i(\mathcal{H}_i^{(1)})} > 0 \quad (i = 1, ..., r).$$

2.1. Resolvent and spectrum of the perturbed Hamiltonian

The spectral decomposition of $h = h^0 + v$ is based on finding a convenient representation of the resolvent operator $R(z) = (h - z)^{-1}$. We shall use a variant of the Feshbach method, taking advantage of the fact that v has finite range, what allows summing the perturbation series in closed form.

We have to solve for f_S, f_i, $i = 1, ..., r$, the system of equations

$$\left\{ \begin{array}{llll} (h_i - z) f_i & + \quad \tau_i^* f_S & = g_i & (i = 1, ...r) \\ \sum_{i=1}^r \tau_i f_i & + (h_S - z) f_S & = g_S, & \end{array} \right. \tag{2.1}$$

where $g = g_S \oplus (\oplus_{i=1}^r g_i) \in \mathcal{H}^{(1)}$ is arbitrary.

If $z \in \mathbb{C} \setminus [e_{\min}, e_{\max}]$, the first line in equation (2.1) provide f_i in terms of f_S:

$$f_i = R_i(z)(g_i - \tau_i^* f_S), \tag{2.2}$$

and the second line becomes

$$(h_{\text{eff}}(z) - z) f_S = Q(z) g, \tag{2.3}$$

where $h_{\text{eff}}(z) : \mathcal{H}_S^{(1)} \to \mathcal{H}_S^{(1)}$ and $Q(z) : \mathcal{H}^{(1)} \to \mathcal{H}_S^{(1)}$ are defined by:

$$\begin{aligned} h_{\text{eff}}(z) &= h_S - \sum_{i=1}^r \tau_i R_i(z) \tau_i^* = h_S - \tau R_{\text{ac}}^0(z) \tau^*, \\ Q(z) &= I^* - \tau R_{\text{ac}}^0(z) J^*. \end{aligned} \tag{2.4}$$

Whenever $h_{\text{eff}}(z) - z$ is invertible, we denote $R_{\text{eff}}(z) = (h_{\text{eff}}(z) - z)^{-1}$, so that Eq. (2.3) has the unique solution

$$f_S = R_{\text{eff}}(z) Q(z) g, \tag{2.5}$$

With f_S given by Eq. (2.5) and f_i given in terms of it by Eq. (2.2), $f = f_S \oplus (\oplus_{i=1}^r f_i) = Q(\bar{z})^* f_S$ provides the solution to the system (2.1). Therefore, remarking that $\cup_{i=1}^r I_i \subset \sigma(h)$ (by the invariance of the essential spectrum under compact perturbations), the following characterization has been proved:

LEMMA **2.1** *The resolvent set of h is*

$$\rho(h) = \{z \in \mathbb{C} \setminus [e_{\min}, e_{\max}];\ \ker(h_{\text{eff}}(z) - z) = \{0\}\}.$$

For all $z \in \rho(h)$,

$$R(z) = J R_{\text{ac}}^0(z) J^* + Q(\bar{z})^* R_{\text{eff}}(z) Q(z). \tag{2.6}$$

The Kato-Rosenblum scattering theory [15] ensures the existence and completeness of the wave operators $W_\pm : \mathcal{H}_R^{(1)} \to \mathcal{H}^{(1)}$ for the unitary groups $\mathrm{e}^{-\mathrm{i}th}$, $\mathrm{e}^{-\mathrm{i}th_{\text{ac}}^0}$, i.e. the existence of the strong limits:

$$W_\pm := (\mathrm{s}) \lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}th} J \mathrm{e}^{-\mathrm{i}th_{\text{ac}}^0}. \tag{2.7}$$

Hence,

LEMMA **2.2** *h has absolutely continuous spectrum $\sigma_{\rm ac}(h) = [e_{\min}, e_{\max}]$ and no singular continuous spectrum. The absolutely continuous part $h_{\rm ac}$ of h, i.e. h restricted $\mathcal{H}_{\rm ac}^{(1)}(h) = W_\pm(\mathcal{H}_R^{(1)})$, is unitarily equivalent to $h_{\rm ac}^0$ via the intertwining relations $h_{\rm ac}W_\pm = W_\pm h_{\rm ac}^0$.*

Finally, we determine the point spectrum of h, $\sigma_{\rm p}(h)$.

Let $z \in \sigma_{\rm p}(h)$, and $f = f_S \oplus (\oplus_{i=1}^r f_i) \neq 0$ be an eigenvector of h with eigenvalue z. Then f is a solution of Eq. (2.1) for $g = 0$.

If, thereby, $\tau_i^* f_S = 0$ for all $i = 1, ..., r$, then $(h_i - z)f_i = 0$, $\forall i$, hence $f_i = 0$, because h_i have no point spectrum. If so, the second line in (2.1) shows that $z \in \sigma_{\rm p}(h_S)$ and that $f_S \in \ker \tau_i^*$ is a corresponding eigenvector. Conversely, if $f_S \in \cap_i \ker \tau_i^*$ is an eigenvector of h_S, then $f_S \oplus 0$ is an eigenvector of h with the same eigenvalue.

Suppose next that $\tau_i^* f_S \neq 0$ for at least one i. If $z \notin [e_{\min}, e_{\max}]$, Eq. (2.2), which expresses f_i in terms of f_S, and Eq. (2.3) show that $f_S \neq 0$ is an eigenvector of $h_{\rm eff}(z)$ with eigenvalue z. Conversely, if $\ker(h_{\rm eff}(z) - z) \ni f_S \neq 0$, then $z \in \sigma_{\rm p}(h)$ and $Q(\bar{z})^* f_S$ is an eigenvector of h with eigenvalue z (in particular, we have that $\Im z = 0$). Let us consider the family of self-adjoint operators $\{h_{\rm eff}(x);\ z = x \in (-\infty, e_{\min})\}$ and let $\lambda_1(x) \leq ... \leq \lambda_N(x)$ be the eigenvalues of $h_{\rm eff}(x)$ and $\psi(x)_S^{(1)}, ..., \psi(x)_S^{(N)}$ the corresponding eigenvectors. As remarked before, $x \in \sigma_{\rm p}(h)$ if, and only if, $x = \lambda_k(x)$ for some $k = 1, ..., N$. As $h_{\rm eff}(x)$ is a decreasing operator-valued function of x in the considered interval, all its eigenvalues $\lambda_k(x)$ are decreasing functions, hence, the equation $x = \lambda_k(x)$ has a simple solution $x = e_k^-$ if, and only if, $\lim_{x \nearrow e_{\min}} \lambda_k(x) < e_{\min}$. Then, every eigenvector of $h_{\rm eff}(e_k^-)$ with eigenvalue e_k^- can be completed to an eigenvector of h with this eigenvalue. Likewise, on $(e_{\max}, \infty)$ the equation $x = \lambda_k(x)$ has a solution e_k^+ if, and only if, $\lim_{x \searrow e_{\max}} \lambda_k(x) > e_{\max}$, implying $e_k^+ \in \sigma_{\rm p}(h)$.

Next, let $f_S \oplus f$ be an eigenvector of h corresponding to x in $(e_{\min}, e_{\max})$ and such that $\tau_i^* f_S \neq 0$ for some $i = 1, ..., r$. Let $z = x + \mathrm{i}y$, with $\Im z = y > 0$. We have, by the first line of equations (2.1), $f_k = R_k(x + \mathrm{i}y)(h_k - x - \mathrm{i}y)f_k = -R_k(x + \mathrm{i}y)\tau_k^* f_S - \mathrm{i}yR_k(x + \mathrm{i}y)f_k$, which, plugged into the second equation, implies, in particular, that

$$\begin{aligned}(f_S, (h_{\rm eff}(x + \mathrm{i}y) - x)f_S) &= \mathrm{i}y \sum_{k=1}^r (\tau_k^* f_S, R_k(x + \mathrm{i}y)f_k) \\ &= \mathrm{i}y \sum_{k=1}^r (\|f_k\|^2 - \mathrm{i}y(f_k, R_k(x + \mathrm{i}y)f_k)).\end{aligned}$$

Equating the imaginary parts of this equality, letting $y \searrow 0$ and using

$\|R_k(x+\mathrm{i}y)\| = 1/y$, we arrive at

$$\Im(f_S, \tau_k R_k(x+\mathrm{i}0)\tau_k^* f_S) = 0, \ \forall k,$$

which contradicts assumption 2.3.

In summary:

LEMMA **2.3** *The point spectrum of h in $\mathbb{R} \setminus \{e_{\min}, e_{\max}\}$ consists, besides the possible eigenvalues of h_S possessing eigenvectors $f_S \in \bigcap_{i=1}^{r} \ker \tau_i^*$, of the solutions $e_k^- \in (-\infty, e_{\min})$ and $e_k^+ \in (e_{\max}, \infty)$ of the equations $\lambda_k(x) = x$. The latter exist if, and only if, $\lambda_k(e_{\min} - 0) < e_{\min}$ and $\lambda_k(e_{\max} + 0) > e_{\max}$, respectively.*

The values $e_{\min}$ or $e_{\max}$ may be eigenvalues of h, either if they are eigenvalues of h_S with eigenvector $f_S \in \bigcap_{i=1}^{r} \ker \tau_i^*$, or if $\lambda_k(x) = x$ and the corresponding eigenvector $\psi(x)^{(k)}$ fulfills $\lim_{x' \to x} \|R_i(x')\tau_i^* \psi(x')^{(k)}\| < \infty$, $\forall i$. The latter condition, being dependent on the structure of h^0 and τ_i, is to be checked for each concrete model.

2.2. Wave operators and scattering matrix

In this subsection we derive the expressions of the wave operators and S-matrix using the formalism of stationary scattering theory [15], [17]. Namely, with the spectral representation of the unitary groups $\mathrm{e}^{-\mathrm{i}th} = \int \mathrm{e}^{-\mathrm{i}tx} \mathrm{d}E(x)$, $\mathrm{e}^{-\mathrm{i}th_i} = \int \mathrm{e}^{-\mathrm{i}tx} \mathrm{d}E_i(x)$, we can express the wave operators in terms of the resolvent $R(z)$ of h. We have

$$\begin{aligned} W_+ &= (\mathrm{s}) \lim_{\epsilon \searrow 0} \epsilon \int_0^\infty \mathrm{e}^{-t\epsilon} \exp(\mathrm{i}th) J \exp(-\mathrm{i}th^0) \mathrm{d}t \\ &= (\mathrm{s}) \lim_{\epsilon \searrow 0} \epsilon \int \mathrm{d}E(x') \int J \mathrm{d}E_{\mathrm{ac}}^0(x) \int_0^\infty \mathrm{d}t \mathrm{e}^{\mathrm{i}t(x'-x+\mathrm{i}\epsilon)} \\ &= (\mathrm{s}) \lim_{\epsilon \searrow 0} (\mathrm{i}\epsilon) \int R(x - \mathrm{i}\epsilon) J \mathrm{d}E_{\mathrm{ac}}^0(x). \end{aligned} \tag{2.8}$$

where we denoted $E_{\mathrm{ac}}^0(x) = \oplus_{i=1}^r E_i(x)$. Similar calculations are valid for W_-. Using Eq. (2.6) for $R(z)$, taking into account that $\mp \mathrm{i}\epsilon R_{\mathrm{ac}}^0(x \pm \mathrm{i}\epsilon) \mathrm{d}E_{\mathrm{ac}}^0(x) = \mathrm{d}E_{\mathrm{ac}}^0(x)$ and Assumption 2.2, the following representation is obtained:

$$W_\pm = J - (\mathrm{s}) \lim_{\epsilon \searrow 0} \int Q(x \pm \mathrm{i}\epsilon)^* R_{\mathrm{eff}}(x \mp \mathrm{i}\epsilon) \tau \mathrm{d}E_{\mathrm{ac}}^0(x). \tag{2.9}$$

Also,

$$W_\pm^* = J^* - (\mathrm{s})\lim_{\epsilon'\searrow 0}\int \mathrm{d}E^0_{\mathrm{ac}}(x')\tau^* R_{\mathrm{eff}}(x'\pm \mathrm{i}\epsilon')Q(x'\pm\mathrm{i}\epsilon'). \tag{2.10}$$

Eqs. (2.9), (2.10) give for the S-matrix:

$$\begin{aligned} S = W_+^* W_- = 1 \quad & -J^*\int Q(x-\mathrm{i}0)^* R_{\mathrm{eff}}(x+\mathrm{i}0)\tau \mathrm{d}E^0_{\mathrm{ac}}(x) \\ & -\int \mathrm{d}E^0_{\mathrm{ac}}(x')\tau^* R_{\mathrm{eff}}(x'+\mathrm{i}0)Q(x'+\mathrm{i}0)J \\ & +\lim_{\epsilon'\searrow 0}\{\lim_{\epsilon\searrow 0}\int \mathrm{d}E^0_{\mathrm{ac}}(x')\tau^* R_{\mathrm{eff}}(x'+\mathrm{i}\epsilon')Q(x'+\mathrm{i}\epsilon') \\ & \qquad \times \int Q(x-\mathrm{i}\epsilon)^* R_{\mathrm{eff}}(x+\mathrm{i}\epsilon)\tau \mathrm{d}E^0_{\mathrm{ac}}(x)\}. \end{aligned} \tag{2.11}$$

We calculate the last term using the resolvent equation, which implies

$$\begin{aligned} & Q(x'+\mathrm{i}\epsilon')Q(x-\mathrm{i}\epsilon)^* = 1+\tau R^0_{\mathrm{ac}}(x'+\mathrm{i}\epsilon')R^0_{\mathrm{ac}}(x+\mathrm{i}\epsilon)\tau^* \\ & = 1+(x'-x+\mathrm{i}(\epsilon'-\epsilon))^{-1}\tau[R^0_{\mathrm{ac}}(x'+\mathrm{i}\epsilon')-R^0_{\mathrm{ac}}(x+\mathrm{i}\epsilon)]\tau^* \\ & = (x'-x+\mathrm{i}(\epsilon'-\epsilon))^{-1}[(h_{\mathrm{eff}}(x+\mathrm{i}\epsilon)-x-\mathrm{i}\epsilon)-(h_{\mathrm{eff}}(x'+\mathrm{i}\epsilon')-x'-\mathrm{i}\epsilon')]. \end{aligned}$$

Each term of the latter expression, when plugged into Eq. (2.11), is sandwiched between R_{eff}, what, after making the obvious simplification, allows one of the integrals to be performed (e.g. $\int \mathrm{d}E^0_{\mathrm{ac}}(x')(x'-x+\mathrm{i}(\epsilon'-\epsilon))^{-1}\tau^* = R^0_{\mathrm{ac}}(x-\mathrm{i}(\epsilon'-\epsilon))\tau^* = J^*Q(x-\mathrm{i}(\epsilon-\epsilon'))^*$). Therefore, after taking the iterated limit, the last term of Eq. (2.11) equals

$$\int J^*Q(x+\mathrm{i}0)^*R_{\mathrm{eff}}(x+\mathrm{i}0)\tau\mathrm{d}E^0_{\mathrm{ac}}(x)+\int \mathrm{d}E^0_{\mathrm{ac}}(x')\tau^*R_{\mathrm{eff}}(x'+\mathrm{i}0)Q(x'+\mathrm{i}0)J.$$

As $Q(z)J = -\tau R^0_{\mathrm{ac}}(z)$, one obtains finally

$$S = 1+2\mathrm{i}\int \Im(R^0_{\mathrm{ac}}(x+\mathrm{i}0))\tau^* R_{\mathrm{eff}}(x+\mathrm{i}0)\tau\mathrm{d}E^0_{\mathrm{ac}}(x). \tag{2.12}$$

REMARK **2.1** *It is sometimes useful to represent the Hilbert space $\mathcal{H}_{\mathrm{ac}}(h^0)$ as a direct integral over energy of Hilbert "eigenspaces" $\mathcal{K}_x$, i.e. there exists a unitary $U : \mathcal{H}_{\mathrm{ac}}(h^0) \to \int^\oplus_{[e_{\min},e_{\max}]}\mathcal{K}_y \mathrm{d}y =: \mathcal{K}$, such that $UE^0_{\mathrm{ac}}(\Lambda)U^* = \chi_\Lambda(\cdot)$ (the operator of multiplication with the indicator of the measurable set Λ). It is clear that, for $\psi(\cdot)\in\int^\oplus_{[e_{\min},e_{\max}]}\mathcal{K}_y\mathrm{d}y$, $(UR^0(z)U^*\psi)(y) = (y-z)^{-1}\psi(y)$. Also, $\tau U^*\psi = \int_{[e_{\min},e_{\max}]}\tau_y(\psi(y))\mathrm{d}y$, where $\tau_y : \mathcal{K}_y \to \mathcal{H}_S^{(1)}$. Eq. (2.12) shows that, in this representation, the S-matrix is diagonal, i.e. $USU^* = \int^\oplus_{[e_{\min},e_{\max}]} S_x\mathrm{d}x$, where $S_x : \mathcal{K}_x\to\mathcal{K}_x$ equals*

$$S_x = 1+2\pi\mathrm{i}\tau_x^* R_{\mathrm{eff}}(x+\mathrm{i}0)\tau_x =: 1+T_x. \tag{2.13}$$

T_x is called the on-shell T-matrix.

Calculating, for $f \in \mathcal{H}_{\rm ac}^{(1)}$, separately the component $I^*W_\pm f \in \mathcal{H}_S^{(1)}$ and $J^*W_\pm f \in \mathcal{H}_{\rm ac}^{(1)}$ of Eq. (2.9), one obtains

$$\begin{array}{lcl} I^*W_\pm f & = & -\int R_{\rm eff}(x \mp {\rm i}0)\tau_x(Uf)(x){\rm d}x, \\ \left[UJ^*W_\pm f\right](x) = & & (Uf)(x)+ \\ & & +\int \frac{1}{x-x'\mp {\rm i}0}\tau_x^* R_{\rm eff}(x' \mp {\rm i}0)\tau_{x'}(Uf)(x'){\rm d}x'. \end{array} \tag{2.14}$$

Also, the action of $W_\pm^*$ on $f \in \mathcal{H}^{(1)}$ is given by

$$\begin{array}{rl} (UW_\pm^* f)(x) = & (UJ^*f)(x)- \\ & -\int \frac{1}{x-x'\pm {\rm i}0}\tau_x^* R_{\rm eff}(x \pm {\rm i}0)\tau_{x'}(UJ^*f)(x'){\rm d}x'- \\ & -\tau_x^* R_{\rm eff}(x \pm {\rm i}0)I^*f. \end{array} \tag{2.15}$$

2.3. An example: two half-infinite lattice reservoirs coupled by a wire

In this subsection we describe, as an illustration of the more general setting of the model, a particular geometry and dynamics: the system consisting of two particle reservoirs, R_1, R_2, connected by a one-dimensional wire, S.

The reservoirs, R_i, $i = 1, 2$, are taken as infinitely extended lattice quantum gases. The particles in the reservoirs live, respectively, on the two (left, respectively, right) half-infinite lattices,

$$L_i = \mathbb{Z}_i^d = \left\{ r = (r', r^d);\ r' \in \mathbb{Z}^{d-1},\ (-1)^i r^d = 1, 2, ... \right\}. \tag{2.16}$$

The Hilbert space of one-particle states in R_i is therefore

$$\mathcal{H}_i^{(1)} = l_2(L_i) = \left\{ f = (f_r)_{r \in L_i};\ \|f\|^2 = \sum_{r \in L_i} |f_r|^2 < \infty \right\}. \tag{2.17}$$

The kinetic energy operator of one particle in R_i is 1/2 times the lattice Laplace operator with free boundary conditions, i.e.

$$(h_i f)_r = d f_r - \frac{1}{2} \sum_{q \in L_i, |q-r|=1} f_q. \tag{2.18}$$

A complete set of generalized eigenvectors of h_i are $\psi^i(k) \in l_\infty(L_i)$, $k \in \mathbb{T}_i^d$, where the index sets $\mathbb{T}_i^d = \{k = (k', k^d);\ k' \in [0, 2\pi)^{d-1}, k^d \in (0, \pi)\}$ are identical (the subscript i has the only role to make the difference between the two reservoirs, e.g. by $\mathbb{T}_1^d \cup \mathbb{T}_2^d$ we mean the disjoint union of two copies this set), and

$$\psi^i(k)_r = 2(2\pi)^{-d/2} \exp(\mathrm{i}k'r') \sin(k^d |r^d|). \tag{2.19}$$

$\psi^i(k)$ corresponds to the generalized eigenvalue

$$\omega_i(k) = 2 \sum_{\alpha=1}^{d} \sin^2(k^\alpha/2). \tag{2.20}$$

Again, though the two dispersion laws (2.20) are identical, we keep the label i to mark the reservoir they correspond to. Therefore the spectra of h_i are absolutely continuous and coincide with the intervals $I_1, I_2 \subset \mathbb{R}$ (both equal to $[0, 2d]$). In fact, we define the unitary operators $u_i : \mathcal{H}_i^{(1)} \to L_2(\mathbb{T}_i^d)$ by

$$u_i f = (\psi^i(\cdot), f); \tag{2.21}$$

then, $u_i h_i u_i^*$ is the operator of multiplication with the function $\omega_i(k)$ on $L_2(\mathbb{T}_i^d)$.

The sample S, providing our model of a nanowire, is a free quantum gas in which particles live on the finite set of sites $\{1, 2, ..., N\}$. The states with one particle are vectors $f = (f_1, ..., f_N) \in \mathcal{H}_S^{(1)} = l_2(\{1, 2, ..., N\}) \equiv \mathbb{C}^N$ and their evolution is controlled by the Hamiltonian

$$(h_S f)_i = (1+e_{\mathrm{g}})f_i - 1/2(f_{i-1} + f_{i+1}),\ i = 1, ..., N \ \ (f_0 = f_{N+1} = 0), \tag{2.22}$$

where the parameter e_{g} plays the role of an adjustable gate potential. The eigenvalues of h_S are $\varepsilon_m = e_{\mathrm{g}} + 2\sin^2(q_m/2); m = 1, ..., N$, where $q_m = m\pi/(N+1)$, with eigenvectors $\psi^{(m)}$:

$$\psi_i^{(m)} = \sqrt{\frac{2}{N+1}} \sin(q_m i). \tag{2.23}$$

The one-particle Hilbert space for the entire system, $S + R_1 + R_2$ is

$$\mathcal{H}^{(1)} = \mathcal{H}_S^{(1)} \oplus \mathcal{H}_1^{(1)} \oplus \mathcal{H}_2^{(1)} = l_2(L), \text{ where } L = \{1, 2, ..., N\} \cup L_1 \cup L_2. \tag{2.24}$$

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

$$h^0 = h_S \oplus h_1 \oplus h_2 \tag{2.25}$$

At $t=0$, tunneling junctions are turned on between the reservoirs and the ends of the wire through the pairs of sites ($\alpha_1=(0',-1),\{1\}$) and ($\alpha_2=(0',1),\{N\}$), $N>0$. On $\mathcal{H}^{(1)}$, this is given by the one-particle operator v defined by the matrix

$$v_{r,s}=\begin{cases} t, & \text{if either } \{r,s\}=\{\alpha_1,1\} \text{ or } \{\alpha_2,N\} \\ 0, & \text{otherwise,} \end{cases} \tag{2.26}$$

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

$$h=h^0+v. \tag{2.27}$$

PROPOSITION **2.1** *The model defined above fulfills the assumptions* 2.1–2.3. *Thereby, h has no eigenvalue embedded in* $(0,2d)$.

Proof. Assumptions 2.1 and 2.2 are obvious, with $r=2$ and τ_1,τ_2 having all matrix elements equal to 0, but for $(\tau_1)_{1,\alpha_1}=(\tau_2)_{N,\alpha_2}=t$. We have that

$$(\tau_1 R_1(z)\tau_1^*)_{i,j}=t^2\delta_{i,1}\delta_{j,1}g(z), \tag{2.28}$$

where

$$\begin{aligned} g(z) = {} & 4(2\pi)^{-d}\int_{\mathbb{T}^d}\sin^2(k^d)(\omega_1(k)-z)^{-1}\mathrm{d}k \\ = {} & 4(2\pi)^{-d}\int_0^{2d}(y-z)^{-1}\mathrm{d}y\int_{\mathbb{T}^d(y)}\sin^2(k^d)\mathrm{d}\mu_y(k), \end{aligned} \tag{2.29}$$

where $\mathrm{d}\mu_y(k)=|\nabla\omega(k)|^{-1}\mathrm{d}\sigma_y(k)$ is the Gelfand-Leray measure on the level set $\mathbb{T}^d(y)=\{k\in\mathbb{T}^d;\ \omega(k)=y\}$ (where $\mathrm{d}\sigma_y(k)$ is the area measure on this surface). Using the Sokhotski formula $(x-\mathrm{i}0)^{-1}=\mathcal{P}(\frac{1}{x})+\mathrm{i}\pi\delta(x)$ (where $\mathcal{P}$ denotes the principal part), we have

$$\lim_{y\searrow 0}\Im g(x+\mathrm{i}y)=4(2\pi)^{-d}\int_{\mathbb{T}^d(x)}\sin^2(k^d)\mathrm{d}\mu_x(k)>0,\ \forall x\in(0,2d). \tag{2.30}$$

Finally, the eigenfunctions (2.23) of h_S fulfill $\psi_1^{(m)}=\sqrt{\frac{2}{N+1}}\sin(q_m)\neq 0, \forall m=1,...,N$, implying that there are no eigenvalues embedded in $(0,2d)$. □

For this model one may define the unitary U of Remark 2.1 as the composition the unitary $u_1\oplus u_2:\mathcal{H}_{\mathrm{ac}}(H^0)\to\oplus_{i=1}^2 L_2(\mathbb{T}_i^d)$ (where u_i are defined in Eq. (2.21)), with the unitary $v_1\oplus v_2:\oplus_{i=1}^2 L_2(\mathbb{T}_i^d)\to\int_0^{2d\oplus}\mathcal{K}_x\mathrm{d}x$, with $\mathcal{K}_x=\oplus_{i=1}^2 L_2(\mathbb{T}_i^d(x),\mathrm{d}\mu_{i,x}(k))$, where $(v_i f_i)(x)$ is the restriction of f_i to the "energy shell" $\mathbb{T}_i^d(x)$ and $\mathrm{d}\mu_{i,x}$ is the Gelfand-Leray measure on the latter. Then, $\tau f = \int_0^{2d} \mathrm{d}x \tau_x(Uf(x))$, where $\tau_x : \mathcal{K}_x \to \mathcal{H}_S^{(1)}$ is given by:

$$\begin{aligned}(\tau_x \phi)_m &= \delta_{m,1} t \int_{\mathbb{T}_1^d(x)} \overline{\psi^1(k)_{\alpha_1}} \phi_1(k) \mathrm{d}\mu_{1,x}(k) + \\ &\quad + \delta_{m,N} t \int_{\mathbb{T}_2^d(x)} \overline{\psi^2(k)_{\alpha_2}} \phi_2(k) \mathrm{d}\mu_{2,x}(k),\end{aligned} \tag{2.31}$$

and $(U\tau^* f)(x) = \tau_x^* f$, where $\tau_x^* : \mathcal{H}_S^{(1)} \to \mathcal{K}_x$ is given by

$$(\tau_x^* f)(k) = t\psi^1(k)_{\alpha_1} f_1 \oplus t\psi^2(k)_{\alpha_2} f_N. \tag{2.32}$$

We remind that $\psi^i(k)_{\alpha_i} = 2(2\pi)^{-d/2} \sin(k^d)$, see Eq. (2.19).

Upon insertion of Eqs. (2.31), (2.32), the equations of the previous remark are made explicit. For instance, the T-matrix $T_x : \mathcal{K}_x \to \mathcal{K}_x$ appearing in Eq. (2.13) is an integral operator with matrix kernel:

$$T_x(k, k')_{i,j} = \frac{4\mathrm{i}}{(2\pi)^{d-1}} \sin(k^d) R_{\mathrm{eff}}(x + \mathrm{i}0)_{s_i, s_j} \sin(k'^d), \tag{2.33}$$

where $s_1 = 1,\ s_2 = N$.

2.4. An example of direct tunneling between reservoirs

The case when the reservoirs are directly coupled through a tunneling junction without any intermediate sample is special. Indeed, e.g. for two reservoirs, $\mathcal{H}^{(1)} = \mathcal{H}_{\mathrm{ac}}(h^0) = \mathcal{H}_1^{(1)} \oplus \mathcal{H}_2^{(1)}$.

In view of the application to Bose gases, where the surface effects may be drastic, we consider now the translation invariant case of lattice reservoirs, i.e. we suppose that particles live on $L_i = \mathbb{Z}^d$, $i = 1, 2$. The one-particle Hilbert spaces $\mathcal{H}_i^{(1)}$ and reservoir Hamiltonians h_i are defined by Eqs.(2.17), (2.18), respectively. Then, the generalized eigenfunctions of h_i are plane waves

$$\psi^i(k)_r = (2\pi)^{-d/2} \exp(\mathrm{i}kr),\ k \in \mathbb{T}^d = [0, 2\pi)^d, \tag{2.34}$$

with generalized eigenvalues $\omega(k)$, Eq. (2.20), and the unitaries u_i are simply the Fourier transform.

The tunneling is between the origins of L_i, i.e. we take $\alpha_i = 0 \in \mathbb{Z}^d$. Let $\pi_0 = \pi_1 \oplus \pi_2 : \mathcal{H}^{(1)} \to \mathbb{C}^2$ denote the restriction to the pair α_1, α_2 of coupled sites:

$$\pi_0(f_1 \oplus f_2) = (f_1)_0 \oplus (f_2)_0,$$

$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ be the unit matrix in $\mathbb{C}^2$ and $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ be the first Pauli matrix (interchange of 1 and 2). The interaction can be represented as

$$v = t\pi_0^*\sigma_1\pi_0 \tag{2.35}$$

One can simplify significantly the expressions of $R(z)$, $\Omega_\pm$, S by using the Fourier representation (2.21) on both spaces: $u = u_1 \oplus u_2 : \oplus_{i=1}^2 \mathcal{H}_i^{(1)} \to \oplus_{i=1}^2 L_2(\mathbb{T}_i^d)$. The resolvent equation $(h-z)f = g$ reduces in $\pi_0\mathcal{H}^{(1)}$ to the equation $(\sigma_0 + t\pi_0 R^0(z)\pi_0^*\sigma_1)(\pi_0 f) = \pi_0 R^0(z) g$, which amounts to inverting a 2×2 matrix. Thereby,

$$\pi_0 R^0(z)\pi_0^* = \tilde{g}(z)\sigma_0, \tag{2.36}$$

with $\tilde{g}(z)$ given by

$$\tilde{g}(z) = (2\pi)^{-d}\int_{\mathbb{T}^d} \frac{dk}{\omega(k) - z}. \tag{2.37}$$

It should be remarked that $\Im\tilde{g}(x + \mathrm{i}0) > 0$ for all $x \in (0, 2d)$ (and is, as a matter of fact, π times the density of states of the lattice Laplaceian (2.18)) and, for $d \geq 3$, goes to 0 at the spectrum ends $x = 0, 2d$.

We obtain finally:

LEMMA **2.4** *In the direct-coupling model described above*

1. *The resolvent of $h = h^0 + v$ has the representation:*

$$\begin{aligned} R(z) = R_0(z) - tR_0(z)\pi_0^*(\sigma_1 + t\tilde{g}(z)\sigma_0)^{-1}\pi_0 R_0(z), \\ (z \in \mathbb{C} \setminus [0, 2d],\ t^2\tilde{g}(z)^2 \neq 1). \end{aligned} \tag{2.38}$$

2. $\sigma_{\mathrm{ac}}(h) = [0, 2d]$.
3. *If $\lim_{x \nearrow 0} \tilde{g}(x) > 1/t$, the equation $t^2\tilde{g}(z)^2 = 1$ has two real solutions $e_0 < 0$ and $2d - e_0$, which are simple eigenvalues of h; otherwise, $\sigma_{\mathrm{p}}(h) = \emptyset$.*

Using this representation in Eq. (2.8) (in this case, $J = 1$), one finds that the wave operators have the form $W_\pm = 1 - K_\pm$, where $uK_\pm u^*$ are integral operators in $L_2(\mathbb{T}^d) \oplus L_2(\mathbb{T}^d)$ with 2×2-matrix kernels

$$K_\pm(k, k') = \frac{t(2\pi)^{-d}}{\omega(k) - \omega(k') \pm \mathrm{i}0}(\sigma_1 + t\tilde{g}(\omega(k') \mp \mathrm{i}0)\sigma_0)^{-1}. \tag{2.39}$$

The S-matrix acquires the form $S = 1 + T$ with uTu^* having the generalized kernel

$$t(k, k') = \frac{\mathrm{i}\delta(\omega(k) - \omega(k'))}{(2\pi)^{d-1}}(\sigma_1 + t\tilde{g}(\omega(k') + \mathrm{i}0)\sigma_0)^{-1}. \tag{2.40}$$

3. Quasi-free Fermion models

3.1. The algebra of observables, the C^*-dynamics and the reference state

We consider the physical situation described in the Introduction, with r reservoirs of free Fermi gases at equilibrium, coupled via a tunneling junction with a sample consisting of free Fermi particles with a finite-dimensional one-particle state space. The dynamics is supposed quasi-free, specified by the one-particle Hamiltonian $h = h^0 + v$, fulfilling the assumptions of Sec. 2. This subsection is devoted to a precise definition of the quantum system under consideration. We use the notation of subsections 2.1., 2.2..

We start with defining the *C^*-dynamical system*:

Let $\mathcal{F}(\mathcal{H}^{(1)})$ be the antisymmetric Fock space over the one-particle space of Assumption 2.1, and denote $a^*(f)/a(f)$ the usual creation/annihilation operators of one particle in the state $f \in \mathcal{H}^{(1)}$; $a^*(f)$ is linear and $a(f)$ is antilinear with respect with $f \in \mathcal{H}^{(1)}$. The following anticommutation relations hold: for $f, g \in \mathcal{H}^{(1)}$,

$$\{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0, \ \{a(f), a^*(g)\} = (f, g). \tag{3.1}$$

It follows that $\|a(f)\| = \|a^*(f)\| = \|f\|$. The norm-closed operator algebra generated by them, denoted $CAR(\mathcal{H}^{(1)})$ (called the the algebra of canonical anticommutation relations), is taken as *the algebra of local observables* of the system. As an instance, we shall consider elements in $CAR(\mathcal{H}^{(1)})$ which are the second quantization of one-particle operators: for a trace-class operator a acting in $\mathcal{H}^{(1)}$ with canonical form $a = \sum s_k(f_k, \cdot)g_k$ (where s_k are the singular values of a), $d\Gamma(a) = \sum s_k a^*(g_k)a(f_k) \in CAR(\mathcal{H}^{(1)})$.

The one-particle Hamiltonians h^0 and h define two (strongly continuous) groups of automorphisms of $CAR(\mathcal{H}^{(1)})$ (corresponding to the uncoupled and coupled dynamics, respectively) by

$$\alpha^t(a^\sharp(f)) = a^\sharp(\mathrm{e}^{\mathrm{i}h^0 t} f), \quad \tau^t(a^\sharp(f)) = a^\sharp(\mathrm{e}^{\mathrm{i}ht} f). \tag{3.2}$$

Also, let ϕ^θ denote the gauge automorphism group of $CAR(\mathcal{H}^{(1)})$, i.e.

$$\phi^\theta(a^\sharp(f)) = a^\sharp(\mathrm{e}^{\mathrm{i}\theta} f). \tag{3.3}$$

Corresponding to the decomposition $\mathcal{H}^{(1)} = \mathcal{H}_S^{(1)} \oplus (\oplus_{i=1}^r \mathcal{H}_i^{(1)})$, one can define gauge automorphisms ϕ_i $(i = 1, ..., r)$, ϕ_S of the kinematical algebras $CAR(\mathcal{H}_i^{(1)})$ $(i = 1, ..., r)$, $CAR(\mathcal{H}_S^{(1)})$ of the reservoirs and of the sample.

The states of the system are positive linear functionals $\omega : CAR(\mathcal{H}^{(1)}) \to \mathbb{C}$ of norm $\|\omega\| = \omega(1) = 1$. A state ω is gauge invariant (i.e. $\omega \circ \phi^\theta = \omega$) if, and only if, $\omega(\prod_{i=1}^{n} a^*(g_i) \prod_{i=1}^{m} a(f_i)) = 0$, $\forall n \neq m$. For any state ω, the formula

$$\omega(a^*(g)a(f)) = (g, \rho_\omega f) \tag{3.4}$$

defines a self-adjoint operator $0 \leq \rho_\omega \leq 1$ on $\mathcal{H}^{(1)}$, called its density operator.

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

$$\omega_\rho(a^*(g_m)...a^*(g_1)a(f_1)...a(f_n)) = \delta_{m,n} \det\{(f_i, \rho g_j)\}. \tag{3.5}$$

If the initial state ω^0 of our system is quasi-free and α^t-invariant, what happens if its density operator ρ^0 commutes with h^0, its evolution ω^t under the perturbed dynamics τ^t is likewise a quasi-free state with density operator:

$$\rho^t = [\mathrm{e}^{-\mathrm{i}th^0}\mathrm{e}^{\mathrm{i}th}]^* \rho^0 \mathrm{e}^{-\mathrm{i}th^0}\mathrm{e}^{\mathrm{i}th}; \tag{3.6}$$

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

$$\begin{aligned}\omega^t(a^*(g)a(f)) &:= \omega^0(\tau^t(a^*(g)a(f))) = \omega^0(\alpha^{-t} \circ \tau^t(a^*(g)a(f))) = \\ &= \omega^0(a^*(\mathrm{e}^{-\mathrm{i}th^0}\mathrm{e}^{\mathrm{i}th}g)a(\mathrm{e}^{-\mathrm{i}th^0}\mathrm{e}^{\mathrm{i}th}f)) = (\mathrm{e}^{-\mathrm{i}th^0}\mathrm{e}^{\mathrm{i}th}g, \rho^0\mathrm{e}^{-\mathrm{i}th^0}\mathrm{e}^{\mathrm{i}th}f).\end{aligned}$$

The initial state is taken as a product state $\omega^0 = \omega_S \otimes (\otimes_{i=1}^r \omega_i)$, where ω_i are the equilibrium states of two lattice free Fermi gases with one-particle state spaces $\mathcal{H}_i^{(1)}$ and one-particle Hamiltonians h_i and ω_S is an invariant state of the isolated sample.

It is well-known [4] that, at given values of the temperature $\beta^{-1} \geq 0$ and chemical potential $\mu \in \mathbb{R}$, a free Fermi gas has a unique equilibrium state: it is the gauge-invariant quasi-free state with density operator $f_{\beta,\mu}(h)$, where h is the one-particle Hamiltonian, and $f_{\beta,\mu}$ is the Fermi-Dirac function:

$$f_{\beta,\mu}(x) = \frac{1}{1 + \mathrm{e}^{\beta(x-\mu)}} \tag{3.7}$$

This defines in particular the initial states of the reservoirs ω_i.

3.2. Convergence to the NESS and currents

We present here the main results of [2] within the framework defined by Assumptions 2.1–2.3. As with our assumptions no regularization is necessary, the proof can be made considerably more transparent, so we shall sketch the argument for reader's convenience.

As all states involved are quasi-free and gauge-invariant, it is sufficient, in view of Eq. (3.5), to establish the convergence of the state on elements of the form $a(g)a^*(f)$. This means to calculate the limit density operator as a *weak* limit of the density operators ρ^t.

As shown in Sec. 2, $\mathcal{H}^{(1)} = \mathcal{H}_{\rm ac}(h) \oplus \mathcal{H}_{\rm p}(h)$, with $\mathcal{H}_{\rm p}(h)$ finite-dimensional. Let $P_{\rm ac}, P_{\rm p}$ denote the corresponding orthogonal projections. We calculate the density operator:

$$\rho_+ = ({\rm w}) \lim_{T\to+\infty} (1/T) \int_0^T \rho^t {\rm d}t. \tag{3.8}$$

For $f \in \mathcal{H}_{\rm ac}(h)$, we have, in view of Eq. (3.6),

$$\lim_{t\to+\infty} \rho^t f = W_- \rho^0 W_-^* f$$

because $\lim_{t\to+\infty} {\rm e}^{-ith^0}{\rm e}^{ith} f = W_-^* f$ exists. On the other hand, if $f \in \mathcal{H}_{\rm p}(h)$, it is a finite combination of eigenvectors, so, we can suppose that f is an eigenvector of h with eigenvalue e,

$$({\rm w}) \lim_{t\to+\infty} P_{\rm ac} {\rm e}^{-ith} \rho^0 {\rm e}^{ith} f = ({\rm w}) \lim_{t\to+\infty} P_{\rm ac} {\rm e}^{-{\rm i}t(h-e)} (\rho^0 f) = 0$$

by the Riemann-Lebesgue lemma, while, for any eigenvector g of h with eigenvalue e',

$$\lim_{T\to+\infty} (1/T) \int_0^T (g, \rho^t f) {\rm d}t = \lim_{T\to+\infty} (1/T) \int_0^T {\rm e}^{{\rm i}t(e-e')} (g, \rho^0 f) {\rm d}t = \delta_{e,e'} (g, \rho^0 f).$$

In summary,

PROPOSITION **3.1** *The following limit exists for $A \in CAR(\mathcal{H}^{(1)})$*

$$\lim_{T\to+\infty} (1/T) \int_0^T \omega^t(A) {\rm d}t = \omega_+(A) \tag{3.9}$$

and is the quasi-free gauge invariant state of density operator

$$\rho_+ = W_- \rho^0 W_-^* + \sum_{e\in\sigma_{\rm p}(h)} P_e \rho^0 P_e, \tag{3.10}$$

where P_e is the projection onto the eigenspace of h corresponding to the eigenvalue e. Thereby, the restriction of ω_+ to $CAR(\mathcal{H}_{\rm ac}(h))$ is the quasi-free state of density $W_- \rho^0 W_-^*$, and we have

$$\lim_{t\to+\infty} \omega^t(A) = \omega_+(A), \ A \in CAR(\mathcal{H}_{\rm ac}(h)). \tag{3.11}$$

Clearly, the state ω_+ is τ^t-invariant, in particular, for any trace-class operator a on $\mathcal{H}^{(1)}$, $\frac{\mathrm{d}}{\mathrm{d}t}\omega_+(\tau^t(d\Gamma(a))) = 0$, implying that $\mathrm{tr}(\rho_+[h,a]) = 0$. However, if a is not a trace-class operator (but $\rho_+[h,a]$ is trace-class), it may happen that $\mathrm{tr}(\rho_+[h,a]) \neq 0$. This is the case for the extensive conserved charges of the isolated reservoirs, and it expresses the existence of the steady currents in the NESS ω_+ constructed above.

Each of the reservoirs R_i has two conserved quantities, the energy and the particle number, which correspond formally to $d\Gamma(h_0 P_i)$ and $d\Gamma(P_i)$, where P_i is the projection of $\mathcal{H}^{(1)}$ onto $\mathcal{H}_i^{(1)}$. This is expressed by the invariance of their equilibrium states ω_i under the dynamical and gauge automorphism groups, α_i^t and ϕ_i^θ, of the isolated reservoirs. The energy and particle currents from the reservoirs R_i is calculated as the ω_+-expectation of the corresponding fluxes $I_{i,\mathrm{en}} = d\Gamma(-\mathrm{i}[h, h^0 P_i]) = d\Gamma(-\mathrm{i}[v, h^0 P_i])$ and $I_{i,\mathrm{part}} = d\Gamma(-\mathrm{i}[h, P_i]) = d\Gamma(-\mathrm{i}[v, P_i])$, respectively. Remark that, because v is a finite range operator, the commutators are trace-class in $\mathcal{H}^{(1)}$, so the proposition 3.1 applies. As $P_e h = h P_e = e P_e$, the sum over the point spectrum in Eq. (3.10) does not contribute to any of the two currents $J = \omega_+(I)$. Hence,

PROPOSITION **3.2** *The energy and particle currents from the reservoirs R_i are calculated according to the formulas*

$$
\begin{aligned}
J_{i,\mathrm{en}} &= -\mathrm{tr}(\rho^+ \mathrm{i}[v, h_0 P_i]) = -\mathrm{tr}(W_- \rho^0 W_-^* \mathrm{i}[v, h_0 P_i]), \\
J_{i,\mathrm{part}} &= -\mathrm{tr}(\rho^+ \mathrm{i}[v, P_i]) = -\mathrm{tr}(W_- \rho^0 W_-^* \mathrm{i}[v, P_i]).
\end{aligned}
\tag{3.12}
$$

We shall next bring formulas (3.12) to a form, known as Landauer-Büttiker formulas, which make clear that the currents depend in fact only on the on-shell T-matrix T_x. We start with a statement [2] relative to a larger class of conserved reservoir observables.

PROPOSITION **3.3** *Let a be a bounded self-adjoint operator in $\mathcal{H}_{\mathrm{ac}}^{(1)}(h^0)$ commuting with h^0, so that, in the representation of Remark 2.1, $UaU^* = \int^{\oplus} a(x)\mathrm{d}x$, with $a(x)$ bounded self-adjoint operators in $\mathcal{K}_x$. We denote $\hat{a} = JaJ^*$ its counterpart in $\mathcal{H}^{(1)}$. Let*

$$
J(a) := \omega_+(d\Gamma(-\mathrm{i}[h, \hat{a}])) = -\mathrm{tr}_{\mathcal{H}_{\mathrm{ac}}(h)}(W_- \rho^0 W_-^* \mathrm{i}[h, \hat{a}]) \tag{3.13}
$$

be the "current" associated to a. Then,

$$
J(a) = -\int \mathrm{tr}_{\mathcal{K}_x}\{\rho^0(x)[a(x)T_x + T_x^* a(x) + T_x^* a(x) T_x]\} \frac{\mathrm{d}x}{2\pi}. \tag{3.14}
$$

Proof. The equality in Eq. (3.13), meaning that the sum over the point spectrum of h in Eq. (3.10) vanishes, is shown in the same way as for Eq. (3.12).

As, by Assumption 2.2, $v = J\tau^* I^* + I\tau J^*$, the commutator in the r.h.s. of (3.13) equals $[h, \hat{a}] = [v, \hat{a}] = I\tau a J^* - J a \tau^* I^*$, which has finite-range. Using the permutation invariance of the trace,

$$\mathrm{tr}_{\mathcal{H}_{\mathrm{ac}}(h)}(W_- \rho^0 W_-^* [v, \hat{a}]) = \mathrm{tr}_{\mathcal{K}}(U \rho^0 W_-^* [v, \hat{a}] W_- U^*).$$

We show that the operator under trace is an integral operator on $\mathcal{K}$, i.e. of the form $K\psi(x) = \int \mathrm{d}y k(x,y)\psi(y)$, where $k(x,y) : \mathcal{K}_y \to \mathcal{K}_x$ are continuous, trace-class-operator valued functions. Therefore, the trace can be calculated as $\int \mathrm{d}x \mathrm{tr}_{\mathcal{K}_x} k(x,x)$.

To this aim, we factorize the two terms of the commutator as

$$\begin{aligned} UW_-^*[v,\hat{a}]W_-U^* = \; & (UW_-^* I\tau U^*)(UaU^*)(UJ^*W_-U^*) \\ & -(UW_-^*JU^*)(UaU^*)(U\tau^*I^*W_-U^*). \end{aligned}$$

Remembering the representation of τ, τ^* in Remark 2.1 and the expressions (2.14), (2.15) of W_-, W_-^*, the generalized kernels of the operators in brackets are

$$(UW_-^*JU^*)(x,y) = \delta(x-y) + (y-x+\mathrm{i}0)^{-1}\tau_x^* R_{\mathrm{eff}}(x-\mathrm{i}0)\tau_y;$$

$$(UJ^*W_-U^*)(x,y) = \delta(x-y) + (x-y-\mathrm{i}0)^{-1}\tau_x^* R_{\mathrm{eff}}(y+\mathrm{i}0)\tau_y;$$

$$(UW_-^*I\tau U^*)(x,y) = -\tau_x^* R_{\mathrm{eff}}(x-\mathrm{i}0)\tau_y;$$

$$(U\tau^*I^*W_-U^*)(x,y) = -\tau_x^* R_{\mathrm{eff}}(y+\mathrm{i}0)\tau_y.$$

The kernel $k(x,y)$ is obtained as the composition of the kernels of the factors. The continuity with respect with x, y is a consequence of Assumption 2.2. The diagonal $k(x,x)$ equals

$$\begin{aligned} & -\tau_x^* R_{\mathrm{eff}}(x-\mathrm{i}0)\tau_x a(x) + a(x)\tau_x^* R_{\mathrm{eff}}(x-\mathrm{i}0)\tau_x - \\ & -\int \mathrm{d}x' \tau_x^* R_{\mathrm{eff}}(x-\mathrm{i}0)\tau_x' a(x')\tau_{x'}^* R_{\mathrm{eff}}(x+\mathrm{i}0)\tau_x \times \\ & \qquad \times[(x'-x-\mathrm{i}0)^{-1} - (x'-x+\mathrm{i}0)^{-1}] \\ & = \tfrac{1}{2\pi\mathrm{i}}[T_x^* a(x) + a(x)T_x + T_x^* a(x) T_x], \end{aligned}$$

where we used the Sokhotski formula $(x-\mathrm{i}0)^{-1} = \mathcal{P}\left(\frac{1}{x}\right) + \mathrm{i}\pi\delta(x)$ and the definition (2.13) of the T-matrix. Insertion of this calculation in Eq. (3.13) gives Eq. (3.14). $\square$

We take now into account the decomposition $\mathcal{H}^{(1)}_{\rm ac}(h^0) = \bigoplus_i \mathcal{H}^{(1)}_i$. For an energy $x \in [e_{\min}, e_{\max}]$, we have $\mathcal{K}_x = \bigoplus_i \mathcal{K}_{x,i}$; thereby, if $x \notin I_i$, $\mathcal{K}_{x,i} = \{0\}$. Accordingly, the operators under $\mathrm{tr}_{\mathcal{K}_x}$ in Eq. (3.14) have matrix representations. The density $\rho^0(x)$ is the diagonal matrix with $\rho^0(x)_{i,i} = f_{\beta_i,\mu_i}(x)\cdot 1$. Also, $(T_x)_{i,j} = 2\pi\mathrm{i}(\tau_i^*)_x R_{\rm eff}(x+\mathrm{i}0)(\tau_j)_x$, which vanishes for $x \notin I_i \cap I_j$. What concerns $a(x)$, as we are interested in observables associated with the isolated reservoirs, we suppose that its matrix has block-diagonal form: $a(x)_{i,j} = \delta_{i,j} a_i(x)$. In this case,

$$\begin{aligned}&\mathrm{tr}_{\mathcal{K}_x}\{\rho^0(x)[a(x)T_x + T_x^* a(x) + T_x^* a(x) T_x]\} =\\ &\sum_{i=1}^r f_{\beta_i,\mu_i}(x)\mathrm{tr}_{\mathcal{K}_{x,i}}\{a_i(x)(T_x)_{i,i} + (T_x^*)_{i,i} a_i(x) + \sum_{j=1}^r (T_x^*)_{i,j} a_j(x)(T_x)_{j,i}\}.\end{aligned} \tag{3.15}$$

This can be further simplified using the unitarity of the S-matrix:

$$(T_x)_{i,i} + (T_x^*)_{i,i} + \sum_{j=1}^r (T_x)_{i,j}(T_x^*)_{j,i} = 0$$

and the permutation invariance of the trace, whence

$$\begin{aligned}&\sum_{i=1}^r f_{\beta_i,\mu_i}(x)\mathrm{tr}_{\mathcal{K}_{x,i}}\{a_i(x)(T_x)_{i,i} + (T_x^*)_{i,i} a_i(x)\}\\ &= -\sum_{i=1}^r f_{\beta_i,\mu_i}(x)\mathrm{tr}_{\mathcal{K}_{x,i}}\{a_i(x)\sum_{j=1}^r (T_x)_{i,j}(T_x^*)_{j,i}\\ &= -\sum_{j=1}^r f_{\beta_j,\mu_j}(x)\mathrm{tr}_{\mathcal{K}_{x,i}}\{\sum_{j=1}^r (T_x^*)_{i,j} a_j(x)(T_x)_{j,i}.\end{aligned}$$

Hence,

COROLLARY **3.1** *For a self-adjoint operator a in $\mathcal{H}^{(1)}_{\rm ac}(h^0)$ such that $a(x)_{i,j} = \delta_{i,j} a_i(x), \forall x$,*

$$J(a) = \sum_{i,j=1}^r \int [f_{\beta_i,\mu_i}(x) - f_{\beta_j,\mu_j}(x)]\mathrm{tr}_{\mathcal{K}_{x,i}}\{a_i(x)(T_x)_{i,j}(T_x^*)_{j,i}\}\mathrm{d}x. \tag{3.16}$$

Thereby, $(T_x)_{i,j} \neq 0$ only for $x \in I_i \cap I_j$.

In particular, defining the transmission probability between reservoirs R_i and R_j as $t_{i,j}(x) := \mathrm{tr}_{\mathcal{K}_{x,i}}\{(T_x)_{i,j}(T_x^*)_{j,i}\}$,

$$\begin{aligned}J_{i,\rm en} &= \sum_{j=1}^r \int [f_{\beta_i,\mu_i}(x) - f_{\beta_j,\mu_j}(x)] x t_{i,j}(x),\\ J_{i,\rm part} &= \sum_{j=1}^r \int [f_{\beta_i,\mu_i}(x) - f_{\beta_j,\mu_j}(x)] t_{i,j}(x).\end{aligned} \tag{3.17}$$

3.3. Consequences for the model of Sec. 2.3

We specialize here to the case of two reservoirs ($r = 2$) of free lattice Fermi gases described in Sec. 2.3. and draw a few conclusions about its behavior as a function of the dimension of the lattices d_i and of the wire length N.

- *The currents*, Eq. (3.17), *are a sum of two currents*, each obtained when one of the two reservoirs is put in turn in the Fock state (corresponding to the density matrix $f_{+\infty,-\infty}(h_i) = 0$. One may consider therefore only the particle current

$$J_{1,\mathrm{part}}(\beta, \mu) = \int f_{\beta,\mu}(x) t_{1,2}(x). \tag{3.18}$$

- *The transmission probability*

$$t_{1,2}(x) = \int_{\mathbb{T}^d(x)} \mathrm{d}\mu_x(k) \int_{\mathbb{T}^d(x)} \mathrm{d}\mu_x(k) |T(k, k')_{1,2}|^2$$

has a resonant structure. In view of Eq. (2.33), one has to study the energy dependence of the matrix element $R_{\mathrm{eff}}(x + \mathrm{i}0)_{1,N}$. By analytic perturbation theory, as h_S has simple eigenvalues ε_m, the eigenvalues $\lambda_m(x)$, $m = 1, ..., N$ of $h_{\mathrm{eff}}(x + \mathrm{i}0)$ are simple for sufficiently small tunneling constant t. Let $\psi^{(m)}(x)$ be the corresponding eigenvectors; then $\bar{\psi}^{(m)}(x)$ is the dual basis (i.e. $(\bar{\psi}^{(m)}(x), \psi^{(m')}(x)) = \delta_{m,m'}$. Hence,

$$R_{\mathrm{eff}}(x + \mathrm{i}0)_{1,N} \sim \sum_{m=1}^{N} (\lambda_m(x) - x)^{-1} \psi_1^{(m)}(x) \psi_N^{(m)}(x).$$

To lowest order in t, $\lambda_m(x) \sim \varepsilon_m - \frac{2}{N+1} t^2 g(x + \mathrm{i}0) \sin^2 q_m$, where we used Eq. (2.28) and the explicit form (2.23) of the eigenvectors $\psi^{(m)}$ at $t = 0$, which puts into evidence "resonances" at $x = \varepsilon_m - \frac{2}{N+1} t^2 \Re g(x + \mathrm{i}0) \sin^2 q_m$ of "width" $\frac{2}{N+1} t^2 \Im g(x + \mathrm{i}0) \sin^2 q_m$.

- *The density profile*

$$n(r) = \omega_+(a^*(\delta_r) a(\delta_r)) = \sum (P_e \delta_r, \rho^0 P_e \delta_r) + (W_-^* \delta_r, \rho^0 W_-^* \delta_r) \tag{3.19}$$

is a sum over reservoirs of density profiles corresponding to the other reservoir put in its Fock state (due to the block structure of $\rho^0 = \sum_i^{\oplus} \rho_i$). We calculate the second term of (3.19) with $\rho_2 = 0$. We need therefore $P_1 W_-^* \delta_r$, where P_1 is the projection onto $\mathcal{H}_1^{(1)}$. In view of Eq. (2.15), we have

$$(UP_1 W_-^* \delta_r)(x) = -t\psi^1(k)_{\alpha_1} R_{\text{eff}}(x - \text{i}0)_{1,r},$$

if $r \in \{1, ..., N\}$,

$$(UP_1 W_-^* \delta_r)(x) = \psi^1(k)_r + t^2\psi^1(k)_{\alpha_1} R_{\text{eff}}(x - \text{i}0)_{1,1} R_1(x + \text{i}0)_{\alpha_1,r}$$

if $r \in L_1$, and

$$(UP_1 W_-^* \delta_r)(x) = t^2\psi^1(k)_{\alpha_1} R_{\text{eff}}(x - \text{i}0)_{1,N} R_2(x + \text{i}0)_{\alpha_2,r},$$

if $r \in L_2$.

In particular, the density profile inside R_2 (the initially void reservoir), is given by

$$t^4 \int \text{d}k f_{\beta_1,\mu_1}(\omega_1(k))|\psi^1(k)_{\alpha_1} R_{\text{eff}}(\omega_1(k) - \text{i}0)_{1,N}|^2 |R_2(\omega_1(k) + \text{i}0)_{\alpha_2,r}|^2.$$

It is to be remarked that, if $d_2 = 1$ (which is the model of infinite leads used in [6]), the density of transmitted particles has a nonzero limit as $r \to \infty$; this seems improper for a reservoir, which is expected to keep unchanged its "conserved charges" even after coupling it to other reservoirs. For $d_2 > 1$, the density decays like $|r|^{-1}$ irrespective of d_2 [14].

4. Quasi-free Boson models

4.1. The algebra of observables and the reference state

The kinematical C^*-algebra of the model is the canonical commutation relation algebra $CCR(\mathcal{D})$ over a suitable subspace $\mathcal{D} \subset \mathcal{H}^{(1)}$, which is left invariant by the one-particle evolution groups: $\exp(\text{i}th^0)\mathcal{D} = \mathcal{D}$, $\exp(\text{i}th)\mathcal{D} = \mathcal{D}$.

$CCR(\mathcal{D})$ is generated by the Weyl operators $\{\mathcal{W}(f);\ f \in \mathcal{D}\}$, satisfying

$$\mathcal{W}(f)\mathcal{W}(g) = \text{e}^{-\frac{\text{i}}{2}\Im(f,g)}\mathcal{W}(f+g). \tag{4.1}$$

The defining equation (4.1) implies that $\mathcal{W}(0) = 1$ and $\mathcal{W}(f)$ are unitaries ($\mathcal{W}(f)^*\mathcal{W}(f) = 1$). According to a theorem by Slawny, such a C^*-algebra is unique up to an isomorphism; in particular, it can be shown (using the well-known Fock representation) that $\|\mathcal{W}(f) - 1\| \geq \sqrt{2}$ for $f \neq 0$, implying that the application $f \mapsto \mathcal{W}(f)$ cannot be norm-continuous [13].

To any state ω on $CCR(\mathcal{D})$ a function $E : \mathcal{D} \to \mathbb{C}$ is associated by

$$E(f) = \omega(\mathcal{W}(f)), \tag{4.2}$$

named its generating functional. E satisfies: (i) normalization: $E(0) = 1$, (ii) unitarity: $\overline{E(f)} = E(-f)$, and (iii) positivity:

$$\sum_{i,j=1}^{n} z_i E(f_i - f_j) \mathrm{e}^{-\frac{\mathrm{i}}{2}\Im(f_i,f_j)} \bar{z}_j \geq 0,\ \forall n, \forall z_i \in \mathbb{C}, f_i \in \mathcal{D}\,(i = 1, ..., n).$$

Conversely, any E with these properties defines a unique state by Eq. (4.2). Therefore, in describing the initial and evolved states of our model, it will be sufficient to specify the corresponding generating functionals.

A state ω is quasi-free if, and only if, E has the particular form

$$E(f) = \exp\left(\mathrm{i}\sqrt{2}\Re\langle l, f\rangle - \frac{1}{4}Q(f, f)\right), \tag{4.3}$$

where $l \in \mathcal{D}'$ is a linear form and $Q(\cdot,\cdot) \geq 1$ a quadratic form on $\mathcal{D} \times \mathcal{D}$. Quasi-free states ω are regular, i.e. in the associated GNS representation π_ω, for any $f \in \mathcal{D}$, the unitary group $\mathbb{R} \ni t \mapsto \pi_\omega(\mathcal{W}(tf))$ is weakly continuous. Hence, $\forall f \in \mathcal{D}$, there exist self-adjoint operators $\varphi(f)$ – "field operators", such that $\pi_\omega(\mathcal{W}(tf)) = \exp(\mathrm{i}t\varphi(f))$. The fields $\varphi(f)$ are real-linear functions of f. In terms of the fields $\varphi(f)$ one can define creation and annihilation operators by $a^*(f) = 2^{-1/2}(\varphi(f) - \mathrm{i}\varphi(\mathrm{i}f))$, $a(f) = 2^{-1/2}(\varphi(f) + \mathrm{i}\varphi(\mathrm{i}f))$. Then, denoting Ω_ω the cyclic vector of π, one has the following

PROPOSITION **4.1** *In a quasi-free state with generating functional* (4.3), Ω_ω *is in the domain of all powers of* $a^\sharp(f)$, $f \in \mathcal{D}$, *and the following relations hold:*

$$\begin{aligned}(\Omega_\omega, a^*(f)\Omega_\omega) = \overline{(\Omega_\omega, a(f)\Omega_\omega)} = \langle l, f\rangle,\\ (\Omega_\omega, a^*(g)a(f)\Omega_\omega) - (\Omega_\omega, a^*(g)\Omega_\omega)(\Omega_\omega, a(f)\Omega_\omega) = Q(f, g);\end{aligned} \tag{4.4}$$

all other truncated expectations vanish.

The time evolutions α^t, τ^t, for the uncoupled, respectively, coupled reservoirs and sample are the groups of Bogoliubov automorphisms on $CCR(\mathcal{D})$ defined by their action on $\mathcal{W}(f)$:

$$\begin{aligned}\alpha^t(\mathcal{W}(f)) &= \mathcal{W}(\mathrm{e}^{\mathrm{i}h^0 t}f),\\ \tau^t(\mathcal{W}(f)) &= \mathcal{W}(\mathrm{e}^{\mathrm{i}ht}f).\end{aligned} \tag{4.5}$$

In view of the canonical commutation relations (4.1), Eq. (4.5) is sufficient to uniquely define the action of τ^t on all elements of $CCR(\mathcal{D})$. By the remark above, the two automorphism groups are *not* strongly continuous. However, in a quasi-free representation they are implemented by weakly continuous unitary groups. Moreover, the evolution of a quasi-free initial state under a dynamics of the form (4.5) is likewise quasi-free. This means that the evolved state at time $t > 0$ of Boson systems, which, at $t = 0$, were in a quasi-free state, is uniquely determined by the evolved one-point and two-point functions, i.e. by $\langle l_t, f\rangle = \langle l, \mathrm{e}^{\mathrm{i}ht}f\rangle$ and $Q_t(f,g) = Q(\mathrm{e}^{\mathrm{i}ht}f, \mathrm{e}^{\mathrm{i}ht}g)$. In this respect, their study parallels the study of Fermi systems in the previous section and the counterpart of proposition 3.1 holds true. There appear, however, subtleties related to the choice of the initial (reference) state; in particular, unlike in the Fermi case, the domain $\mathcal{D}$ (i.e. the kinematical algebra $CCR(\mathcal{D})$) depends on the reference state. In order to keep the exposition at a reasonable level of complexity, we shall explain them only for the model in Sec. 2.4., i.e. direct tunneling between reservoirs on $\mathbb{Z}^d$ with no intermediate sample. The consideration of the general frame (given by assumptions 2.1–2.3, supplemented with special requirements about the existence of a density of energy levels in the infinite volume limit) is left for another publication.

The equilibrium states of a free Bose gas are quasi-free; they have been studied in detail in the literature [4]. The peculiarity of the free Bose gas is that, under certain conditions, it shows a phase transition at low temperature and high density. It happens that, in the multi-phase region, the canonical and grand-canonical are inequivalent. As we are interested in particle flows between reservoirs, it is natural to use the canonical description for the reservoirs.

We remind below the expressions of the generating functionals for the canonical equilibrium states for our model of reservoir, obtained by an easy adaptation of the derivation by Cannon [4], [11] for the continuum Bose gas.

We start by describing one reservoir R, consisting of a free lattice Bose gas living on $\mathbb{Z}^d$.

Let β, ρ be fixed positive numbers and define:

$$\rho_{\mathrm{cr}}(\beta) = (2\pi)^{-d}\int_{\mathbb{T}_1^d} \frac{1}{\mathrm{e}^{\beta\omega(k)} - 1}\mathrm{d}^d k \leq +\infty, \tag{4.6}$$

where $\omega(k)$ is the dispersion law Eq. (2.20). As $\omega(k) \approx \frac{1}{2}|k|^2$ around its minimum at $k = 0$, one has that $\rho_{\rm cr}(\beta)$ is finite for $d \geq 3$ and is infinite for $d = 1, 2$.

For $\rho < \rho_{\rm cr}(\beta)$, the fugacity z is defined to be the unique solution $z(\beta, \rho)$ of the equation

$$\rho = (2\pi)^{-d} \int\limits_{\mathbb{T}^d} \frac{z}{\mathrm{e}^{\beta\omega(k)} - z} \mathrm{d}^d k,$$

while, for $\rho \geq \rho_{\rm cr}(\beta)$, put $z(\beta, \rho) = 1$. The momentum distribution for $k \neq 0$ at the given β, ρ is proportional to

$$n_{\beta,\rho}(k) = \frac{z(\beta, \rho)}{\mathrm{e}^{\beta\omega(k)} - z(\beta, \rho)}, \tag{4.7}$$

while the condensate density is given by

$$\rho_0 = \max\{0, \rho - \rho_{\rm cr}(\beta)\}. \tag{4.8}$$

Then, the generating functional of the canonical equilibrium state at β, ρ is given by the formula

$$E_{\beta,\rho}(f) = \exp\left\{-\frac{\|f\|^2}{4} - \frac{1}{2}(uf, n_{\beta,\rho}\, uf)\right\} J_0(\sqrt{2(2\pi)^d \rho_0}\, |(uf)(0)|), \tag{4.9}$$

where u is the Fourier transform and J_0 is the Bessel function.

For $\rho \leq \rho_{\rm cr}(\beta)$, the canonical state defined by Eq. (4.9) is extremal, however, if $\rho_{\rm cr}(\beta) < \infty$ and $\rho > \rho_{\rm cr}(\beta)$, it has a nontrivial decomposition into extremal states indexed by a phase $\mathrm{e}^{\mathrm{i}\theta}$:

$$E_{\beta,\rho}(f) = (2\pi)^{-1} \int_0^{2\pi} E^{\theta}_{\beta,\rho}(f) \mathrm{d}\theta, \tag{4.10}$$

where

$$E^{\theta}_{\beta,\rho}(f) = \exp\left\{-\frac{\|f\|^2}{4} - \frac{(uf, n_{\beta,\rho}\, uf)}{2} - \frac{\mathrm{i}\sqrt{2\rho_0}}{(2\pi)^{d/2}} \Re(\mathrm{e}^{-\mathrm{i}\theta}(uf)(0))\right\}. \tag{4.11}$$

Thereby, the test function space $\mathcal{D}$ should be chosen such that the functionals (4.11) are well defined for $f \in \mathcal{D}$, e.g. taking $\mathcal{D} = l^1(\mathbb{Z}^d)$ would suffice. Indeed, with this choice uf is continuous on $\mathbb{T}^d$, ensuring both the integrability of $n_{\beta,\rho}|uf|^2$ and the existence of $(uf)(0)$. We shall impose, however a stronger condition ensuring that uf is Hölder-continuous, and take $\mathcal{D}$ as the space $l^1(\mathbb{Z}^d; |x|^\epsilon)$ for some $\epsilon > 0$, consisting of functions $f : \mathbb{Z}^d \to \mathbb{C}$ for which $\|f\|_{\mathcal{D}} := \sum_{x\in\mathbb{Z}^d} |x|^\epsilon |f_x| < \infty$.

Using the matrix notation associated with the direct sum $\mathcal{H}^{(1)} = \mathcal{H}_1^{(1)} \oplus \mathcal{H}_2^{(1)}$, we take $f = f_1 \oplus f_2 \in \mathcal{D}_1 \oplus \mathcal{D}_2$ (where $\mathcal{D}_i$ are copies of $\mathcal{D}$) and the initial state ω^0 as a product of canonical equilibrium states of R_i at temperatures β_i and densities ρ_i $(i = 1, 2)$, respectively:

$$\omega^0(\mathcal{W}(f)) = E_0(f) = E_{\beta_1,\rho_1}(f_1) E_{\beta_2,\rho_2}(f_2), \tag{4.12}$$

where $E_{\beta_i,\rho_i}(f_i)$ are arbitrary mixtures (with probability measures $\mathrm{d}\mu_{1,2}(\theta_{1,2})$) of the extremal state generating functionals (4.11). Denoting $\rho_{0,i}$ the condensate densities in R_i and

$$\tilde{n}_0 = \begin{pmatrix} n_{\beta_1,\rho_1} & 0 \\ 0 & n_{\beta_2,\rho_2} \end{pmatrix}, \; \tilde{\rho}_0(\theta_1, \theta_2) = \begin{pmatrix} \sqrt{2\rho_{0,1}}\mathrm{e}^{-\mathrm{i}\theta_1} & \sqrt{2\rho_{0,2}}\mathrm{e}^{-\mathrm{i}\theta_2} \end{pmatrix}, \tag{4.13}$$

we have

$$E_0(f) = \int \mathrm{d}\mu_1(\theta_1)\mathrm{d}\mu_2(\theta_2) E_0^{\theta_1,\theta_2}(f), \tag{4.14}$$

where

$$E_0^{\theta_1,\theta_2}(f) = \exp\left\{-\frac{\|f\|^2}{4} - \frac{(uf, \tilde{n}_0\, uf)}{2} - \frac{\mathrm{i}}{(2\pi)^{d/2}} \Re(\tilde{\rho}_0(\theta_1, \theta_2)(uf)(0))\right\}. \tag{4.15}$$

In particular, the canonical states (4.9) are obtained for $\mathrm{d}\mu_i(\theta) = (2\pi)^{-1}\mathrm{d}\theta$.

4.2. The approach to, and properties of, the NESS

We are interested in the time evolution of an initial state ω^0 as defined by Eq. (4.14) (which is α^t-invariant) under the coupled dynamics τ^t, Eq. (4.5). We have

$$\omega^t(\mathcal{W}(f)) = \omega^0(\mathcal{W}(\exp(\mathrm{i}th)f) = \omega^0(\mathcal{W}(\exp(-\mathrm{i}th^0)\exp(\mathrm{i}th)f). \tag{4.16}$$

Using the analysis done in Sec. 2.4., we obtain the following convergence result, which defines the stationary state.

Proposition **4.2** *Under the condition above, the following limit exists and defines a quasi-free invariant state* ω_{stat}: $\forall f \in \mathcal{D}$,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \omega^t(\mathcal{W}(f))\mathrm{d}t = E_{\mathrm{stat}}(f). \tag{4.17}$$

Corresponding to the decomposition (4.14) *of the initial state,*

$$E_{\rm stat}(f) = \int {\rm d}\mu_1(\theta_1){\rm d}\mu_2(\theta_2)E^{\theta_1,\theta_2}_{\rm stat}(f), \tag{4.18}$$

where

$$E^{\theta_1,\theta_2}_{\rm stat}(f) = E^{\theta_1,\theta_2}_0(W^*_- P_{\rm ac}f)E^{\theta_1,\theta_2}_{\rm (p)}(P_{\rm p}f). \tag{4.19}$$

Thereby, the limit in mean is necessary only for the contribution of the point spectrum, i.e. for $f = P_{\rm ac}f$, *the limit* $\lim_{t\to\infty}\omega^t(\mathcal{W}(f))$ *exists and equals* $\int {\rm d}\mu_1(\theta_1){\rm d}\mu_2(\theta_2)E^{\theta_1,\theta_2}_0(W^*_- P_{\rm ac}f)$.

Proof. We isolate, in the quadratic and linear forms appearing at the exponent in $E^{\theta_1,\theta_2}_0({\rm e}^{{\rm i}ht}f)$, the terms which do not depend on $P_{\rm ac}f$, i.e. $T_{\rm p}(t) := -\frac{1}{4}\|P_{\rm p}f\|^2 - \frac{1}{2}(u{\rm e}^{{\rm i}ht}P_{\rm p}f, \tilde{n}_0\, u{\rm e}^{{\rm i}ht}P_{\rm p}f) - {\rm i}(2\pi)^{-3/2}\Re(\tilde{\rho}_0(\theta_1,\theta_2)(u{\rm e}^{{\rm i}ht}P_{\rm p}f)(0))$. The t-dependence of $T_{\rm p}(t)$ comes from exponentials of the form ${\rm e}^{{\rm i}e_0t}$, ${\rm e}^{{\rm i}(2d-e_0)t}$ and ${\rm e}^{{\rm i}2(d-e_0)t}$, where $e_0, 2d-e_0$ are the two eigenvalues of h. Therefore, ${\rm e}^{T_{\rm p}(t)}$ is an almost-periodic function, what ensures that $\lim_{T\to\infty}\frac{1}{T}\int_0^T {\rm e}^{T_{\rm p}(t)}{\rm d}t =: E^{\theta_1,\theta_2}_{\rm (p)}(P_{\rm p}f)$ exists. Remark that $(P_{\rm p}f)_r$ decays exponentially as $r\to\infty$, therefore, if $f\in\mathcal{D}$, $P_{\rm ac}f\in\mathcal{D}$ as well. Hence, $\int_{\mathbb{T}^d(x)}(uP_{\rm ac}f)(k){\rm d}\mu_x(k)$ is Hölder continuous of x, therefore, by the Privalov theorem [7],

$$\begin{aligned}(uW^*_-P_{\rm ac}f)(k) &= (uP_{\rm ac}f)(k) - \\ &-\tfrac{t}{(2\pi)^d}(\sigma_1 + t\tilde{g}(\omega(k)-{\rm i}0)\sigma_0)^{-1}\textstyle\int_{\mathbb{T}^d}\frac{(uP_{\rm ac}f)(k'){\rm d}k'}{\omega(k')-\omega(k)+{\rm i}0}\end{aligned} \tag{4.20}$$

is likewise Hölder continuous of $\omega(k)$ and, as such, belongs to the domain of E^{θ_1,θ_2}_0. By an analysis like that in the proof of Proposition 3.1, the remaining terms have (usual) limits as $t\to\infty$, which proves the assertion. □

In view of the explicit forms (4.15) of the functionals E^{θ_1,θ_2}_0, Proposition 4.2 provides a detailed description of the stationary state and allows the calculation of various quantities of physical interest.

We report below the analytic results for the energy and particle currents. We point out that, like in the Fermi case, the point spectrum of h gives no contribution to the currents and the contribution of the absolutely continuous spectrum may be expressed in terms of the S-matrix alone (Landauer-Büttiker-like formula). We shall not repeat here the proof of the latter, but perform the direct calculation based on Eq. (4.19). Thereby, if $d\geq 3$, we suppose, for simplicity, that we are in the weak coupling regime, where $\sigma_{\rm p}(h) = \emptyset$.

In calculating the currents between pure phases of the reservoirs, we take advantage that the initial state, being a product of extremal equilibrium states, can be approximated by finite-volume states (possibly with weak symmetry-breaking perturbations), what allows to substantiate expressions (of the currents from a reservoir in an extremal state) similar to those in the Fermi case [1]. As a preparation, we calculate, using Eq. (4.20), $W_-^* f$ for a few local functions f appearing in these expressions:

- For $(\delta_0^1)_r = \delta_{0,r}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and δ_0^2 defined analogously for the second reservoir,

$$(uP_jW_-^*\delta_0^i)(k) = \frac{1}{(2\pi)^{d/2}}\left\{\delta_{i,j} - t\tilde{g}(\omega(k)-\mathrm{i}0)[(\sigma_1 + t\tilde{g}(\omega(k)-\mathrm{i}0))^{-1}]_{j,i}\right\},$$

where P_j projects onto the reservoir j and we used the definition (2.37) of $\tilde{g}$;

- For $(h_0^1)_r = (d\delta_{x,0} - \frac{1}{2}\delta_{|x|,1})\begin{pmatrix} 1 \\ 0 \end{pmatrix}$,

$$\begin{array}{l}(uP_jW_-^*h_0^1)(k) = \frac{1}{(2\pi)^{d/2}}\left\{\omega(k)\delta_{j,1} - \right.\\ \left. -t[(\sigma_1 + t\tilde{g}(\omega(k)-\mathrm{i}0))^{-1}]_{j,1}[1+\omega(k)\tilde{g}(\omega(k)-\mathrm{i}0)]\right\}.\end{array}$$

PROPOSITION **4.3** *In the direct tunneling model of Section* 2.4*, the currents flowing from* R_1 *in the stationary state* $\omega_{stat}^{\theta_1,\theta_2}$ *arising from extremal initial states are given by:*

1. *The particle current:*

$$\begin{aligned} J^1_{\rm part}(\theta_1,\theta_2) &= 2t\Im\omega_0^{\theta_1,\theta_2}(a_0^*(W_-^*(\delta_0^1))a_0(W_-^*(\delta_0^2))) \\ &= \frac{2t}{(2\pi)^d}\int(n_1(k)-n_2(k))\frac{\Im\tilde{g}(\omega(k)-\mathrm{i}0))}{|1-t^2\tilde{g}(\omega(k)-\mathrm{i}0))^2|^2}d^3k \\ &+ \frac{2t}{(2\pi)^d}\frac{\sqrt{\rho_{01}\rho_{02}}}{1-\tilde{g}(0)^2}\sin(\theta_2-\theta_1) \end{aligned}$$

2. *The energy current:*

$$\begin{aligned} J^1_{\rm en}(\theta_1,\theta_2) &= 2t\Im\omega_0^{\theta_1,\theta_2}(a_0^*(W_-^*(h_0^1))a_0(W_-^*(\delta_0^2))) \\ &= \frac{2t}{(2\pi)^d}\int(n_1(k)-n_2(k))\frac{\omega(k)\Im\tilde{g}(\omega(k)-\mathrm{i}0))}{|1-t^2\tilde{g}(\omega(k)-\mathrm{i}0))^2}|^2d^3k. \end{aligned}$$

Several remarks are in order:

If both reservoirs are condensed, i.e. $\rho_{0,1}$, and $\rho_{0,2}$ are both different from zero, the particle current shows a peculiar dependence on the phase difference. This is not true for the energy current, where the second term, coming from the expectations of the creation/annihilation operators does not contribute (as expected, as the $k = 0$ states carry no energy). Also, if $\rho_{0,1}\rho_{0,2} \neq 0$ and $\beta_1 = \beta_2$, then $n_1(k) = n_2(k)$, in which case the integral terms in the currents, representing the contribution of the excited states, vanish, therefore particles are exchanged only between the $k = 0$ states, and there is no energy flow.

In order to obtain the currents in the canonical state, we have still to integrate the expressions of the currents over the phases θ_i of the two condensates. This has the effect that the particle currents between the $k = 0$ states are averaged out, and only the first term in the expression of the particle current survives. In particular, there is no current if the temperatures are equal and either $\rho_1 = \rho_2 \leq \rho_{\rm cr}(\beta)$, or both densities are overcritical (irrespective of their values).

As a matter of fact, Proposition 4.3 implies that the presence of the condensates in the reservoirs has little influence on the currents, as long as one considers non-symmetry-breaking states. We conjecture that this holds true for more general junctions.

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