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T-matrix formalism for one space dimension systems with different spatial asymptotics and symmetry relations for ferromagnetic Josephson junctions

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Abstract

We present a study of quantum scattering systems in one space dimension with different spatial asymptotics on the left and right, using as a specific model a ferromagnetic Josephson junction with inhomogeneous magnetization texture. So except for the space dimension there is also a particle–hole and a spin degree of freedom. We focus on the stationary scattering states of such systems and derive appropriate Lippmann–Schwinger equations for them. These lead us to define a channel-dependent T-matrix, as in N-body multichannel scattering theory, where the role of the channels is played by the different asymptotic Hamiltonians and indicates an appropriate temporal evolution. The channel-dependent T-matrix elements are shown to be proportional to the scattering amplitudes and this fact is used to obtain symmetry conditions for them, under the action of anti-unitary transformations. We then present some of the consequences of our findings to the current–phase-relation of ferromagnetic Josephson junctions, the spectrum of Andreev bound states and a simplification of the Furusaki–Tsukada formula for the dc Josephson current.

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1. Introduction

Quantum scattering systems in one space dimension with different spatial asymptotics on the left and right can appear as models describing layered mesoscopic solid state systems. These systems can be described by one-particle wave equations with spatial variation accounted for by the spatial change of certain potential functions, as well as the spatial change of the effective mass. Thus the difference in the spatial asymptotics may result from different limiting values of these functions on the left and right, as for example when the materials used in the layered structures are different from each other. A particular case of such systems are

Josephson junctions. Josephson junctions consist of superconducting electrodes separated by normal materials. The Josephson current that flows through such junctions is intimately related to the phase difference of the order parameter between the electrodes. Thus the Josephson effect is inherently related to a scattering problem with different spatial asymptotics, even if the materials used are identical. For this reason we shall use as a concrete model in our investigation that of a ferromagnetic Josephson junction. The magnetic structure of these systems also provides us with a model with a non-trivial dependence on the spin degree of freedom, as well as the particle–hole degree of freedom characteristic of superconductivity.

There has been considerable work done on the field of one dimensional scattering theory with different spatial asymptotics, both in the time-dependent and in the time-independent formalisms. In [1], the Dirac equation in one dimension was considered, with a potential having different limits on the left and right and with the investigation of the Klein paradox in mind. There the authors recognize the need for separate definitions of Møller operators, depending on the direction of motion of in-coming wavepackets. In [2], the authors start with a half-solid system in mind and define separate Møller operators depending on the direction of incidence or transmission of wavepackets, by introducing the asymptotic projection operators we mention in section 3. In [3], the Jost solutions are used to investigate the spectrum, the resolvent and the resolution of identity in systems with non-zero or periodic spatial asymptotics, different on the left and right. An account of scattering theories with step-like potentials, considering Møller operators and Lippmann–Schwinger equations for stationary scattering states, is given in [4]. However, in what the authors call the multichannel formalism, which is the one we adopt, they do not define a T-matrix, a study of which is made in this work. More recently, [5] provides a study of the time delay of scattering states for step-like potentials and reviews the whole subject, with emphasis on the time-dependent theory and a thorough account of the literature. The above references mostly concentrate on scattering systems with only the spatial degree of freedom. However, consideration of other discrete degrees of freedom is useful, for it accounts for the non-trivial modification of the dispersion relation of one-particle states.

In this work we study the T-matrix theory for scattering systems with one space dimension and different spatial asymptotics on the left and right, in the context of Josephson junction theory. We focus on potentials having well defined limits in the asymptotic regions. The T-matrix method has been used in Josephson junction theory by Ishii [6], who used a kind of mean value T-matrix, to construct the Green's function and calculate the supercurrent in a superconductor–normal metal–superconductor junction in a non-self-consistent approximation. Also T-matrix methods have been used in the quasiclassical theory of superconductivity, in order to formulate appropriate boundary conditions for the quasiclassical Green's functions at interfaces with various properties, separating regions described by different Hamiltonians [7, 8]. These references consider as free states those satisfying hard wall boundary conditions at the interface, an assumption we do not employ in this work.

In the theoretical development of this work, we assume that the pair potential, the normal potential and the magnetization take their true, self-consistent values throughout the junction. Thus our theoretical results are valid in the general case. Although the self-consistent determination of the potentials is difficult, there exist in the literature efficient numerical methods for tackling the problem, such as the recursive Green's function method [9–11], also applied in the Keldysh formalism [12] and the kernel polynomial method [13], applied to inhomogeneous superconducting systems [14–16]. These methods could be used in conjunction with the T-matrix formalism, in order to calculate scattering amplitudes from the accurate determination of the Green's function. Further elaboration could be the subject of future work.

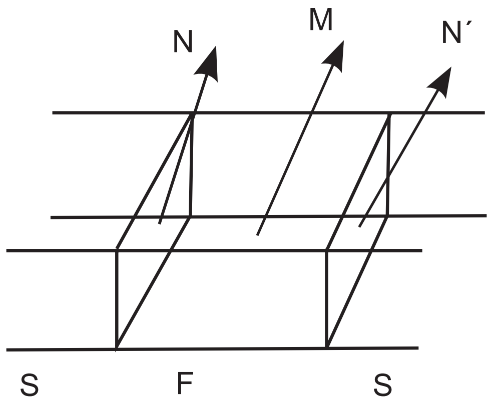

Figure 1. A Josephson junction with one ferromagnetic intermediate layer and spin active interfaces. S stands for superconductor and F for ferromagnet. $\boldsymbol{N}$, $\boldsymbol{N}'$ are the interfacial magnetization vectors. $\boldsymbol{M}$ is the magnetization of the intermediate layer.

This paper is organized as follows: in section 2 we present the model of the ferromagnetic Josephson junction, which we use as a concrete example to develop our scattering theory. In section 3 we review the Møller operator theory and derive from it Lippmann–Schwinger equations appropriate for systems with different spatial asymptotics on the left and right. Then in section 4 we are naturally led to define a channel-dependent T-matrix and relate it to the scattering amplitudes. In section 5 we use this relation to derive formulas for the Green's function, when its spatial arguments lie on the asymptotic regions. These formulas are useful in deriving formulae for the supercurrent in Josephson junctions. In section 6 we select certain anti-unitary operators and, using the T-matrix theory developed, derive symmetry conditions for the scattering amplitudes. Then in section 7 we use these results to prove symmetry relations for the current–phase-relation and the Andreev bound state spectrum of ferromagnetic Josephson junctions and also show a simplification of the Furusaki–Tsukada formula [17] for the dc Josephson supercurrent. We give our conclusions in section 8.

2. Bogoliubov–de Gennes equations and scattering states

As mentioned, we will use as a specific model for developing our theory a ballistic ferromagnetic Josephson junction with conventional superconducting electrodes and inhomogeneous magnetization, possibly with normal as well as magnetic scattering on the interfaces (see figure 1). This system is the simplest one exhibiting non-trivial dependence both on the spin as well as the particle–hole degree of freedom. We assume the model to have one space dimension x, which takes values from minus to plus infinity. We shall use the Blonder–Tinkham–Klapwijk model [18]. Our system is then described by the one-particle Bogoliubov–de Gennes (BdG) equations [19], which read:

$$\mathcal{H}\Psi(x) = E\Psi(x), \tag{1}$$

where E is the energy of the full wavefunction

$$\Psi(x) = \begin{pmatrix} \hat{u}(x) \\ \hat{v}(x) \end{pmatrix}, \tag{2}$$

where $\hat{u}(x) = (u_\uparrow(x), u_\downarrow(x))^T$ is the electron part of the wavefunction, $\hat{v}(x) = (v_\uparrow(x), v_\downarrow(x))^T$ is its hole part and the BdG Hamiltonian is given by

$$\mathcal{H} = \begin{pmatrix} \hat{H}_0 & \hat{\Delta} \\ -\Delta^* & -\hat{H}_0^* \end{pmatrix}. \tag{3}$$

In the above, $\hat{H}_0$ is the normal Hamiltonian, which is given by

$$\hat{H}_0 = -\frac{\mathrm{d}}{\mathrm{d}x}\frac{\hbar^2}{2m(x)}\frac{\mathrm{d}}{\mathrm{d}x} - \mu + U(x) - \boldsymbol{\sigma}\cdot\boldsymbol{M}(x), \tag{4}$$

where the first term is the kinetic energy, $m(x)$ is the effective mass function, μ is the chemical potential, $U(x)$ is the normal potential, which contains also interfacial scattering modelled by delta functions, and $\boldsymbol{M}(x)$ is the magnetization of the system, which contains also interfacial magnetization (spin active interfaces) and is equal to zero for sufficiently large $|x|$. At every point x, we will denote by $\phi(x)$ the azimuthal angle of the magnetization vector and by $\theta(x)$ its polar angle. Also $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices and

$$\hat{\Delta}(x) = \mathrm{i}\sigma_y\Delta(x) = \mathrm{i}\sigma_y|\Delta(x)|\,\mathrm{e}^{\mathrm{i}\chi(x)} \tag{5}$$

is the spin dependent pair potential, which is generally complex and its absolute value is diminished for finite x and attains constant asymptotic values at infinity. Its spin dependence is characteristic of conventional spin singlet superconductors. We denote by $\Delta(x)$ the spatial part of the pair potential and by $\chi(x)$ its phase.

It is known that the study of the one-particle stationary scattering states in Josephson junctions can give useful information about observables, such as the supercurrent, through the analytic continuation in complex energy of the Andreev reflection amplitudes [17]. Therefore, there is interest in studying the scattering states of the BdG equations and their analytic continuation in complex energy. We proceed to describe these states for our model.

As already mentioned, the Hamiltonian of our system has well defined limits for sufficiently large $|x|$. We shall separate the junction into three main regions: the left and right asymptotic regions and the intermediate region. In the asymptotic regions, the Hamiltonian is equal to its limiting values $\mathcal{H}_\ell$ and $\mathcal{H}_r$ in the left and right respectively. These asymptotic Hamiltonians are characterized by zero magnetization and constant normal and pair potentials. The asymptotic regions reside in $x < 0$ in the left and $x > d$ in the right and are sufficiently far apart. The intermediate region resides in between and consists of the ferromagnetic layer and superconducting proximity regions on the left and right, where the pair potential is modified from its bulk values due to the proximity effect. The approximate separation into asymptotic and intermediate regions is legitimate, since we assume that the Hamiltonian attains its limiting values sufficiently rapidly as x tends to infinity. Then the stationary bound and scattering states can be represented as linear combinations of linearly independent solutions in the three specified regions, which are in principle easier to find. The linearly independent solutions in the asymptotic regions are given by

$$\Phi_{\pm ps\nu}(x) = \mathrm{e}^{\pm\mathrm{i}\nu p k_{p\nu}x}\phi_{ps\nu}. \tag{6}$$

We give the definition of the indices p, s, ν that appear in the above, which are assumed to be numbers in mathematical expressions and symbols, when they appear as indices:

$$p = \begin{cases} +1, & (e) \\ -1, & (h) \end{cases} \quad s = \begin{cases} +1, & (\uparrow) \\ -1, & (\downarrow) \end{cases} \quad \nu = \begin{cases} +1, & (\ell) \\ -1, & (r). \end{cases}$$

The index p defines the particle–hole degree of freedom, s defines the spin and ν defines the asymptotic region (left or right) under investigation. The solutions (6) are plane waves with wavenumbers

$$k_{p\nu} = \sqrt{\frac{2m}{\hbar^2}(\mu - U_\nu + p\Omega_\nu)}, \tag{7}$$

where U_ν is the asymptotic value of the normal potential and the branch cut of the square root is taken to be the negative real axis of its domain of definition. Also

$$\Omega_\nu = \sqrt{z^2 - |\Delta_\nu|^2} \tag{8}$$

where z is the complex energy and the branch cut of the square root is chosen to be the interval $[-\infty, -|\Delta_\nu|] \cup [|\Delta_\nu|, \infty]$ of the real energy axis. Thus we also define linearly independent solutions for complex energy, which we shall need in the following sections. The four dimensional spinors appearing in (6) are given by

$$\phi_{e\uparrow\nu} = \left(u_\nu\, \mathrm{e}^{\mathrm{i}\chi_\nu/2}, 0, 0, v_\nu\, \mathrm{e}^{-\mathrm{i}\chi_\nu/2}\right)^T \tag{9a}$$

$$\phi_{e\downarrow\nu} = \left(0, u_\nu\, \mathrm{e}^{\mathrm{i}\chi_\nu/2}, -v_\nu\, \mathrm{e}^{-\mathrm{i}\chi_\nu/2}, 0\right)^T \tag{9b}$$

$$\phi_{h\downarrow\nu} = \left(v_\nu\, \mathrm{e}^{\mathrm{i}\chi_\nu/2}, 0, 0, u_\nu\, \mathrm{e}^{-\mathrm{i}\chi_\nu/2}\right)^T \tag{9c}$$

$$\phi_{h\uparrow\nu} = \left(0, v_\nu\, \mathrm{e}^{\mathrm{i}\chi_\nu/2}, -u_\nu\, \mathrm{e}^{-\mathrm{i}\chi_\nu/2}, 0\right)^T \tag{9d}$$

where χ_ν is the phase of the pair potential in asymptotic region $\nu(=\ell, r)$ and we define the so-called coherence factors as

$$u_\nu = \sqrt{\frac{1}{2}\left(1 + \frac{\Omega_\nu}{z}\right)}, \quad v_\nu = \mathrm{csgn}(z)\sqrt{\frac{1}{2}\left(1 - \frac{\Omega_\nu}{z}\right)}. \tag{10}$$

The complex sign function $\mathrm{csgn}(z)$ is defined as

$$\mathrm{csgn}(z) = \begin{cases} \sqrt{z^2}/z, & \mathrm{Re}(z) \neq 0, \\ -\mathrm{sgn}(\mathrm{Im}(z)), & \mathrm{Re}(z) = 0. \end{cases} \tag{11}$$

In the above, the square roots are defined with branch cuts at the negative real axis of their domain of definition, except the square root in Ω_ν. Also we note that the minus sign in the definition of the complex sign function for imaginary energies is essential, otherwise the wavefunctions (6) do not satisfy the BdG equations.

Thus, for incidence of a one-particle stationary state from the left, we can write down the full stationary scattering state as:

$$\Psi^+_{ps\ell}(x) = \begin{cases} \Phi_{ps\ell}(x) + \sum_{p's'} \alpha^\ell_{ps,p's'} \Phi_{-p's'\ell}(x), & x < 0 \\ \sum_i \beta^\ell_{ps,i} \Psi_{I,i}(x), & 0 < x < d \\ \sum_{p's'} \gamma^\ell_{ps,p's'} \Phi_{-p's'r}(x), & x > d. \end{cases} \tag{12}$$

where the z-dependent quantities, defined in this section, that appear in the above equation have $z = E + \mathrm{i}0$. The scattering state $\Psi^+_{ps\ell}(x)$ is the stationary state that in the remote past consisted of an incident from the left free state with variables p, s. We denote by $\alpha^\ell_{ps,p's'}$ the reflection amplitude that this state is reflected to a state with variables $p's'$ moving to the left. A similar interpretation is assumed for the transmission amplitude $\gamma^\ell_{ps,p's'}$. The superscript ℓ stands for left incidence. For right incidence we use the superscript r in scattering amplitudes and always denote by α^ν the reflection and γ^ν the transmission amplitudes ($\nu = \ell, r$). The amplitudes $\beta^\ell_{ps,i}$ combine the linearly independent solutions $\Psi_{I,i}(x)$ ($i = 1, \ldots, 8$) of the BdG equations in the intermediate region to form the stationary scattering state. For bound states, as the Andreev bound states in Josephson junctions [20], the wavefunction is given by a similar equation, with the term corresponding to the incident state missing. All the coefficients in the wavefunction, describing a scattering or a bound state, can be calculated using the well known matching conditions for the wavefunction and its spatial derivative at the interfaces $x = 0$ and d. Thus the coefficients of scattering states can be calculated for all complex energies, except for poles in the real interval $[-\min(|\Delta_\ell|, |\Delta_r|), \min(|\Delta_\ell|, |\Delta_r|)]$ that correspond to bound states and branch cuts on the real energy axis outside this interval.

If the stepwise pair potential approximation is used, the solutions to the BdG equations in the intermediate region are easy to find, since then the Hamiltonian in this region is that of a homogeneous Stoner ferromagnet. Details about these solutions can be found for example in [21, 22].

For a bulk superconductor with constant normal and pair potential, the Green's function can be easily proved to be given by the formula

$$\mathcal{G}_\nu(x, x'; z) = \sum_{ps} \left(-\frac{\mathrm{i} m_\nu z}{\hbar^2 k_{p\nu}(z) \Omega_\nu(z)} \right) \phi_{ps\nu}(z) \tilde{\phi}^T_{ps\nu}(z)\, \mathrm{e}^{\mathrm{i} p k_{p\nu}(z)|x-x'|}. \tag{13}$$

Here m_ν ($\nu = \ell, r$) is the effective mass in the left or right asymptotic region. Also the tilde over the spinor $\phi_{ps\nu}$ means that we change the sign of the phase of the pair potential χ_ν. We shall use this equation for the Green's function in the following sections.

3. Lippmann–Schwinger equations

Having set the model on which we shall base our discussion, we proceed to derive Lippmann–Schwinger equations for the stationary scattering states, taking into account the difference in asymptotic Hamiltonians on the left and right. We shall use the method of [23], which makes use of the Møller operators, and take into account the modification of this (time-dependent) theory by the different asymptotic Hamiltonians, which is described e.g. in [5].

We will briefly review the theory of the Møller operators in systems with different spatial asymptotics on the left and right. The central idea behind this theory is to relate wavepackets evolving under the influence of the free asymptotic Hamiltonians to wavepackets evolving under the influence of the full Hamiltonian at some finite time instant, in such a way that under both evolutions, the wavepackets coincide in the remote past or the distant future. The systems we are concerned with have the property that for every free scattering state there is a scattering state of the full Hamiltonian with the same asymptotics at infinite times (positive or negative) and vice versa. This property is related to the unitarity of the S-matrix. The Møller operators act on free scattering states at some finite instant of time and give the true scattering state at the same instant. In the case of different spatial asymptotics on the left and right, the Møller operators are divided in two parts, as follows:

$$W^\pm = W^\pm_\ell + W^\pm_r, \tag{14}$$

where

$$W^\pm_\ell = \lim_{t \to \mp\infty} \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathcal{H}}\, \mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathcal{H}_\ell} \mathcal{F}^\pm_\ell(\mathcal{H}_\ell) \tag{15}$$

and

$$W^\pm_r = \lim_{t \to \mp\infty} \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathcal{H}}\, \mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathcal{H}_r} \mathcal{F}^\pm_r(\mathcal{H}_r). \tag{16}$$

The plus and minus superscripts indicate whether the scattering states related by the Møller operator coincide in the remote past (plus sign) or the distant future (minus sign)[3]. Operator $W^\pm_\ell$ gives the full scattering state, when it acts on the free scattering state that is incident from the left (plus sign) or evolves to the left (minus sign). A similar interpretation holds for $W^\pm_r$, with ℓ and r interchanged. The Møller operator $W^\pm$ is the sum of the above two operators. The Møller operators are time independent.

[3] Note that this convention is the traditional one, but opposite to that of [5].

The operators $\mathcal{F}_\nu^\pm(\mathcal{H}_\nu)$ $(\nu = \ell, r)$ are asymptotic projection operators that project free scattering states, evolving under the action of asymptotic Hamiltonian $\mathcal{H}_\nu$, on their components that have incidence (plus sign superscript) from asymptotic region ν or evolution (minus sign superscript) to the ν asymptotic region in the distant future [2]. They are defined as follows:

$$\mathcal{F}_\ell^\pm(\mathcal{H}_\ell) = \lim_{t\to\mp\infty} \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathcal{H}_\ell}\mathcal{P}_\ell\, \mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathcal{H}_\ell}\mathcal{P}_c(\mathcal{H}_\ell) \tag{17}$$

and

$$\mathcal{F}_r^\pm(\mathcal{H}_r) = \lim_{t\to\mp\infty} \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathcal{H}_r}\mathcal{P}_r\, \mathrm{e}^{\frac{-\mathrm{i}t}{\hbar}\mathcal{H}_r}\mathcal{P}_c(\mathcal{H}_r), \tag{18}$$

where $\mathcal{P}_c(\mathcal{H}_\nu)$ $(\nu = \ell, r)$ are the projections on the space of scattering states of the Hamiltonian $\mathcal{H}_\nu$, which for our model are equal to unity due to the absence of bound states for the asymptotic Hamiltonians. Also $\mathcal{P}_\nu$ are operators that project the wavefunctions on the space region of the ν (left or right) asymptotic region. The operators $\mathcal{F}_\nu^\pm(\mathcal{H}_\nu)$ are time independent.

Next we are going to apply the Møller operators on stationary scattering states of the asymptotic Hamiltonians in order to obtain the stationary scattering states of the full Hamiltonian, as suggested for example in [23]. To this end we shall treat the free stationary scattering states as very extended Gaussian modulated plane wavepackets at times $t = 0$ and afterwards consider the limit of the Gaussian modulation tending to unity. Thus we are going to consider states like $|e^{-ax^2}\Phi_{\pm ps\nu}(x)\rangle$ and after calculations take the limit $a \to 0^+$. We shall not explicitly show this procedure in presented formulas, but we shall always keep it in mind.

Thus, in the case of different spatial asymptotics on the left and right, we can represent the stationary scattering states of the full Hamiltonian with incidence from the left and right respectively as

$$|\Psi_{ps\ell}^+(x)\rangle = W_\ell^+|\Phi_{ps\ell}(x)\rangle \tag{19}$$

and

$$|\Psi_{psr}^+(x)\rangle = W_r^+|\Phi_{psr}(x)\rangle. \tag{20}$$

From the above equations we can derive Lippmann–Schwinger equations for systems with different spatial asymptotics on the left and right, by writing the Møller operators as integrals of their derivative with respect to time and keeping in mind that the operators $\mathcal{F}_\nu^\pm(\mathcal{H}_\nu)$ are time independent. Then, for example, we have

$$W_\ell^+ = \mathcal{F}_\ell^+(\mathcal{H}_\ell) + \lim_{\epsilon\to0^+}\int_0^{-\infty} \mathrm{d}t\, \mathrm{e}^{\epsilon t}\frac{\mathrm{i}}{\hbar}\, \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathcal{H}}\mathcal{V}_\ell\, \mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}\mathcal{H}_\ell}\mathcal{F}_\ell^+(\mathcal{H}_\ell), \tag{21}$$

where the exponential factor $\mathrm{e}^{\epsilon t}$ does not affect, but makes more obvious the convergence of the above time integral [23]. Also we have and will use the following separation of the full Hamiltonian

$$\mathcal{H} = \mathcal{H}_\ell + \mathcal{V}_\ell = \mathcal{H}_r + \mathcal{V}_r, \tag{22}$$

where $\mathcal{H}_\nu$ $(\nu = \ell, r)$ are the Hamiltonians of the system in the asymptotic regions and $\mathcal{V}_\nu$ are the potentials in the full Hamiltonian associated with them. Acting with (21) on the left incident free stationary scattering state, keeping in mind that $\mathcal{F}_\ell^+(\mathcal{H}_\ell)|\Phi_{ps\ell}(x)\rangle = |\Phi_{ps\ell}(x)\rangle$ and the fact that the free stationary scattering state is an improper eigenfunction of $\mathcal{H}_\ell$ with energy E, we have

$$|\Psi_{ps\ell}^+(x)\rangle = |\Phi_{ps\ell}(x)\rangle + \lim_{\epsilon\to0^+}\int_0^{-\infty} \mathrm{d}t\frac{\mathrm{i}}{\hbar}\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}(E+\mathrm{i}\epsilon-\mathcal{H})}\mathcal{V}_\ell|\Phi_{ps\ell}(x)\rangle, \tag{23}$$

where we have rescaled the variable ϵ $(\epsilon \to \epsilon/\hbar)$. Performing the integration with respect to t, we obtain

$$|\Psi_{ps\ell}^+(x)\rangle = |\Phi_{ps\ell}(x)\rangle + \lim_{\epsilon\to0^+}\mathcal{G}(E+\mathrm{i}\epsilon)\mathcal{V}_\ell|\Phi_{ps\ell}(x)\rangle, \tag{24}$$

where

$$\mathcal{G}(z) = (z - \mathcal{H})^{-1} \tag{25}$$

is the Green's function for the full Hamiltonian. By a similar procedure, starting with (20), we can derive the equation

$$|\Psi^{+}_{psr}(x)\rangle = |\Phi_{psr}(x)\rangle + \lim_{\epsilon\to 0^{+}} \mathcal{G}(E + \mathrm{i}\epsilon)\mathcal{V}_r|\Phi_{psr}(x)\rangle. \tag{26}$$

Equations (24) and (26) are Lippmann–Schwinger equations for scattering systems with different spatial asymptotics on the left and right and for states that are well-defined free scattering states in the remote past. We observe that, according to the type of incidence, the potential function that appears in the right hand side of the Lippmann–Schwinger equations is the left or right potential $\mathcal{V}_\nu$. Similar equations have been given in [4], in the context of a model with only the spatial degree of freedom. In the next section we shall work on the Lippmann–Schwinger equations in order to relate the scattering amplitudes to the elements of the *T*-matrix.

4. *T*-matrix and scattering amplitudes

In this section we shall derive the form of the *T*-matrix that is appropriate for systems with different spatial asymptotics on the left and right and relate it to the scattering amplitudes described in section 2. We shall see that, according to the type of incidence and transmission that the scattering amplitude describes, the *T*-matrix is defined differently, in analogy to *N*-body many-channel quantum scattering problems [23, 24]. Here the channels consist of the left and right incidence or transmission and, as remarked in [5], they are orthogonal to each other and depend on the sign of the time variable. This time dependence appears in the stationary state formulation of the problem as the need for an appropriate selection of a channel component of the *T*-matrix.

We proceed to define the channel components of the *T*-matrix. For reasons that will become apparent soon, we give the following definitions

$$\mathcal{G}_\ell(z)\mathcal{T}_{\ell\ell}(z) = \mathcal{G}(z)\mathcal{V}_\ell, \tag{27a}$$

$$\mathcal{G}^{(+)}_r(E)(z)\mathcal{T}_{r\ell}(z) = \mathcal{G}(z)\mathcal{V}_\ell, \tag{27b}$$

where $\mathcal{G}_{\ell,r}(z)$ is the free Green's function of the asymptotic Hamiltonian $\mathcal{H}_{\ell,r}$, as given at the end of section 2. The above channel components of the *T*-matrix will be utilized to express scattering amplitudes for left incidence as their matrix elements between free asymptotic states. Making use of the equation

$$\mathcal{G}^{-1}_\nu(z)\mathcal{G}(z) = 1 + \mathcal{V}_\nu\mathcal{G}(z) \tag{28}$$

($\nu = \ell, r$), we can write generally

$$\mathcal{T}_{\nu'\nu}(z) = \mathcal{V}_\nu + \mathcal{V}_{\nu'}\mathcal{G}(z)\mathcal{V}_\nu, \tag{29}$$

which are appropriate for expressing scattering amplitudes for the left or right incidence of an excitation and $\nu, \nu' = \ell, r$. At this point we note that the potential $\mathcal{V}_\nu$ is the one appearing as the first term in the right hand side of the above equation for the *T*-matrix $\mathcal{T}_{\nu'\nu}(z)$. However, when $\nu \neq \nu'$ and the matrix element of $\mathcal{T}_{\nu'\nu}(z)$ is between asymptotic stationary scattering states $\langle\Phi_{-p's'\nu'}|$ and $|\Phi_{ps\nu}\rangle$ with the same value of the energy, then the first term can be either $\mathcal{V}_\nu$ or $\mathcal{V}_{\nu'}$. For then the two definitions of the *T*-matrix have a difference equal to $\mathcal{H}_\ell - \mathcal{H}_r$, whose matrix element is zero. This situation also has an analogue in *N*-body many channel scattering theory [23, 24]. With this remark in mind, we can write

$$(\mathcal{T}_{\nu\nu'}(z))^{\dagger} = \mathcal{T}_{\nu'\nu}(z^{*}). \tag{30}$$

Having defined the various channel components of the T-matrix, we can establish their connection to the scattering amplitudes. We shall do this by comparing the stationary scattering state of (12) to the Lippmann–Schwinger equations, in which we substitute the definitions (27*a*) and (27*b*). Thus, substituting from definition (27*a*) to (24) and restricting the space variable x to lie on the left asymptotic region ($x < 0$), we obtain

$$\Psi^{+}_{ps\ell}(x) = \Phi_{ps\ell}(x) + \int \mathrm{d}x'\,\mathrm{d}y\,\mathcal{G}^{(+)}_{\ell}(x,x';E)\mathcal{T}^{(+)}_{\ell\ell}(x',y;E)\Phi_{ps\ell}(y), \tag{31}$$

where $\mathcal{G}^{(+)}_{\ell}(x,x';E)$ and $\mathcal{T}^{(+)}_{\ell\ell}(x',y;E)$ are the retarded Green's function and T-matrix from the left to the left channel in the co-ordinate representation, which in the ferromagnetic Josephson junction model are also 4×4 matrices, because of the spin and particle–hole degrees of freedom dependence. At this point we note that the integration over x' extends over all space except the left asymptotic region, due to the fact that $\mathcal{V}_\ell$ is equal to zero there by definition. But the variable x lies exactly in that region, so it can be considered to be always less than x'. This has the consequence that $x-x'$ has a constant sign and the absolute value in the exponential of relation (13) can be dropped. Then the exponential can be separated in its x and x' dependence, as the spinors $\phi_{ps\ell}$ do. The part depending on x can be passed outside the integral and inside the integral we are left with a matrix element of the T-matrix. Comparing this equation with (12), for $x<0$, we obtain

$$\alpha^{\ell}_{ps,p's'}(E^+) = -\frac{\mathrm{i}m_\ell E}{\hbar^2 k_{p'\ell}(E^+)\Omega_\ell(E^+)}\langle\Phi_{-p's'\ell}|\mathcal{T}^{(+)}_{\ell\ell}|\Phi_{ps\ell}\rangle, \tag{32}$$

where $E^+ = E + \mathrm{i}0$ and we have used the notation

$$\langle\Phi_{-p's'\ell}|\mathcal{T}^{(+)}_{\ell\ell}|\Phi_{ps\ell}\rangle = \int \mathrm{d}x'\,\mathrm{d}y(\Phi_{-p's'\ell}(x'))^{\dagger}\mathcal{T}^{(+)}_{\ell\ell}(x',y;E)\Phi_{ps\ell}(y). \tag{33}$$

Therefore we have come to the conclusion that the matrix element of the T-matrix from the left to the left channel, between the free stationary states of incidence from the left and reflection to the left, is proportional to the reflection amplitude. Although $\mathcal{T}_{\ell\ell}$, through the potential $\mathcal{V}_\ell$, as its first term does not vanish on the right asymptotic region, we have no convergence issue, because of the assumption we made about the Gaussian modulation of the free stationary states (for details see appendix A). A similar result holds for right incidence and we can write generally

$$\alpha^{\nu}_{ps,p's'}(E^+) = -\frac{\mathrm{i}m_\nu E}{\hbar^2 k_{p'\nu}(E^+)\Omega_\nu(E^+)}\langle\Phi_{-p's'\nu}|\mathcal{T}^{(+)}_{\nu\nu}|\Phi_{ps\nu}\rangle. \tag{34}$$

In order to derive a similar relation for the transmission amplitudes, we substitute from (27*b*) into the Lippmann–Schwinger equation (24), obtaining

$$|\Psi^{+}_{ps\ell}(x)\rangle = |\Phi_{ps\ell}(x)\rangle + \mathcal{G}^{(+)}_{r}(E)\mathcal{T}^{(+)}_{r\ell}(E)|\Phi_{ps\ell}(x)\rangle, \tag{35}$$

or

$$|\Psi^{+}_{ps\ell}(x)\rangle = |\Phi_{ps\ell}(x)\rangle + \mathcal{G}^{(+)}_{r}(E)(\mathcal{V}_\ell + \mathcal{V}_r\mathcal{G}^{(+)}(E)\mathcal{V}_\ell)|\Phi_{ps\ell}(x)\rangle,$$

or

$$|\Psi^{+}_{ps\ell}(x)\rangle = |\Phi_{ps\ell}(x)\rangle + \mathcal{G}^{(+)}_{r}(E)(\mathcal{V}_\ell - \mathcal{V}_r)|\Phi_{ps\ell}(x)\rangle + \mathcal{G}^{(+)}_{r}(E)(\mathcal{V}_r + \mathcal{V}_r\mathcal{G}^{(+)}(E)\mathcal{V}_\ell)|\Phi_{ps\ell}(x)\rangle.$$

However, $\mathcal{V}_\ell - \mathcal{V}_r = \mathcal{H}_r - \mathcal{H}_\ell$ by definition and the second term in the above equation becomes

$$\mathcal{G}^{(+)}_{r}(E)(\mathcal{H}_r - \mathcal{H}_\ell)|\Phi_{ps\ell}(x)\rangle = \mathcal{G}^{(+)}_{r}(E)(\mathcal{H}_r - E)|\Phi_{ps\ell}(x)\rangle = -|\Phi_{ps\ell}(x)\rangle.$$

Note in the above that the wavefunction is not an eigenstate of $\mathcal{H}_r$ with energy E and thus the last equality follows[4]. As a result we have

$$|\Psi^+_{ps\ell}(x)\rangle = \mathcal{G}_r(\mathcal{V}_r + \mathcal{V}_r\mathcal{G}^{(+)}(E)\mathcal{V}_\ell)|\Phi_{ps\ell}(x)\rangle. \tag{36}$$

We then set x to lie on the right asymptotic region ($x > d$). Since the potential $\mathcal{V}_r$ is zero in the right asymptotic region by definition, when we write the above equation in the co-ordinate representation, we can separate the Green's function $\mathcal{G}_r$, just like we did in handling the reflection amplitude. The operator in parentheses is equivalent to the T-matrix from the left to the right channel, when sandwiched between free scattering states of the left and right asymptotic Hamiltonians with the same energy. Then, comparing to (12) for $x > d$, we conclude that

$$\gamma^{\ell}_{ps,p's'}(E^+) = -\frac{\mathrm{i}m_r E}{\hbar^2 k_{p'r}(E^+)\Omega_r(E^+)}\langle\Phi_{-p's'r}|\mathcal{T}^{(+)}_{r\ell}|\Phi_{ps\ell}\rangle. \tag{37}$$

Therefore, the transmission amplitudes for left incidence are proportional to the matrix element of the T-matrix from the left to the right channel, between free scattering states of incidence and transmission. Although $\mathcal{T}_{r\ell}$, through the potential $\mathcal{V}_\ell$ or $\mathcal{V}_r$ as its first term, does not vanish on the right or left asymptotic region respectively, we have no convergence issue, because of the assumption we made about the Gaussian modulation of the free stationary states (for details see appendix A). A similar result holds for the transmission amplitudes for right incidence, which is obtained from (37) by interchanging everywhere the indices r and ℓ.

The argument we used to relate the transmission amplitudes to the T-matrix is general and does not rely on the specific model of the ferromagnetic Josephson junction. Therefore, the result holds for different situations also. However, there is interest in deriving it for the Josephson junction model, as will be seen in the next section. To this end, we write the Lippmann–Schwinger equation in the co-ordinate representation and $x > d$ in the right asymptotic region:

$$\Psi^+_{ps\ell}(x) = \Phi_{ps\ell}(x) + \int \mathrm{d}x'\,\mathrm{d}y\,\mathcal{G}^{(+)}_r(x,x';E)\mathcal{T}^{(+)}_{r\ell}(x',y;E)\Phi_{ps\ell}(y). \tag{38}$$

The T-matrix $\mathcal{T}_{r\ell}$, as given in (29), has the potential $\mathcal{V}_\ell$ as its first term, which vanishes by definition on the left asymptotic region but not on the right one. Since $x > d$ and the argument x' can lie in the right asymptotic region, the separation of the x and x' dependence of the free Green's function $\mathcal{G}_r$ cannot be made. Therefore, if we want to proceed by brute force, we have to calculate the integral without performing the separation mentioned. To this end, we separate from the integral of (38) the term that follows

$$X = \left(\int_d^x \mathrm{d}x' + \int_x^{+\infty}\mathrm{d}x'\right)\mathcal{G}^{(+)}_r(x,x';E)\mathcal{V}_\ell(x')\Phi_{ps\ell}(x'). \tag{39}$$

Since by hypothesis the potential $\mathcal{V}_\ell$ is constant for $x > d$ (or perhaps depends also on the momentum operator, if there is a difference in effective mass between the asymptotic regions) the integrations in the above term X are easy to perform, for the Green's function has exponential dependence on the co-ordinates x, x'. Then we can find terms in X, which result from the limits of integration containing x, that constitute an expression X' and can be proved [22] to be equal to

$$X' = -\Phi_{ps\ell}(x), \tag{40}$$

[4] The product $\mathcal{G}^{(+)}_r(E)(E-\mathcal{H}_r)$ can be easily shown to be a projection operator in the complement of the space of the eigenstates of $\mathcal{H}_r$ with energy E. Thus only if it acts on these eigenstates does it not equal unity, but is equal to zero. $|\Phi_{ps\ell}(x)\rangle$ can contain components in these directions, but their weight is infinitesimal, so it is not affected.

if the ferromagnetic Josephson junction model is used[5]. Thus the X' terms cancel the free incident wavefunction in (38). This cancellation happens in the first Born approximation, we can say. The rest of the terms in X of (39) are combined with the rest of the integral in (38) to give the matrix element of the T-matrix, confirming the result (36). However expression X' should be equal to minus the incident wavefunction whatever model we use, since there is no other way that we can reach the general result (36). We shall use (40) in section 5.

4.1. A note on the S-matrix

We now give the relation of the on-shell T-matrix elements to the S-matrix. We follow [23], but generalize to the case of different spatial asymptotics. The definition of the S-matrix through the Møller operators is

$$S = W^{-\dagger}W^{+}. \tag{41}$$

As mentioned, in problems with different spatial asymptotics the Møller operator is the sum of two parts, each of which handles the part of the wavefunction according to its incoming or outgoing behaviour. Using this fact, we can write for the S-matrix [5]

$$S = \sum_{\nu,\nu'} S_{\nu'\nu}, \tag{42}$$

where ν, $\nu' = \ell, r$ and

$$S_{\nu'\nu} = W_{\nu'}^{-\dagger}W_{\nu}^{+}. \tag{43}$$

Using (15) and (16) as well as the fact that operators $\mathcal{F}_{\nu}^{\pm}(\mathcal{H}_{\nu})$ are time independent, we can write the channel component $S_{\nu'\nu}$ of the S-matrix as the integral of its derivative and obtain

$$S_{\nu'\nu} = \mathcal{F}_{\nu'}^{-}\mathcal{F}_{\nu}^{+} + \mathrm{i}\lim_{\epsilon\to 0^+}\int_0^{-\infty} \mathrm{d}t\, \mathrm{e}^{\epsilon t/\hbar}\mathcal{F}_{\nu'}^{-}\left(\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H_{\nu'}}\mathcal{V}_{\nu'}\mathrm{e}^{\frac{2\mathrm{i}t}{\hbar}H}\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H_{\nu}} + \mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H_{\nu'}}\mathrm{e}^{\frac{2\mathrm{i}t}{\hbar}H}\mathcal{V}_{\nu}\,\mathrm{e}^{-\frac{\mathrm{i}t}{\hbar}H_{\nu}}\right)\mathcal{F}_{\nu}^{+}. \tag{44}$$

where the exponential factor $\mathrm{e}^{\epsilon t/\hbar}$ does not affect, but makes more obvious the convergence of the above time integral [23]. We note that the product $\mathcal{F}_{\nu'}^{-}\mathcal{F}_{\nu}^{+}$ is equal to zero, if $\nu = \nu'$; we shall focus in the sequel on the case $\nu \neq \nu'$, as the case $\nu = \nu'$ is quite straight forward.

We now take matrix elements of $S_{\nu'\nu}$ between free scattering states $\langle\Phi_{-p's'\nu'}|$ and $|\Phi_{ps\nu}\rangle$, which are not affected by the operators $\mathcal{F}_{\nu'}^{-}$, $\mathcal{F}_{\nu}^{+}$ and are improper eigenfunctions of $\mathcal{H}_{\nu'}$ and $\mathcal{H}_{\nu}$ with eigenvalues $E'_{\nu'}$ and E_{ν} respectively, the last two being different in general. We focus on the integral of the right hand side of (44), which we call Y and, after acting on the eigenfunctions, we perform the time integration. Then we have

$$Y = \frac{1}{2}\left\{\langle\Phi_{-p's'\nu'}|\mathcal{V}_{\nu'}\mathcal{G}\left(\frac{E'_{\nu'}+E_{\nu}}{2}+\mathrm{i}0\right) + \mathcal{G}\left(\frac{E'_{\nu'}+E_{\nu}}{2}+\mathrm{i}0\right)\mathcal{V}_{\nu}|\Phi_{ps\nu}\rangle\right\}. \tag{45}$$

We utilize the easily obtained formulae, valid for complex energy z:

$$\mathcal{G}\mathcal{V}_{\nu} = \mathcal{G}_{\nu'}\mathcal{T}_{\nu'\nu} \tag{46}$$

and

$$\mathcal{V}_{\nu'}\mathcal{G} = (\mathcal{H}_{\nu} - \mathcal{H}_{\nu'})\mathcal{G}_{\nu} + \mathcal{T}_{\nu'\nu}\mathcal{G}_{\nu}, \tag{47}$$

[5] This result holds even when the energy assumes complex values z, possibly with some restrictions that give meaning to T-matrix elements (see appendix A).

where we have used the fact that $\mathcal{V}_{\nu'} - \mathcal{V}_{\nu} = \mathcal{H}_{\nu} - \mathcal{H}_{\nu'}$. Substituting from (46) and (47) into (45) and then to (44) we see that the first term in the right hand side of (47) cancels the first term in the right hand side of (44) and we get

$$\langle \Phi_{-p's'\nu'} | S_{\nu'\nu} | \Phi_{ps\nu} \rangle = -2\pi \mathrm{i} \delta(E'_{\nu'} - E_{\nu}) \langle \Phi_{-p's'\nu'} | \mathcal{T}_{\nu'\nu}(E_{\nu}^{+}) | \Phi_{ps\nu} \rangle, \tag{48}$$

which holds also for $\nu = \nu'$. We have also made use of the fact that the free Green's function is diagonal, when acting on the bra–ket's states. The delta function appears as a result of the difference of the Green's functions' eigenvalues.

We conclude that the bra–ket of a particular channel component of the S-matrix, being the probability amplitude that connects the in-coming asymptote with a particular out-going asymptote, is proportional to the matrix element of the corresponding channel component of the on-shell retarded T-matrix. The delta function assures that this probability amplitude is zero, when energy is not conserved. This simple result is the generalization of a similar formula holding in the case of equal spatial asymptotics on the left and right.

5. Green's function in the asymptotic regions

It is interesting and useful to develop a simple way of deriving the Green's function, when its co-ordinate arguments lie in the asymptotic regions in the left and right, by employing the theory we have developed so far. For example, the Green's function in the asymptotic regions can be used to derive simple and powerful formulae for the supercurrent in Josephson junctions [17]. Our starting point is the Dyson equation, a form of which is (28). We rewrite this equation as

$$\begin{aligned} \mathcal{G}(z) &= \mathcal{G}_{\ell}(z) + \mathcal{G}_{\ell}(z)\mathcal{V}_{\ell}\mathcal{G}(z) \\ &= \mathcal{G}_{\ell}(z) + \mathcal{G}(z)\mathcal{V}_{\ell}\mathcal{G}_{\ell}(z). \end{aligned} \tag{49}$$

We first consider the case when x, x' lie in the left asymptotic region, i.e. $x, x' < 0$. Then (49) can be written in the co-ordinate representation, taking into account definition (27*a*), as

$$\mathcal{G}(x, x'; z) = \mathcal{G}_{\ell}(x, x'; z) + \int \mathrm{d}y\, \mathrm{d}y' \mathcal{G}_{\ell}(x, y)\mathcal{T}_{\ell\ell}(y, y'; z)\mathcal{G}_{\ell}(y', x'). \tag{50}$$

The y, y' variables of integration take values everywhere, except the left asymptotic region, where x, x' lie. Therefore, the signs of $x - y$ and $x' - y'$ in the exponents of the free Green's functions are constant and their exponential co-ordinate dependence can be separated, as already mentioned. Then replacing the free Green's function from (13), we obtain

$$\mathcal{G}(x, x'; z) = \mathcal{G}_{\ell}(x, x'; z) - \sum_{ps,p's'} \frac{\mathrm{i} m_{\ell} z}{\hbar^2 k_{p\ell}(z)\Omega_{\ell}(z)} \alpha^{\ell}_{ps,p's'}\, \mathrm{e}^{-\mathrm{i}p'k_{p'\ell}x - \mathrm{i}pk_{p\ell}x'} \phi_{p's'\ell}(z)\tilde{\phi}^{T}_{ps\ell}(z), \tag{51}$$

where

$$\alpha^{\ell}_{ps,p's'}(z) = -\frac{\mathrm{i} m_{\ell} z}{\hbar^2 k_{p'\ell}(z)\Omega_{\ell}(z)} \int \mathrm{d}y\, \mathrm{d}y'\, \mathrm{e}^{\mathrm{i}p'k_{p'\ell}y} \tilde{\phi}^{T}_{p's'\ell}(z)\mathcal{T}_{\ell\ell}(y, y'; z)\, \mathrm{e}^{\mathrm{i}pk_{p\ell}y'} \phi_{ps\ell}(z). \tag{52}$$

We remind the reader that the tilde over the spinors $\phi_{ps\ell}$ means that we have to change the sign of the phase of the pair potential χ_{ℓ}, wherever it appears. Therefore, in the above equation, we recognize the analytic continuation to complex energy of the reflection amplitudes. However, in order for (51) to hold true, the integrals in (52) must converge (taking into account the Gaussian modulation of the free wavefunctions) and have a finite limit as $a \to 0^{+}$, at least in some neighbourhood of z in the complex plane. If this is true, then the result (51) can be analytically continued to the whole z plane (except for poles and branch cuts on the real axis), since the scattering amplitudes have been defined in this region by the methods described in section 2. We show in appendix A that this is true and we have therefore proved the validity of (51) in the complex energy plane, except for poles and branch cuts in the real energy axis.

Similar equations hold for the Green's function with co-ordinate arguments in the right asymptotic region. We just have to replace in (51) the indices ℓ with r and change the sign of the wavevectors in the exponentials.

We next proceed to derive the Green's function in the asymptotic regions, when the first argument $x > d$ lies in the right asymptotic region and the second $x' < 0$ lies in the left asymptotic region. Then we write the Dyson equation as

$$\begin{aligned}\mathcal{G}(z) &= \mathcal{G}_\ell(z) + \mathcal{G}(z)\mathcal{V}_\ell\mathcal{G}_\ell(z)\\ &= \mathcal{G}_\ell(z) + \mathcal{G}_r(z)\mathcal{G}_r^{-1}(z)\mathcal{G}(z)\mathcal{V}_\ell\mathcal{G}_\ell(z)\\ &= \mathcal{G}_\ell(z) + \mathcal{G}_r(z)\mathcal{V}_\ell\mathcal{G}_\ell(z) + \mathcal{V}_r\mathcal{G}(z)\mathcal{V}_\ell\mathcal{G}_\ell(z).\end{aligned} \tag{53}$$

In this case, we cannot use the simple trick we used for the Lippmann–Schwinger equations in the right asymptotic region, for both the left and the right asymptotic Green's functions must have separable space dependent exponentials. Thus we proceed by writing the second term in the last line of the above equations in the co-ordinate representation as follows

$$X = \int \mathrm{d}y\, \mathcal{G}_r(x, y; z)\mathcal{V}_\ell(y)\mathcal{G}_\ell(y, x'; z). \tag{54}$$

Then the integration over y extends over all space except the left asymptotic region. Therefore, $y > x'$ and the Green's function's $\mathcal{G}_\ell$ spinor and spatial dependence can be separated. But then we have encountered this integral over y in the quantity X of section 4 and we know that part of this integral cancels the first term in the last line of (53). The rest of the terms complete the matrix element of the T-matrix. Thus we have

$$\mathcal{G}(x, x'; z) = \int \mathrm{d}y\, \mathrm{d}y' \mathcal{G}_r(x, y; z)\mathcal{T}_{r\ell}(y, y'; z)\mathcal{G}_\ell(y', x'; z), \tag{55}$$

where we assume that the parts of the Green's function $\mathcal{G}_r$ in the x and y variables can be separated. Then, substituting the free Green's functions from (13), we have

$$\mathcal{G}(x, x'; z) = \sum_{ps,p's'} \left(-\frac{\mathrm{i}m_\ell z}{\hbar^2 k_{p\ell}(z)\Omega_\ell(z)}\right) \gamma^\ell_{ps,p's'}\, \mathrm{e}^{\mathrm{i}p'k_{p'r}x - \mathrm{i}pk_{p\ell}x'} \phi_{p's'r}(z)\tilde{\phi}^T_{ps\ell}(z), \tag{56}$$

where x lies in the right asymptotic region, x' lies in the left one and

$$\gamma^\ell_{ps,p's'}(z) = -\frac{\mathrm{i}m_r z}{\hbar^2 k_{p'r}(z)\Omega_r(z)} \int \mathrm{d}y\, \mathrm{d}y'\, \mathrm{e}^{-\mathrm{i}p'k_{p'r}y} \tilde{\phi}^T_{p's'r}(z)\mathcal{T}_{r\ell}(y, y'; z)\, \mathrm{e}^{\mathrm{i}pk_{p\ell}y'} \phi_{ps\ell}(z). \tag{57}$$

In the above equation, we recognize the analytic continuation of the transmission amplitudes. Similar remarks hold in this case about the convergence of the T-matrix integral (see appendix A). In case x lies in the left and x' in the right asymptotic region, a similar equation to (56) holds, if we replace the index ℓ by r and vice versa and change the sign of the wavevectors in exponentials.

It should be stressed that scattering amplitudes have poles on the energies of bound states and branch cuts on the interval $[-\infty, -\min(|\Delta_\ell|, |\Delta_r|)] \cup [\min(|\Delta_\ell|, |\Delta_r|), \infty]$. We also note that the Green function with co-ordinate arguments in the asymptotic regions can be utilized to obtain formulae for the calculation of observables, such as the Josephson supercurrent [17].

6. Transformations of the BdG Hamiltonian and symmetries of the scattering amplitudes

In this section, we lay the ground for applications of the T-matrix theory in the dc Josephson effect for ferromagnetic Josephson junctions. We shall use certain anti-unitary operators that leave the BdG Hamiltonian invariant, with the exception of changing the sign of some of the parameters of the system, including the Hamiltonian itself. We shall confine ourselves to the model of ferromagnetic Josephson junctions that we described in section 2.

In the state space of the BdG Hamiltonian, we follow [25] and define an anti-unitary operator, which we call the Ruijsenaars–Bogoliubov (RB) conjugation, as

$$\mathcal{U}_{\mathrm{RB}} = \begin{pmatrix} \hat{0} & \hat{1}C \\ \hat{1}C^{*} & \hat{0} \end{pmatrix}, \tag{58}$$

where $\hat{1}$ and $\hat{0}$ are the 2×2 unit and the zero matrix respectively and C is the complex conjugation operator, which satisfies $C^{*} = C$ and $C^{\dagger} = C$. The importance of operator (58) is that every other unitary or anti-unitary operator in the state space of the BdG Hamiltonian has to commute with $\mathcal{U}_{\mathrm{RB}}$, in order that in the Fock space constructed by the transformed basis there are creation and annihilation operators that satisfy the fermion anti-commutation relations [25]. This requirement demands that unitary or anti-unitary operators in the state space of the BdG Hamiltonian have 2×2 block diagonal elements that are complex conjugate to each other and block anti-diagonal elements that are also complex conjugate to each other, apart from conditions that guarantee the (anti-)unitary property. These conditions are met by the RB conjugation itself and we shall use it in the following. The other transformations that we shall use are block diagonal and do not mix the particle and hole degree of freedom. In this case we have

$$\mathcal{U}\begin{pmatrix} \hat{u}(x) \\ \hat{v}(x) \end{pmatrix} = \begin{pmatrix} \hat{U} & \hat{0} \\ \hat{0} & \hat{U}^{*} \end{pmatrix}\begin{pmatrix} \hat{u}(x) \\ \hat{v}(x) \end{pmatrix}. \tag{59}$$

The block diagonal transformations that we shall use are complex conjugation $\mathcal{U}_C$, with $\hat{U} = C$ and time reversal $\mathcal{U}_T$, with $\hat{U} = \hat{T} = \hat{R}_{\pi}(\boldsymbol{y})C$, where $\hat{R}_{\pi}(\boldsymbol{y})$ is the rotation in spin space about the y axis through 180°.

The transformations $\mathcal{U}_C, \mathcal{U}_T$ and $\mathcal{U}_{\mathrm{RB}}$ transform the BdG Hamiltonian as follows

$$\mathcal{U}_C\mathcal{H}(\chi,\phi)\mathcal{U}_C^{\dagger} = \mathcal{H}(-\chi,-\phi), \tag{60a}$$

$$\mathcal{U}_T\mathcal{H}(\chi,\boldsymbol{M})\mathcal{U}_T^{\dagger} = \mathcal{H}(-\chi,-\boldsymbol{M}), \tag{60b}$$

$$\mathcal{U}_{\mathrm{RB}}\mathcal{H}\mathcal{U}_{\mathrm{RB}}^{\dagger} = -\mathcal{H}, \tag{60c}$$

where $\chi = \chi_r - \chi_\ell$ is the phase difference between the superconducting asymptotic regions. We note that the transformations actually change the sign of the phase of the pair potential at all points x of the junction. Also ϕ represents the azimuthal angles at every point x of the junction and $\boldsymbol{M}$ represents the magnetization vector at all points x of the junction. The RB conjugation has no effect on the phase difference χ and the magnetization, but changes the sign of the BdG Hamiltonian.

Similar transformation equations hold for potentials and Green's functions. The latter also change their energy argument to its complex conjugate, because the transformations we employ are anti-unitary:

$$\mathcal{U}_C\mathcal{G}(z;\chi,\phi)\mathcal{U}_C^{\dagger} = \mathcal{G}(z^{*};-\chi,-\phi), \tag{61a}$$

$$\mathcal{U}_T \mathcal{G}(z;\chi,\boldsymbol{M})\mathcal{U}_T^\dagger = \mathcal{G}(z^*;-\chi,-\boldsymbol{M}), \tag{61b}$$

$$\mathcal{U}_{\mathrm{RB}} \mathcal{G}(z)\mathcal{U}_{\mathrm{RB}}^\dagger = -\mathcal{G}(-z^*). \tag{61c}$$

Thus the transformation equations for the T-matrices are

$$\mathcal{U}_C \mathcal{T}_{\nu'\nu}(z;\chi,\phi)\mathcal{U}_C^\dagger = \mathcal{T}_{\nu'\nu}(z^*;-\chi,-\phi), \tag{62a}$$

$$\mathcal{U}_T \mathcal{T}_{\nu'\nu}(z;\chi,\boldsymbol{M})\mathcal{U}_T^\dagger = \mathcal{T}_{\nu'\nu}(z^*;-\chi,-\boldsymbol{M}), \tag{62b}$$

$$\mathcal{U}_{\mathrm{RB}} \mathcal{T}_{\nu'\nu}(z;\chi)\mathcal{U}_{\mathrm{RB}}^\dagger = -\mathcal{T}_{\nu'\nu}(-z^*;\chi). \tag{62c}$$

We shall also need the transformation properties of the free stationary scattering states of real as well as complex energies. We will change the notation of these states to Dirac's ket notation, in order to facilitate the discussion. Thus, for real energy solutions of the free BdG equations, we have

$$\mathcal{U}_C|k_{p\nu}s;\chi_\nu\rangle = |-k_{p\nu}s;-\chi_\nu\rangle. \tag{63}$$

We see that complex conjugation changes the sign of the wavevector and the phase of the pair potential, but leaves the spin of the state unaffected. For the action of time reversal, we obtain

$$\mathcal{U}_T|k_{p\nu}s;\chi_\nu\rangle = ps|-k_{p\nu}\bar{s};-\chi_\nu\rangle. \tag{64}$$

Here we see that the wavevectors change sign, the spin s changes to its complementary value $\bar{s}$, the phase χ_ν changes sign and there is also a sign ps in front of the transformed wavefunction. All these changes are typical of time reversal. The RB conjugation gives

$$\mathcal{U}_{\mathrm{RB}}|k_{p\nu}s;E^+,\chi_\nu\rangle = s\cdot\mathrm{sgn}(E)|-k_{p\nu}\bar{s};-E^-,\chi_\nu\rangle, \tag{65}$$

where we have used the relations (B.1), (B.2) of appendix B. In (65) we see that the RB conjugation changes the sign of the wavevector and spin, the sign of the energy (together with the direction of the limit to the real energy axis, where a branch cut exists for $|E| > \min(|\Delta_\ell|,|\Delta_r|)$), but leaves the phase χ_ν invariant.

For complex energies, we will need the effect of the RB conjugation on the solutions to the asymptotic BdG equations. Using the relations of appendix B, we obtain:

$$\mathcal{U}_{\mathrm{RB}}|pk_{p\nu}s;z\rangle = -s|\overline{p}k_{\overline{p}\nu}s;-z^*\rangle, \tag{66}$$

for $\mathrm{Re}(z)\neq 0$, while for imaginary $z = \mathrm{i}\omega$, we have

$$\mathcal{U}_{\mathrm{RB}}|pk_{p\nu}s;\mathrm{i}\omega\rangle = -s\cdot\mathrm{sgn}(\omega)|\overline{p}k_{\overline{p}\nu}s;\mathrm{i}\omega\rangle. \tag{67}$$

In order to obtain symmetry conditions for the scattering amplitudes, we transform the matrix elements of the T-matrix according to the transformations mentioned above. We shall do this in two ways: (a) transform the real energy matrix elements and then analytically continue the result into the complex energy plane, (b) consider the analytic continuation of the matrix elements and then apply the transformations. The way the transformations are to be applied is given symbolically below:

$$\begin{aligned}\langle A|\mathcal{T}|B\rangle &= \langle A|\mathcal{U}^\dagger\mathcal{U}\mathcal{T}\mathcal{U}^\dagger\mathcal{U}|B\rangle\\ &= \langle\mathcal{U}(A)|\mathcal{U}\mathcal{T}\mathcal{U}^\dagger|\mathcal{U}(B)\rangle^*\\ &= \langle A'|\mathcal{T}'|B'\rangle^*\\ &= \langle B'|(\mathcal{T}')^\dagger|A'\rangle\\ &= \langle B'|\mathcal{T}''|A'\rangle.\end{aligned}$$

Note in the second line of the above equations that the action of the anti-unitary transformation on the bra requires that we take the complex conjugate of the matrix element [26]. We terminate the above procedure in the third line, when dealing with the analytic continuation of the matrix elements, i.e. for complex energy functions. The rest of the lines in the above equation are executed when transforming real energy matrix elements, where we make use of property (30). Here we shall transform the analytically continued matrix elements only under the RB conjugation. More transformations of this case are considered in [22].

We also have to clarify the legitimacy of acting, in the second step of the previous equation, with $\mathcal{U}$ on the bra, when we handle the analytic continuation of the matrix elements. For this we have to extend the definition of the tilde over the spinors of (52) and (57) to mean that the complex conjugate of everything under it is taken, except for the energy variable z. This definition of a kind of complex conjugation can be given, because in our case complex numbers and functions of z appear as products. Then, since our anti-unitary transformations do not depend on the energy, their action on the bra is legitimate.

Now we are ready to present the symmetries of the scattering amplitudes that stem from the transformations we have considered. The transformation of complex conjugation $\mathcal{U}_C$ gives for the reflection amplitudes

$$\frac{\alpha^{\nu}_{ps,p's'}(z;\chi,\phi)}{k_{p\nu}(z)} = \frac{\alpha^{\nu}_{p's',ps}(z;-\chi,-\phi)}{k_{p'\nu}(z)} \tag{68}$$

and for the transmission amplitudes

$$\frac{m_\ell}{k_{p\ell}(z)\Omega_\ell(z)}\gamma^{\ell}_{ps,p's'}(z;\chi,\phi) = \frac{m_r}{k_{p'r}(z)\Omega_r(z)}\gamma^{r}_{p's',ps}(z;-\chi,-\phi). \tag{69}$$

We see that complex conjugation relates scattering amplitudes that differ in the sign of the phase difference χ and the azimuthal angle of the magnetization vectors of the junction. Symmetry properties (68) and (69) are generalizations of symmetry properties appearing in [17].

Time reversal $\mathcal{U}_T$ gives for the reflection amplitudes

$$\frac{\alpha^{\nu}_{ps,p's'}(z;\chi,\boldsymbol{M})}{k_{p\nu}(z)} = psp's'\frac{\alpha^{\nu}_{p'\bar{s}',p\bar{s}}(z;-\chi,-\boldsymbol{M})}{k_{p'\nu}(z)} \tag{70}$$

and for the transmission amplitudes

$$\frac{m_\ell}{k_{p\ell}(z)\Omega_\ell(z)}\gamma^{\ell}_{ps,p's'}(z;\chi,\boldsymbol{M}) = psp's'\frac{m_r}{k_{p'r}(z)\Omega_r(z)}\gamma^{r}_{p'\bar{s}',p\bar{s}}(z;-\chi,-\boldsymbol{M}). \tag{71}$$

Here also we see that time reversal relates scattering amplitudes that differ in the sign of the phase difference χ and the sign of the magnetization vectors of the junction. It changes the spin also, as it should.

From the RB conjugation we get

$$\frac{\alpha^{\nu}_{ps,p's'}(z,\chi)}{k_{p\nu}(z)} = s's\frac{\alpha^{\nu}_{p'\bar{s}',p\bar{s}}(-z,\chi)}{k_{p'\nu}(-z)} \tag{72}$$

and

$$\frac{m_\ell}{k_{p\ell}(z)\Omega_\ell(z)}\gamma^{\ell}_{ps,p's'}(z,\chi) = s's\frac{m_r}{k_{p'r}(-z)\Omega_r(-z)}\gamma^{r}_{p'\bar{s}',p\bar{s}}(-z,\chi). \tag{73}$$

The RB conjugation leaves the phase difference χ as well as the magnetization vectors invariant, but changes the sign of the complex energy z. Also, when applied to the analytic continuation of the T-matrix elements, gives the following symmetry relations

$$\alpha^{\nu}_{ps,p's'}(z;\chi) = s's\alpha^{\nu}_{\bar{p}s,\bar{p}'s'}(-z^*;\chi)^* \tag{74}$$

and

$$\gamma^{\nu}_{ps,p's'}(z;\chi) = s's\gamma^{\nu}_{\bar{p}s,\bar{p}'s'}(-z^*;\chi)^*. \tag{75}$$

Making use of the property of the wavevectors $k_{p\nu}(z) = k_{\bar{p}\nu}(-z^*)^*$, we can also write

$$\frac{1}{k_{p\nu}(z)}\alpha^{\nu}_{ps,p's'}(z;\chi) = s's\left(\frac{1}{k_{\bar{p}\nu}(-z^*)}\alpha^{\nu}_{\bar{p}s,\bar{p}'s'}(-z^*;\chi)\right)^*. \tag{76}$$

The above symmetry relations for the scattering amplitudes have been numerically confirmed, using the stepwise pair potential approximation. They will be utilized in section 7 for deriving symmetries of the current–phase-relation and simplifying the Furusaki–Tsukada formula for the dc Josephson current.

7. Effect on the current–phase-relation, Andreev bound states and Furusaki–Tsukada formula

The symmetry relations for the scattering amplitudes furnish us with one way to derive symmetries for the current–phase-relation of Josephson junctions. This is accomplished by the use of the Furusaki–Tsukada formula for the supercurrent [17] which, in a compact notation, reads

$$I = \nu\frac{e|\Delta_\nu|}{\hbar\beta}\sum_{\omega_n}\frac{1}{4\overline{\Omega}_\nu}\left\{\sum_{ps}(k_{p\nu}+k_{\bar{p}\nu})p\frac{\alpha^{\nu}_{ps,\bar{p}\bar{s}}}{k_{p\nu}}\right\}, \tag{77}$$

where I is the supercurrent, e the absolute value of the electronic charge, $\beta = 1/k_BT$ the inverse temperature, ω_n the fermion Matsubara frequencies and

$$\overline{\Omega}_\nu = \sqrt{\omega_n^2 + |\Delta_\nu|^2}. \tag{78}$$

The symmetry relations for the reflection amplitudes (68), that stem from complex conjugation, together with the Furusaki–Tsukada formula (77), give the following symmetry for the current–phase-relation:

$$I(\chi,\phi) = -I(-\chi,-\phi). \tag{79}$$

The above equation means that the supercurrent is odd with respect to $\chi = 0$ (or $\chi = \pi$, due to 2π periodicity in χ of the current–phase-relation), as long as we change the sign of all azimuthal angles of the magnetization of the junction. We note that, if the magnetization vectors of the system lie on the zx plane, then all azimuthal angles are equal to zero and (79) becomes

$$I(\chi) = -I(-\chi). \tag{80}$$

This symmetry property prohibits the existence of a zero phase difference supercurrent, when the magnetization vectors of the junction all lie on the same plane. The choice of the zx plane to prove this result is immaterial, for the current–phase-relation is invariant under a simultaneous rotation of all the magnetization vectors. In addition, we note that complex conjugation is identical with a combination of a rotation in spin space on the zx plane around 180° and time reversal (as defined here), which was considered in [21, 27] in connection with the prohibition of the zero phase difference supercurrent in ferromagnetic Josephson junctions with co-planar magnetization vectors. Also it must be stressed that (79) holds true for all magnetization vector geometries.

In a similar manner, taking advantage of (70), we can derive the following symmetry of the current–phase-relation:

$$I(\chi,\boldsymbol{M}) = -I(-\chi,-\boldsymbol{M}). \tag{81}$$

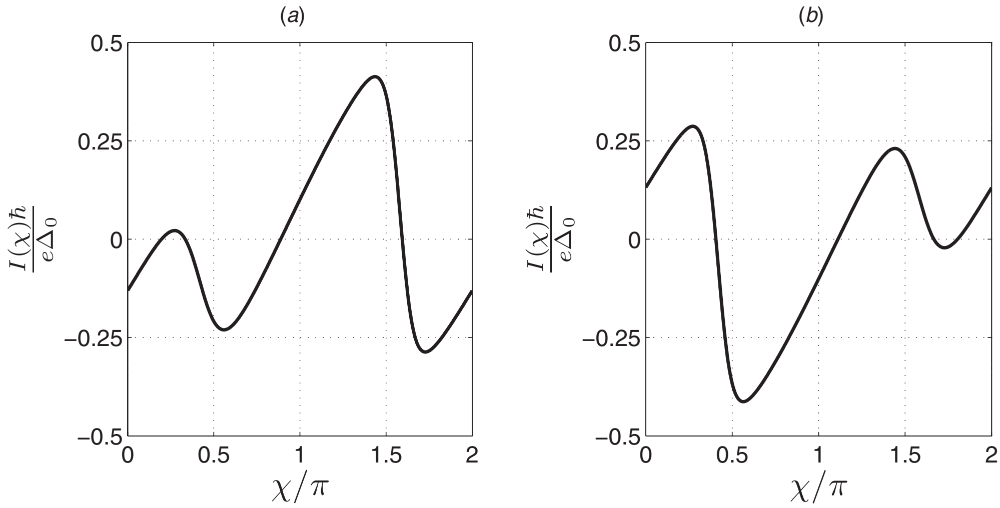

Figure 2. Current–phase-relation for two Josephson junctions with one ferromagnetic intermediate layer and spin active interfaces: (*a*) with magnetization geometry z, x, y, (*b*) with magnetization geometry $z, x, -y$ or $-z, -x, -y$. The rest of the parameters are temperature $T/T_c = 0.1$, zero temperature pair potential $\Delta_{0\ell,r}/E_F = 0.001$, normalized interface normal and magnetic scattering strengths $Z_{n\ell,r} = 0$, $Z_{m\ell,r} = 1$ respectively, normalized length and the magnetization of intermediate layers $k_F d = 20$ and $M/E_F = 0.5$ respectively.

This symmetry also holds true regardless of the magnetization geometry. Properties (79) and (81) can be seen in figure 2. The form of the current–phase-relation is the result of the combination of several features appearing in inhomogeneous ferromagnetic Josephson junctions. The $I(\chi)$ curve is far from sinusoidal, contrary to the case of small transmission junctions; there is a strong zero phase supercurrent due to the non-coplanarity of the magnetization vectors. There appear higher harmonics and the saw-tooth behaviour, which exists in normal metal weak links, is shifted in χ due to the strong and inhomogeneous magnetization of the junction.

We would like also to mention the symmetries of the Andreev bound state spectrum of ferromagnetic Josephson junctions that result from the transformations we have employed. These can be found from the eigenvalue equations of the BdG Hamiltonian. Thus, complex conjugation implies

$$E_n(\chi, \phi) = E_n(-\chi, -\phi), \tag{82}$$

that is, the Andreev bound state spectrum is symmetric with respect to $\chi = 0$ (or $\chi = \pi$, due to 2π periodicity in χ of the spectrum), as long as we change the sign of all azimuthal angles of the magnetization of the junction. On the other hand, time reversal implies that

$$E_n(\chi, \boldsymbol{M}) = E_n(-\chi, -\boldsymbol{M}). \tag{83}$$

The RB conjugation forces Andreev bound states to be symmetric with respect to the Fermi energy $E = 0$. All the above properties can be seen in figure 3 for a junction identical to that of figure 2. As expected for a junction with a short intermediate layer width, there are four branches. For a non-ferromagnetic metallic intermediate layer, there is spin degeneracy and the two branches can be classified as right and left going excitations, which will be mixed in the case of interfacial normal scattering. The spin degeneracy is removed with a weak exchange field for a single ferromagnetic layer and the spin up and down branches are

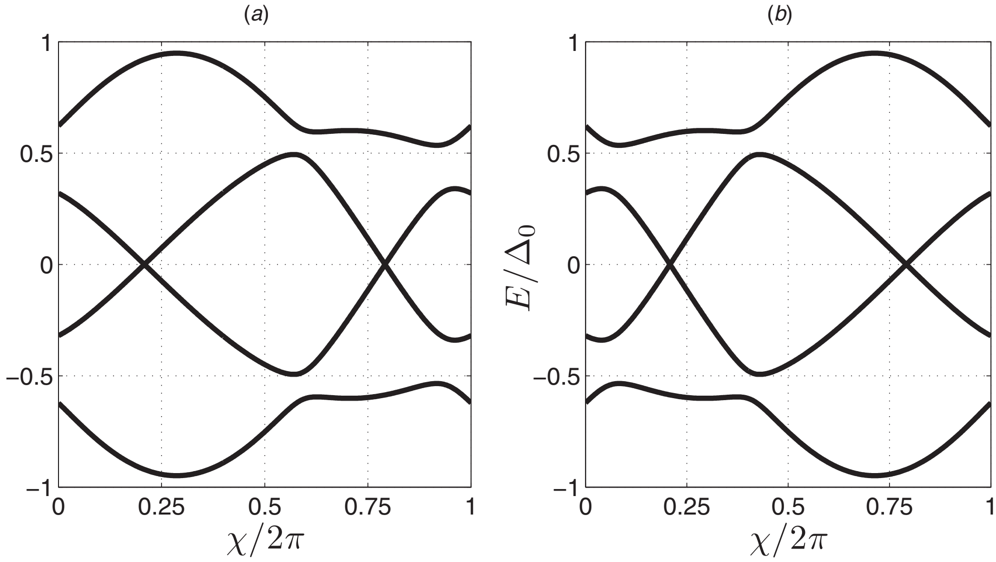

Figure 3. Andreev bound state spectrum for two Josephson junctions with one ferromagnetic intermediate layer and spin active interfaces: (*a*) with magnetization geometry z, x, y and (*b*) with magnetization geometry z, x, $-y$ or $-z$, $-x$, $-y$. The rest of the parameters are as in figure 2.

shifted horizontally in opposite χ directions. For a strong and inhomogeneous exchange field, the shifting is more complicated. In the plot, we also see both branch crossings and branch avoidance, the latter due to hybridization. In addition, the non-coplanarity of the magnetization gives asymmetry around $\chi = \pi$.

Finally, we mention the effect of the RB conjugation on the Furusaki–Tsukada formula for the dc Josephson supercurrent. From the use of (72) on the Furusaki–Tsukada formula, we conclude that the sum over the Matsubara frequencies is symmetric and that we can only sum positive Matsubara frequencies and multiply by a factor of 2. Also (76) leads to a simplification of the Furusaki–Tsukada formula, which reads

$$I = \nu \frac{e|\Delta_\nu|}{\hbar\beta} \sum_{\omega_n > 0} \frac{1}{\overline{\Omega}_\nu} (k_{e\nu} + k_{h\nu}) \mathrm{Re}\left\{ \frac{\alpha^{\nu}_{e\uparrow,h\downarrow}}{k_{e\nu}} + \frac{\alpha^{\nu}_{e\downarrow,h\uparrow}}{k_{e\nu}} \right\} \tag{84}$$

and in which the Andreev reflection amplitudes with hole incidence have been eliminated in favour of the real part of the electron incidence Andreev reflection amplitudes. Also it is obvious from the above, since the wavevectors $k_{e\nu}$ and $k_{h\nu}$ in the Matsubara frequency domain are complex conjugate to each other, that the supercurrent given by (84) is a real number, as it should be. Equation (84) can facilitate analytical and numerical calculations of the dc Josephson supercurrent.

8. Concluding remarks

In summary, we have considered quantum scattering systems in one space dimension with different asymptotics on the left and right, that are characterized by short range potentials with well defined limits in the asymptotic regions. We used as a concrete model throughout that of ferromagnetic Josephson junctions, in which the phase difference between the superconducting asymptotic regions makes the spatial asymptotics different on the left and right, even if the superconducting electrodes are of the same material. By developing the theory of the Lippmann–Schwinger equations, we were naturally led to define a channel-dependent T-matrix, the matrix elements of which are proportional to the scattering amplitudes. Then we considered certain anti-unitary transformations, the use of which led us to symmetries of the scattering amplitudes, which in turn were derived, through the elements of the T-matrix, essentially from the transformation properties of the full Hamiltonian and the stationary scattering states of the asymptotic Hamiltonians. The consequences of these symmetry relations to the current–phase-relation and the Andreev bound states were then presented, as well as a useful simplification of the Furusaki–Tsukada formula for the dc Josephson supercurrent.

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Appendix A. Finiteness of T-matrix elements

In this appendix, we give information about the finiteness of the T-matrix elements that represent the scattering amplitudes. These matrix elements contain integrals over the position variables; we want to examine whether they give finite results in the limit $a \to 0^+$ of no Gaussian modulation. For example, we have the matrix-element

$$\int \mathrm{d}x \Phi_{-p's'r}(x)\mathcal{V}_\ell(x)\Phi_{ps\ell}(x) + \int \mathrm{d}x\,\mathrm{d}x'\,\Phi_{-p's'r}(x)\mathcal{V}_r(x)\mathcal{G}(x,x')\mathcal{V}_\ell(x')\Phi_{ps\ell}(x'). \tag{A.1}$$

We consider the parts of the above integrals with integration of x and x' over the asymptotic regions, to check whether they are finite. The second term in the above expression has a similar treatment to the first one and we therefore focus on the latter. Since the potential $\mathcal{V}_\ell$ is constant in the right asymptotic region, the nontrivial part of the above integral has the form

$$P = \lim_{a\to 0^+} \int_0^{+\infty} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}bx}\, \mathrm{e}^{-ax^2}, \tag{A.2}$$

where we have shown explicitly the Gaussian modulation, the lower limit of integration is chosen as zero without loss of generality and b is some sum or difference of appropriate wavevectors and is generally complex. Completing the square in the exponent of expression P and making a change of variables, we have

$$P = \lim_{a\to 0^+} \int_{-\frac{\mathrm{i}b}{2\sqrt{a}}}^{+\infty} \frac{\mathrm{d}y}{\sqrt{a}}\, \mathrm{e}^{-y^2}\, \mathrm{e}^{-\frac{b^2}{4a}}, \tag{A.3}$$

where $y = \sqrt{a}(x - \mathrm{i}b/2a)$. If $\mathrm{Im}(b) > 0$ and anticipating the limit is $a \to 0^+$, we see that the lower limit of integration in (A.3) has a real part that tends to $+\infty$ and the leading term in an asymptotic expansion of P, closely related to the so-called probability integral (see [28]), tends to $-1/ib$ as $a \to 0^+$. When $\mathrm{Im}(b) < 0$, the lower limit of integration has a real part that tends to $-\infty$ and the leading term in the asymptotic expansion is proportional to $1/\sqrt{a}$, which multiplied by $\mathrm{e}^{-b^2/4a}$ in expression P has a limit equal to zero, as $a \to 0^+$, provided that $|\mathrm{Re}(b)| > |\mathrm{Im}(b)|$. The next term in the asymptotic expansion has limit $-1/ib$. Thus we see that the limit of expression P is equal to the integral of e^{ibx}, between 0 and $+\infty$, as if the antiderivative of this function were zero at $+\infty$. Therefore, the only requirement for the convergence of these integrals is that $|\mathrm{Re}(b)| > |\mathrm{Im}(b)|$, which can be met simultaneously for all scattering amplitudes in at least a neighbourhood of the complex plane, when the wavevectors comprising b are close to large enough real numbers. In the pathological case that b is the difference of equal wavevectors and thus zero, which can happen in Josephson junctions with identical superconducting electrodes, then the corresponding matrix elements turn out to be zero, due to the other (non-spatial) degrees of freedom [22].

Appendix B. Properties of coherence factors and wavevectors

The relations for the coherence factors used to derive the transformation of real energy states by the RB conjugation are:

$$u_\nu(E^+) = -\mathrm{sgn}(E)v_\nu(-E^-), \tag{B.1}$$

$$v_\nu(E^+) = \mathrm{sgn}(E)u_\nu(-E^-). \tag{B.2}$$

For the transformation of states with complex energy by the RB conjugation, we use the relations:

$$u_\nu(z)^* = u_\nu(-z^*), \tag{B.3}$$

$$v_\nu(z)^* = -v_\nu(-z^*), \tag{B.4}$$

for $\mathrm{Re}(z) \neq 0$, while for imaginary $z = \mathrm{i}\omega$

$$u_\nu(\mathrm{i}\omega)^* = \mathrm{sgn}(\omega)u_\nu(\mathrm{i}\omega) \tag{B.5}$$

$$v_\nu(\mathrm{i}\omega)^* = -\mathrm{sgn}(\omega)v_\nu(\mathrm{i}\omega). \tag{B.6}$$

We also make use of the relation

$$k_p(z)^* = k_{\overline{p}}(-z^*), \tag{B.7}$$

where $\bar{p}$ is the complementary value to p.

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