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Spin–charge conductance in nanoscale electronic devices

Huan-Qiang Zhou[1] **and Sam Young Cho**[2]

[1] Department of Physics, Chongqing University, Chongqing 400044, People's Republic of China and
Centre for Mathematical Physics, University of Queensland, 4072, Australia
[2] Department of Physics, University of Queensland, 4072, Australia

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Abstract

We introduce a spin–charge conductance matrix as a unifying concept underlying charge and spin transport within the framework of the Landauer–Büttiker conductance formula. It turns out that the spin–charge conductance matrix provides a natural and gauge covariant description for electron transport through nanoscale electronic devices. We demonstrate that the charge and spin conductances are gauge invariant observables which characterize transport phenomena arising from spin-dependent scattering. Tunnelling through a single magnetic atom is discussed to illustrate our theory.

1. Introduction

Spintronics is a promising and intriguing subject which aims to bring novel functionalities to conventional electronic devices via the manipulation of spin degrees of freedom of electrons (for a recent review, see, e.g., [1]). This is achieved by implementing various means such as imposing external electrical and magnetic fields to control and manipulate charge and spin dynamics. Although significant advances have been made over the years in diverse areas including spin transport, spin dynamics, and spin relaxation, the full potential of spintronic applications in nanoscale electronic devices remains to be developed.

Electrons as carriers carry both charge and spin degrees of freedom. This makes it impossible to consider separately charge and spin transport in solid-state devices, since any manipulation of one degree of freedom influences the other, although the detection of charge and spin currents does require different kinds of experimental set-ups. A fundamental issue is how to characterize spin conduction associated with a given charge current, which is well understood in conventional electronics. In this paper, we will address this issue for a specific problem, i.e., electron transport in solids, which has been systematically studied by Landauer and Büttiker [2, 3]. In their approach, charge transport in mesoscopic systems is described in terms of the probability for an electron to be transmitted through a given channel. The theory has been successfully confirmed in remarkable experiments [4, 5] which exhibit quantized conductance in a quantum point contact. On the other hand, if one tries to incorporate spin degrees of freedom into the Landauer–Büttiker formalism, it is necessary to introduce a spin conductance which describes effects arising from spin-dependent scattering processes in nanoscale electronic devices, because the charge conductance is not enough to give a proper and complete description of the spin-dependent scattering. This motivates us to define a spin–charge conductance matrix which presents a unifying concept underlying spin and charge transport based on the scattering matrix formalism for nanoscale electronic devices. It turns out that the charge and spin conductances are two physical observables which one may construct from the spin–charge conductance matrix as gauge invariants. This results from the unitary freedom in choosing the incoming and outgoing wavefunctions for a spin-dependent scatterer. We stress that the charge and spin conductance matrix constitutes a natural spintronic analogue of the scalar conductance encountered in the Landauer–Büttiker formalism, which plays a fundamental role in mesoscopic physics. We also mention a relevant work by Pareek [6] in which an extension of the Landauer–Büttiker formula to spin-dependent transport was discussed. However, in contrast to our approach, his theory is only applicable to systems with multiple leads.

To illustrate the theory, we consider tunnelling through a single magnetic atom, in which spin flip processes play a dominant role. The exact solvability of the model Hamiltonian makes it a good example for illustrating our general formalism. The experimental set-up required to measure the spin currents associated with tunnelling from a scanning tunnelling microscope tip through a magnetic atom is indicated.

2. A mesoscopic system and the Landauer–Büttiker charge conductance

Consider a quantum mesoscopic device consisting of a scatterer connected to two ideal leads. For each ideal lead, there are $2M$ channels, where the factor 2 comes from the spin degeneracies and M is the number of different transverse modes which electrons are allowed to populate. Without loss of generality, we restrict ourselves to the case where only one mode is populated, i.e., $M = 1$. This amounts to assuming that there is no scattering from one transverse mode to another. This may be achieved by ensuring that the transverse confining potential does not vary along the longitudinal direction. Then electron transport through the scatterer is described by a scattering matrix $\boldsymbol{S}$ [7] connecting the outgoing wave amplitudes to the incoming wave amplitudes at the different leads. $\boldsymbol{S}$ is unitary, ensuring current conservation. Taking into account the internal spin space describing the spin degrees of freedom, we see that $\boldsymbol{S}$ is a 4×4 matrix, defined in terms of four 2×2 block matrices $\boldsymbol{r}$, $\boldsymbol{r}'$, $\boldsymbol{t}$, and $\boldsymbol{t}'$, which are the reflection and transmission matrices from the left and right leads, respectively. The indices σ $(=\pm)$ and σ' $(=\pm)$ will be used to denote partial reflection and transmission entries. For example, $r_{\sigma\sigma'}$ denotes the reflection coefficient with spin σ' for electrons incident from the left lead with spin σ. According to Landauer [2], the (charge) conductance G_{C} is related to the transmission probabilities in the linear response regime. In our case, the charge conductance [7] is given by

$$G_{\mathrm{C}} = \frac{e^2}{h} \mathrm{Tr}\, \boldsymbol{t}\,\boldsymbol{t}^{\dagger}, \tag{1}$$

where the trace of the product of the transmission matrices is taken over the internal spin space. Intuitively it is quite plausible that the charge conductance is proportional to the ease with which electrons can transmit through the scatterer.

3. A spin–charge conductance matrix (charge and spin conductances)

$\boldsymbol{S}$ is not unique because of the unitary freedom in choosing the incoming and outgoing wavefunctions associated with a given lead. The unitary freedom allows different choices of the scattering matrix: $\boldsymbol{S}' = \boldsymbol{\Omega S}$ with $\boldsymbol{\Omega}$ a diagonal block matrix, each block of which is a 2×2 unitary matrix $\boldsymbol{\omega}$. This amounts to the fact that there is a (global) gauge group $\boldsymbol{U}(2)$ ($\ni \boldsymbol{\omega}$) originating from the unitary freedom. Physically, left multiplication of the scattering matrix $\boldsymbol{S}$ by $\boldsymbol{\Omega}$ just redistributes the scattering particles among different incoming channels associated with a certain lead. Such a redistribution should not affect correlations at the scatterer and so one may expect the physics to remain the same. This kind of gauge transformation has appeared in the discussion of quantum adiabatic pumping [8, 9]. The gauge transformation for the scattering matrix induces a transformation for the transmission matrix $\boldsymbol{t}$: $\boldsymbol{t} \to \boldsymbol{\omega t}$.

Physical information on spin-dependent scattering through the scatterer encoded in the amplitudes of the transmission matrix is relevant to charge and spin transport through nanoscale electronic devices. However, the charge conductance defined in equation (1) does not exhaust all the encoded information. To help understand transport phenomena arising from spin-dependent scattering, let us define a spin–charge conductance matrix as follows:

$$\boldsymbol{G} = \frac{e^2}{h} \boldsymbol{t} \boldsymbol{t}^{\dagger}. \tag{2}$$

One sees that such a conductance matrix transforms covariantly: $\boldsymbol{G}' = \boldsymbol{\omega G} \omega^{-1}$. Therefore, the spin–charge conductance matrix $\boldsymbol{G}$ is itself gauge dependent. However, as we will see below, the gauge invariants that one can construct from $\boldsymbol{G}$ determine the physical observables such as the charge conductance.

To show why we need to introduce such a conductance matrix, we consider a system in which the spin is conserved, i.e., the spin flip processes are absent. In such a case, the transmission matrix $\boldsymbol{t}$ is diagonal in the internal spin space, i.e., only t_{++} and t_{--} are non-zero in a properly chosen basis (gauge). Following Landauer and Büttiker, one may write down the conductances G_{++} and G_{--} as $G_{\sigma\sigma} = (e^2/h)|t_{\sigma\sigma}|^2$. This corresponds to the case where the conductance matrix introduced above is diagonal. However, this is only true in a specific gauge; generically, a covariant spin–charge conductance matrix as defined above is needed. Physically, the conductance matrix results from the fact that charge and spin transport should be proportional to the ease with which electrons can transmit through the scatterer, combining with the spin dependence of the scatterer which can flip spins of electrons when they traverse it.

Now we rewrite the conductance matrix $\boldsymbol{G}$ as $\boldsymbol{G} = \sum_{\alpha \in \{0,x,y,z\}} G_\alpha \boldsymbol{\sigma}^\alpha/2$, where $G_\alpha = (e^2/h) \mathrm{Tr}\ \boldsymbol{t}^\dagger \boldsymbol{\sigma}^\alpha \boldsymbol{t}$. Here, $\boldsymbol{\sigma}^0$ is the identity matrix and $\boldsymbol{\sigma}^x$, $\boldsymbol{\sigma}^y$, and $\boldsymbol{\sigma}^z$ are the Pauli matrices. One may establish that G_0 is just the charge conductance, G_{C}, appearing in the Landauer–Büttiker formula in equation (1). Under a gauge transformation, as one may expect, G_0 is invariant, whereas G_x, G_y, and G_z are themselves gauge dependent. However, G_x, G_y, and G_z transform like a vector under the induced rotation group in the internal spin space. Then we have another gauge invariant quantity, $G_x^2 + G_y^2 + G_z^2$. Indeed, the spin–charge conductance matrix may be rewritten in terms of these gauge invariants, i.e., charge and spin conductances:

$$\boldsymbol{G} = \tfrac{1}{2} \left(G_{\mathrm{C}} \boldsymbol{\sigma}^0 + G_{\mathrm{S}} \boldsymbol{\sigma}^s \right), \tag{3}$$

where the spin conductance vector is defined as $\boldsymbol{G}_{\mathrm{S}} = G_{\mathrm{S}} \boldsymbol{\sigma}^s$. The amplitude of the spin conductance vector takes the form

$$G_{\mathrm{S}} = \sqrt{G_x^2 + G_y^2 + G_z^2} \tag{4}$$

and $\boldsymbol{\sigma}^s = (G_x\boldsymbol{\sigma}^x + G_y\boldsymbol{\sigma}^y + G_z\boldsymbol{\sigma}^z)/G_S$ is the unit directional vector for the spin conductance. It should be noted that the charge conductance, G_0, and the amplitude of the spin conductance, G_S, are gauge invariant. Since the $\boldsymbol{\sigma}^s$ is not gauge invariant, $\boldsymbol{G}$ is itself gauge dependent. Then G_x, G_y, and G_z are the projection components of a vector in internal spin space for the spin conductance. As in the case of a quantum spin, they cannot be observed simultaneously. In other words, the spin conductance defined contains a unique spin conduction for spin scattering but the components of the spin conductance depend on how the basis has been chosen.

4. Charge and spin currents

The essential issue now is how to observe the above-defined spin and charge conductances. Let us consider gauge invariant quantities which can be constructed from the spin–charge conductance matrix. One sees that the eigenvalues of $\boldsymbol{G}$ are gauge invariant. They are denoted by G_+ and G_-. From equation (3), we have $G_\pm = (G_C \pm G_S)/2$. This is obtained by performing a gauge transformation defined by $\boldsymbol{\omega}\boldsymbol{\sigma}^s\boldsymbol{\omega}^{-1} = \boldsymbol{\sigma}^z$. Now we address the connection between the defined conductances and physical observables. Actually, in our case, there are two independent simultaneous observables which are charge currents flowing into two spin channels, I_σ. As observables, the I_σ must be gauge invariant. Therefore they must be some functions of the gauge invariants G_C and G_S, i.e., $I_\sigma = f_\sigma(G_C, G_S)$ with the f_σ being model-independent functions to be determined, since our argument only involves the gauge invariance. From scattering processes without spin flips, we have

$$I_\sigma = \tfrac{1}{2}(G_C + G_S)\Delta V, \qquad I_{\bar{\sigma}} = \tfrac{1}{2}(G_C - G_S)\Delta V. \tag{5}$$

Here ΔV is the voltage bias across the device. From the two charge currents, we may define the charge current, $I_C = I_\sigma + I_{\bar{\sigma}}$, and the spin current, $I_S = I_\sigma - I_{\bar{\sigma}}$. Then the charge and spin conductances are directly connected to the charge and spin currents by

$$I_{C(S)} = G_{C(S)}\Delta V. \tag{6}$$

The above consideration amounts to the statement that in order to incorporate spin degrees of freedom into the conventional Landauer–Büttiker theory, it is necessary to introduce a 2×2 current matrix $\boldsymbol{I}$:

$$\boldsymbol{I} \equiv \begin{pmatrix} I_{\sigma\sigma} \, I_{\sigma\bar{\sigma}} \\ I_{\bar{\sigma}\sigma} \, I_{\bar{\sigma}\bar{\sigma}} \end{pmatrix} = \boldsymbol{G}\Delta V. \tag{7}$$

The equation is covariant under a gauge transformation. The appearance of a current matrix instead of a current vector characterizes the difference between the conventional Landauer–Büttiker theory and ours. The two charge currents I_σ turn out to be the eigenvalues of the current matrix so defined. Therefore, the defined spin conductance, G_S, is indeed the observable physical quantity characterizing spin-dependent scattering within the Landauer–Büttiker framework for electron transport in nanoscale electronic devices.

5. The extension to a system with multiple leads

It is straightforward to extend the above discussion to a system with N leads. In such a case, $\boldsymbol{S}$ becomes a $2N \times 2N$ matrix, which may be defined in terms of $N^2 2 \times 2$ block matrices, i.e., the matrices for reflection from the αth lead $\boldsymbol{r}_{\alpha\alpha}$ and the matrices for transmission from the αth lead to the βth lead $\boldsymbol{t}_{\alpha\beta}$. Then the 2×2 current matrix (for flow into the αth lead) takes the form

$$\boldsymbol{I}_\alpha = \sum_\beta \boldsymbol{G}_{\alpha\beta}\Delta V_{\alpha\beta}. \tag{8}$$

Here $\Delta V_{\alpha\beta}$ is the voltage bias between the αth and βth leads, and $\boldsymbol{G}_{\alpha\beta}$ is a 2×2 charge and spin conductance matrix defined by $\boldsymbol{G}_{\alpha\beta} = (e^2/h)\, \boldsymbol{t}_{\alpha\beta}\, \boldsymbol{t}^{\dagger}_{\alpha\beta}$. The currents $\boldsymbol{I}_{\alpha\sigma}$ are two eigenvalues of the current matrix above, which are gauge invariant under a gauge transformation $\boldsymbol{t}_{\alpha\beta} \to \boldsymbol{\omega}_{\alpha}\boldsymbol{t}_{\alpha\beta}$ induced from the unitary freedom in choosing the incoming and outgoing bases, where $\boldsymbol{\omega}_{\alpha}$ denotes the αth diagonal block in $\boldsymbol{\Omega}$.

6. Tunnelling through a single magnetic atom

Consider a mesoscopic system consisting of two normal leads coupled to a single site, the magnetic spin of which has an exchange interaction J with a magnetic atom. The model Hamiltonian takes the form [9, 10]

$$H = \sum_{k\sigma\in \mathrm{L,R}} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} + J \sum_{\sigma,\sigma'} d^{\dagger}_{\sigma} \Omega_{\sigma\sigma'} d_{\sigma'} + \sum_{k\sigma\in \mathrm{L,R}} (V_k c^{\dagger}_{k\sigma} d_{\sigma} + \mathrm{H.c.}). \tag{9}$$

Here, $c^{\dagger}_{k\sigma}$ and $c_{k\sigma}$ denote, respectively, the creation and destruction operators for an electron with momentum k and spin σ in either the left (L) or the right (R) lead, whereas $d^{\dagger}_{\sigma}$ and d_{σ} are the creation and destruction operators for the single electron with spin σ at the magnetic spin site. ϵ_k are the single-particle energies of conduction electrons in the two leads. As usual, it is convenient to linearize the ϵ_k around the Fermi points, i.e., $\epsilon_k = v_{\mathrm{F}}(|k| - k_{\mathrm{F}})$, where v_{F} is the Fermi velocity and k_{F} is the Fermi momentum. For brevity, it is assumed that $v_{\mathrm{F}} = 1$ and $k_{\mathrm{F}} = 0$. The latter implies that the momentum is measured from the Fermi surface for electrons in leads. The electrons on the spin site are connected to those in the two leads with the tunnelling matrix elements V_k. For simplicity, we assume symmetric tunnelling barriers between the local spin, i.e., $V_{\mathrm{L}} = V_{\mathrm{R}} = V$. Then the entries of the coupling matrix Ω take the form $\Omega_{++} = -\Omega_{--} = \cos\theta$ and $\Omega_{+-} = \Omega^{*}_{-+} = \sin\theta \exp(-\mathrm{i}\phi)$, where the angle between the magnetic spin of the atom and magnetic field is denoted by θ and the azimuthal angle is ϕ.

The model Hamiltonian is exactly solvable. The elements of the transmission matrix, $\boldsymbol{t}$, take the following form:

$$t_{++} = \frac{1}{2}\left(-1 + \mathrm{e}^{\mathrm{i}\delta_1}\cos^2\frac{\theta}{2} + \mathrm{e}^{\mathrm{i}\delta_2}\sin^2\frac{\theta}{2}\right), \tag{10}$$

$$t_{+-} = \frac{1}{2}\mathrm{e}^{-\mathrm{i}\phi}\left(\mathrm{e}^{\mathrm{i}\delta_1} - \mathrm{e}^{\mathrm{i}\delta_2}\right)\sin\frac{\theta}{2}\cos\frac{\theta}{2}, \tag{11}$$

$$t_{-+} = \frac{1}{2}\mathrm{e}^{+\mathrm{i}\phi}\left(\mathrm{e}^{\mathrm{i}\delta_1} - \mathrm{e}^{\mathrm{i}\delta_2}\right)\sin\frac{\theta}{2}\cos\frac{\theta}{2}, \tag{12}$$

$$t_{--} = \frac{1}{2}\left(-1 + \mathrm{e}^{\mathrm{i}\delta_1}\sin^2\frac{\theta}{2} + \mathrm{e}^{\mathrm{i}\delta_2}\cos^2\frac{\theta}{2}\right), \tag{13}$$

where the δ_i ($i = 1, 2$) are the phase shifts defined by $\delta_1 = -2\tan^{-1}(\Gamma/(k - J))$ and $\delta_2 = -2\tan^{-1}(\Gamma/(k + J))$ with the tunnelling rate $\Gamma = V^2$. As a result, the charge and spin conductances take the forms

$$G_{\mathrm{C}} = \frac{e^2}{h}\left(\sin^2\frac{\delta_1}{2} + \sin^2\frac{\delta_2}{2}\right), \tag{14}$$

$$G_{\mathrm{S}} = \frac{e^2}{h}\left(\sin^2\frac{\delta_1}{2} - \sin^2\frac{\delta_2}{2}\right), \tag{15}$$

respectively, where the unit directional vector for the spin conductance is $\boldsymbol{\sigma}^s = \cos\phi\sin\theta\boldsymbol{\sigma}^x + \sin\phi\sin\theta\boldsymbol{\sigma}^y + \cos\theta\boldsymbol{\sigma}^z$. As one might expect, the amplitude of the spin conductance does not depend on the details of the specified coordinates for the spin of the magnetic atom, contrasting with the fact that G_x, G_y, and G_z are rather dependent on the specified coordinates. When

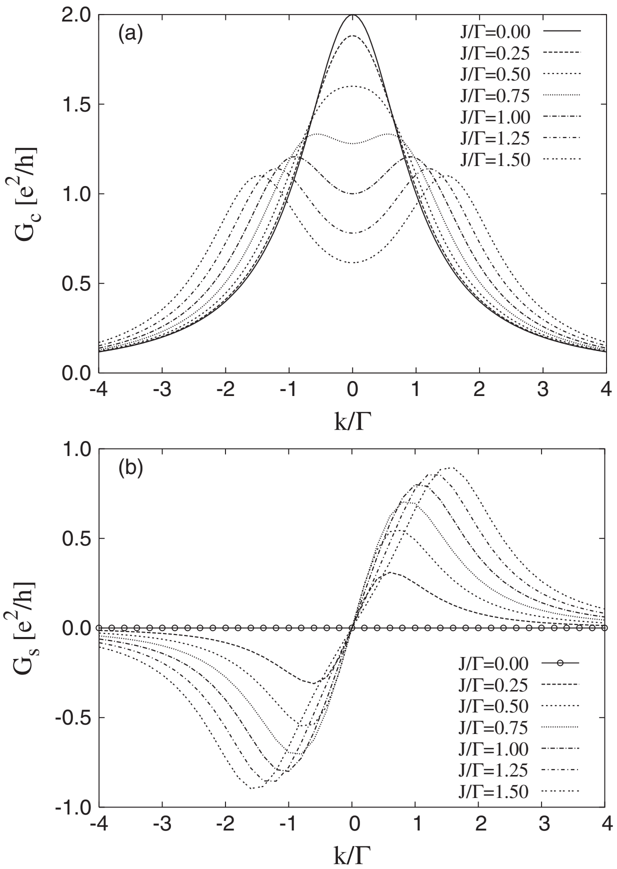

Figure 1. (a) Charge and (b) spin conductances through a single magnetic spin for various spin exchange interactions, J. The strength of the coupling between the magnetic atom and the leads is denoted by Γ.

$\delta_1 = \delta_2(J = 0)$, the amplitude of the spin conductance becomes $G_S = 0$, as it should. At the Fermi energy, a resonant peak occurs in the charge conductance. Figure 1 shows the spin and charge conductances as a function of k/Γ for various spin exchange interactions. As the exchange interaction increases from zero, the peak of the charge conductance for $J = 0$ splits into two peaks around the resonant scattering, $k = \pm J$. As we defined the spin current as the difference between two charge currents associated with opposite spins, the sign change of the spin conductance implies that the dominance of one given charge current is taken over by the other. In addition, the spin current through the magnetic atom reaches its maximum value around the resonant charge transport. It is shown that the exchange interaction inducing a spin flip scattering determines the spin conduction through the scatterer.

The spin polarization, P, can be written in terms of the spin and charge conductances:

$$P = \frac{I_\sigma - I_{\bar{\sigma}}}{I_\sigma + I_{\bar{\sigma}}} = \frac{G_S}{G_C}. \tag{16}$$

In our case, the spin polarization through the magnetic atom is given by $P = (\sin\delta_1/2 - \sin\delta_2/2)/(\sin\delta_1/2 + \sin\delta_2/2)$. The maximum polarization is shown to be at resonant charge transport. As shown in figure 1(b), it reaches a perfect spin polarization as the spin exchange interaction increases.

Detection of spin currents. To do this, one could replace one of the normal metal leads by a ferromagnetic one. Then the charge currents in both the normal and ferromagnetic leads should be measured, which tells us the spin current I_S via the relations

$$\begin{pmatrix} I_C^F \\ I_S^F \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & \cos\zeta \\ \cos\zeta & 1 \end{pmatrix} \begin{pmatrix} I_C \\ I_S \end{pmatrix}, \tag{17}$$

where ζ is an angle between the z-axis and the magnetization in the ferromagnetic lead. We believe recent advances in electron spin resonance and scanning tunnelling microscope experiments [11–13] make it possible to observe spin currents discussed here.

7. Conclusion

The scalar conductance which appears in the Landauer–Büttiker formalism has been generalized to incorporate the spin degrees of freedom, thus revealing a unifying concept underlying charge and spin transport in nanoscale electronic devices. The connection between the charge and spin currents and the eigenvalues of the conductance matrix was established and the experimental set-up for measuring spin currents was discussed. To demonstrate the nontriviality of the effect, we considered tunnelling via a single magnetic atom in which the presence of spin flip processes makes it possible to generate spin currents whose full description requires a proper understanding of the non-Abelian character of the spin degrees of freedom.

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