Spin-dependent conductance statistics in systems with spin-orbit coupling

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Abstract. Transfer-matrix methods are used for a tight-binding description of electron transport in the presence of spin-orbit (SO) couplings. Spin-dependent partial conductances are evaluated. We show that, as the magnitude of SO interactions increases, the separation of spin-switching channels from non-spin-switching ones is gradually erased. We examine procedures designed to produce spin-polarised incident beams, namely: (i) imposing spin-dependent amplitudes on the incident wavefunctions; and (ii) including a Zeeman-like term in the Hamiltonian, while keeping the incident beams fully spin-unpolarised. For procedure (ii) we show that the exiting polarisation displays a maximum as a function of the intensity of SO couplings. For moderate site disorder, and both weak and strong SO interactions, no evidence is found for a decay of exiting polarisation against increasing system length. With very low site disorder, as well as weak SO couplings, a spin-filter effect takes place, as polarisation increases with increasing system length.

Keywords: quantum transport, quantum disordered systems, numerical simulations

1. Introduction

In this paper we consider electronic transport in two-dimensional (2D) systems with spin-orbit (SO) interactions. While single-parameter scaling predicts that noninteracting electron states in 2D are generally localized by disorder [1], in this marginal dimension the enhancement of forward scattering provided by SO effects partially offsets disorder-induced quantum interference, thus giving rise to a conducting phase [2] [3] [4].

Our purpose here is to study the statistics of the direct-current (DC) conductance of such systems, in particular its spin-dependent properties and their dependence on various externally-imposed parameters. We compare selected results, especially those pertaining to spin polarisation, to those obtained for a variant of the similar (though classical) problem of directed flow with exclusion which mimicks the Pauli principle by allowing for conditional site double-occupation [5].

Section 2 below recalls selected existing results, as well as some technical aspects of the transfer-matrix (TM) method used in our calculations. In Sec. 3 we give numerical
results for the statistics of spin-dependent conductances, first for spin-unpolarised systems and then, with the help of some additional working hypotheses, for the polarised case. For the latter we also investigate the behaviour of the polarisation itself, and of spin-correlation functions. In Sec. 4 we summarize and discuss our results.

2. Theory

The model one-electron Hamiltonian for this problem is

\[ \mathcal{H} = \sum_{i,\sigma} \varepsilon_i c_{i\sigma} c_{i\sigma} + \sum_{\langle i,j \rangle} \sum_{\sigma,\sigma'} V_{ij} c_{i\sigma} c_{j\sigma'}, \]

(1)

where \( c_{i\sigma} \) are creation and annihilation operators for a particle with spin eigenvalues \( \sigma = \pm 1 \) at site \( i \), and the self-energies \( \varepsilon_i \) are independently-distributed random variables; \( V_{ij} \) denotes the \( 2 \times 2 \) spin-dependent hopping matrix between pairs of nearest-neighbour sites \( \langle i, j \rangle \), whose elements must be consistent with the symplectic symmetry of SO interactions [6, 7]. In Eq. (1) we describe SO couplings via an effective Hamiltonian with a single (s-like) orbital per site [4]. Several possible forms may be considered for the hopping term, depending on whether one is specifically considering Rashba- or Dresselhaus-like couplings [4, 8], or (as is the case here) the focus is simply on the basic properties of systems in the symplectic universality class [9, 10, 11].

Here we use the implementation of [9, 10], namely:

\[ V_{ij} = I + \mu \sum_{k=x,y,z} V^k \sigma^k = \begin{pmatrix} 1 + i\mu V^z & \mu V^y + i\mu V^x \\ -\mu V^y + i\mu V^x & 1 - i\mu V^z \end{pmatrix}, \]

(2)

where \( I \) is the \( 2 \times 2 \) identity matrix, \( \sigma^k \) are the Pauli matrices, and \( \mu \) gives the intensity of the SO coupling; below we consider the (real) \( \{V^k\} \) uniformly distributed in \([-1/2, 1/2]\]. Thus all energies will be written in units of the \( \mu \equiv 0 \) nearest-neighbour hopping.

Similarly the \( \varepsilon_i \) will generally be taken from a random uniform distribution in \([-W/2, W/2]\).

The form Eq. (2) for the hopping term does not exhibit the explicit multiplicative coupling between momentum and spin degrees of freedom, characteristic of Rashba-like Hamiltonians [4, 8]. In two dimensions one should not expect significant discrepancies between results from either type of approach, as long as one is treating systems without lateral confinement.

Since we shall not attempt detailed numerical comparisons to experimental data, the simplified formulation described in the preceding paragraphs seems adequate for our purposes.

We apply the TM approach specific to tight-binding Hamiltonians like Eq. (1) [12, 13, 14]. Consider a strip of the square lattice, cut along one of the coordinate directions. For the orthogonal universality class with site disorder, denoting by \( k = 1, \ldots, M \) the successive columns, and \( i = 1, \ldots, N \) the respective positions of sites within each column of a strip, the recursion relation for an electronic wave function at energy \( E \) is given
in terms of its local amplitudes (which can all be assumed real), \( \{ a_{ik}(E) \} \), and tight-binding orbitals \( |ik\rangle \), as:

\[
( \psi_{k+1} \psi_k ) = \begin{pmatrix} P_k & -I \\ I & 0 \end{pmatrix} \begin{pmatrix} \psi_k \\ \psi_{k-1} \end{pmatrix}, \quad \psi_k \equiv \begin{pmatrix} a_{1k} \\ a_{2k} \\ \cdots \\ a_{Nk} \end{pmatrix},
\]

(3)

where \( I \) is the \( N \times N \) identity matrix, the energy dependence has been omitted for clarity and (invoking periodic boundary conditions across the strip),

\[
P_k = \begin{pmatrix}
E - \varepsilon_{1k} & -1 & 0 & \cdots & -1 \\
-1 & E - \varepsilon_{2k} & -1 & \cdots & 0 \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
-1 & 0 & \cdots & -1 & E - \varepsilon_{Nk}
\end{pmatrix}.
\]

(4)

The introduction of SO couplings along the bonds, see Eqs. (1) and (2), means that the \( a_{ik} \) are now spinors, written on the basis of the eigenvectors of \( \sigma^z \) as:

\[
a_{ik} = (a_{ik}^\uparrow a_{ik}^\downarrow),
\]

(5)

where the \( a_{ik}^\uparrow, a_{ik}^\downarrow \) are complex. The matrices \( P_k \) and the subdiagonal \( I \) of Eq. (3) are now \( 2N \times 2N \), while the diagonal terms of \( P_k \) are doubly degenerate, and the non-zero off-diagonal ones are replaced either by the (bond-dependent) negative of matrix \( V_{ij} \) of Eq. (2) or that of its hermitean adjoint \( V_{ij}^\dagger \), depending on whether they are supra- or sub-diagonal \[15\]. The negative unitary elements of the (now \( 2N \times 2N \)) supradiagonal identity matrix of Eq. (3) are replaced by the bond-dependent negative of \( V_{ij} \).

In our calculations of the two-terminal DC conductance we follow the procedure described in \[16\], in which the TM of Eq. (3), with the adaptations delineated above for incorporating SO effects, is iterated and projected in such a way that the transmissivity matrix \( t \) can be retrieved \[16, 17, 18\]. From that the zero-field conductance \( g \) is evaluated by the Landauer formula \[18, 19\]

\[
g = \text{Tr} \ t t^\dagger = \sum_{i,j} |t_{ij}|^2,
\]

(6)

where the sum runs over all entry (\( j \)) and exit (\( i \)) channels.

In this scheme one considers a disordered system described by Eq. (1), with \( N \) sites across and length \( M \) sites, connected to pure leads at both ends (that is, where all \( \varepsilon_i \equiv 0, \mu \equiv 0 \)). It is seen that Eq. (6) gives the total conductance, i.e., considering both spin directions. The methods of \[16\] were used to evaluate the probability distribution of the total conductance \[20, 21, 22, 23\], at the metal-insulator transition for 2D systems with SO couplings.

For spin-dependent properties one considers the partial conductances \( g_{\sigma\sigma'} \), where

\[
g_{\sigma\sigma'} = \sum |t_{\sigma\sigma'}|^2,
\]

(7)

with \( t_{\sigma\sigma'} \) being the transmission coefficient from the left lead with spin \( \sigma' \) to the right lead with spin \( \sigma \) \[24, 25\]. The sum runs over all such pairs of channels with fixed \( \sigma, \sigma' \).
3. Numerics

3.1. Introduction

For numerical implementation of the procedures just outlined, here we take the energy $E = 0$, corresponding to the Fermi energy of a non-disordered system with $W = \mu = 0$. At $E = 0$, $\mu = 2.0$ the critical disorder for the metal–insulator transition on a square lattice is estimated as $W_c = 8.55 (5)$ \cite{10}.

For the spinless case treated in \cite{16} one starts with a plane wave-like state propagating to the right along the $x$ direction, incident on the left boundary of the sample. For example, with the notation given in Eq. (4), $a_{i0}^\uparrow = 1; a_{i1}^\uparrow = e^{ik_x}, i = 1, \ldots, N$ where the lattice parameter is taken as unitary. In practice one finds that final results for the conductance do not depend strongly on the precise value of $k_x$, as long as it is not too close to zero. In some cases, e.g., when free boundary conditions across the strip must be obeyed \cite{24, 25}, a transverse wavevector $k_y$ is included. This is generally made of order $1/N$, as the zero-field conductance of interest depends mostly on the lowest-lying vacant states close to the Fermi energy $E_F$. Here, $k_y$ can be set to zero since we only consider periodic boundary conditions in the transverse direction.

In what follows, for each set of $E$, $\mu$, and $W$ studied we take $N_s = (1 - 5) \times 10^5$ independent realizations of disorder, which enables us to obtain smooth curves for the distributions of conductances and associated quantities.

3.2. Unpolarised beams

In order to make contact with extant results, initially we consider a system in a square geometry with $N = 40$ at $E = 0$, $W = W_c$ and evaluate the probability distribution function $P(g)$ for the total conductance $g$, as well as the $P(g_{\sigma\sigma'})$ for the partial ones. The plane wave-like incident states used are straightforward adaptations of those given for the spinless case, with the spinors of Eq. (5) having equal components, i.e., $a_{i0}^\uparrow = a_{i0}^\downarrow$ and similarly for the $a_{i1}^\uparrow, a_{i1}^\downarrow$. So in this case the incident beam is fully spin-unpolarised.

Fig. 1 shows $P(g)$, $P(g_{++})$, and $P(g_{+-})$. Data for $P(g)$ are compressed (stretched) along the horizontal (vertical) axis to account for the doubling in number of transmission channels for this case, compared to the fixed-spin ones. The curve for $P(g)$ is in very good quantitative agreement with that given in Fig. 3 of \cite{22}. Qualitatively, its most salient feature is the steep drop around $g = 2$, reflecting the one dimensional-like character of the incipient percolating cluster at the transition \cite{22}. $P(g_{++})$ and $P(g_{+-})$ are identical within simulational fluctuations; as we shall see below, this occurs for strong SO coupling, but is not verified as these interactions become weaker. Also, $P(g_{--})$ and $P(g_{-+})$ (not shown) coincide, respectively, with $P(g_{++})$ and $P(g_{+-})$, which is in line with the symmetry of the Hamiltonian, and of the input vectors. While $P(g)$ is the convolution of the $P(g_{ab}), a, b = \pm$, the only significant difference between (the properly scaled shape of) the former and any of the latter is the steep drop referred to above, which is rather rounded off for the $g_{ab}$. This follows from the relatively high degree of
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Figure 1. Probability distributions for total \(g\) and partial \((g_{++}, g_{+-})\) conductances of system with \(M = N = 40\) sites for energy \(E = 0\), at the metal-insulator transition point with \(\mu = 2.0, W = 8.55\), see Eqs. (1) and (2). \(N_s = 5 \times 10^5\) independent samples.

mutual correlation among the \(g_{ab}\), via the association of each individually occurring set of those with the same realization of quenched disorder.

Away from the metal-insulator transition point, the conductance distributions in the conducting phase are expected to be Gaussian \([21, 26]\).

Still with \(E = 0, \mu = 2.0\) we took \(W = 3\), well within the metallic phase. Then, keeping \(W\) fixed we lowered the SO coupling by an order of magnitude, making \(\mu = 0.2\). For this \(\mu\) the critical disorder at the centre of the unperturbed band is \(W_c \approx 5.3\). The results for the \(g_{ab}\) are displayed in Fig. 2 confirming to a very good extent the Gaussian nature of such quantities. Denoting ensemble averages by \(\langle \cdots \rangle\) and with the cumulants \(C_n \equiv \langle (g_{ab} - \langle g_{ab} \rangle)^n \rangle\), the dimensionless skew \([27]\) \(S \equiv C_3/C_2^{3/2}\) of all curves shown in the Figure is only slightly positive, never exceeding 0.2.

While for \(\mu = 2.0\) all four curves coincide just as at the metal-insulator transition, there is a split between the spin-conserving and spin-flipping groups at \(\mu = 0.20\) where the SO effects are weaker. For the lower \(\mu\) the peaks of the \((+-), (-+)\) group are located at a value of \(g\) some 3.7\% less than those of \((++), (--)\). For comparison, for \(\mu = 2.0\) the (non-systematic) spread among the peak locations for all four distributions is of order 0.3\%.

We have checked that close to the metal-insulator transition for \(\mu = 0.2\), the partial conductance distributions split into two groups in the same manner as the metallic-state data of Fig. 2 (though assuming a non-trivial shape rather similar to that exhibited in Fig. 1 for \(\mu = 2.0\)).
Figure 2. Probability distributions for partial conductances \( g_{ab} \), \( a, b = \pm \) of system with \( M = N = 40 \) sites for energy \( E = 0, W = 3.0 \), with \( \mu = 0.20 \) (leftmost curves) and 2.0, see Eqs. (1) and (2), both in the metallic phase. \( N_s = 10^5 \) independent samples for each case.

3.3. Spin-polarised beams

When attempting to represent unbalanced (i.e., spin-polarised) mixtures of plus and minus spins with the methods of [16], the following procedures may be devised in order to set a specific incoming polarisation: either (i) impose a constraint on the input state vectors, see Eqs. (3) and (5), or (ii) suitably modify the Hamiltonian Eq. (1) while keeping the input vectors unconstrained.

In the following we consider each of these possibilities in turn.

3.3.1. Constraining input states

One can set up an incident beam with a given polarisation \( \mathcal{P} \geq 0 \) by writing the spinors of Eq. (5) as:

\[
\begin{pmatrix}
a_{i0}^\uparrow \\
a_{i0}^\downarrow 
\end{pmatrix} = \begin{pmatrix} a_0 \sqrt{(1 + \mathcal{P})/2} \\ a_0 \sqrt{(1 - \mathcal{P})/2} \end{pmatrix}, \quad i = 1, \ldots, N.
\]

The \( a_{i1}^\uparrow, a_{i1}^\downarrow \) follow by adding the phase factor \( e^{ikz} \) to the \( a_{i0}^\uparrow, a_{i0}^\downarrow \).

This is a straightforward adaptation, to the quantum context, of the procedures used in the classical problem of directed flow with exclusion to simulate injection of a spin-unbalanced particle beam [5].

The time-reversal symmetry of the Hamiltonian Eq. (1) means that in terms of the incoming concentrations \( x_{\pm}^{\text{in}} = (1 \pm \mathcal{P})/2 \), and their outgoing counterparts \( x_{\pm}^{\text{out}} \),
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Figure 3. Scaled probability distributions, see Eq. (9), for partial conductances $g_{ab}$, $a,b = \pm$ of system with $M = N = 40$ sites for energy $E = 0$, at the metal-insulator transition point with $\mu = 2.0$, $W = 8.55$, see Eqs. (1) and (2), and incoming polarisations $\mathcal{P} = 1/4$, $1/2$, and $3/4$. $N_s = 3 \times 10^5$ independent samples for each case.

one has $x_{\text{out}} = x_{\text{in}}$, i.e., the average polarisation is conserved [18]. Thus, the channel-specific conductances $g_{ab}$ will be modulated by the respective incoming and outgoing concentrations $x_b$, $x_a$.

At the critical point of the metal-insulator transition with strong SO coupling $\mu = 2.0$, the resulting picture is similar to that for unpolarised incoming beams, once the modulation effects just referred to are incorporated.

For given $x_+$ one has the following relationship for the associated probability distributions:

$$\frac{P(g_{ab})}{x_a x_b} = f(g_{ab} x_a x_b),$$

where $f(u)$ is the same function of the generic variable $u$ for all combinations $a,b = \pm$. This generalizes the results displayed for $x_+ = x_- = 1/2$ in Fig. 1.

Furthermore, as illustrated in Fig. 3 at this point we have the same $f(u)$ also for all $x_+ \in [1/2, 1)$ (as $x_+ \to 1$ the methods of [16] run into numerical difficulties related to the existence, in the matrices involved, of lines full of vanishing elements; so we leave the full-polarisation case out of our considerations).

The $\mathcal{P} = 0$ $g_{ab}$ curves, of which those for $g_{++}$ and $g_{+-}$ are depicted in Fig. 1, also coincide with those of Fig. 3 when scaled by the common factor $x_+ x_- = 1/4$. The same is not true, however, of the $\mathcal{P} \neq 0$ probability distributions for $P(g)$, which cannot be brought into a good collapse with the $\mathcal{P} = 0$ one by the use of a single factor analogous...
Figure 4. Scaled probability distributions, see Eq. (9), for partial conductances $g_{ab}$, $a, b = \pm$ of system with $M = N = 40$ sites for energy $E = 0$, $W = 3.0$, with $\mu = 0.20$ (leftmost curves) and 2.0, see Eqs. (1) and (2), both in the metallic phase, and incoming polarisation $P = 3/4$. $N_s = 10^5$ independent samples for each case.

to the $\{x_a x_b\}$. This is of course because, for fixed $P$, the unscaled $g_{ab}$ which add up to $g$ can have widely differing ranges of variation, the more so as $P$ increases.

In the metallic phase, for ease of comparison with the cases considered in Sec. 3.2 we took $P = 3/4$, $E = 0$, $W = 3$, and both $\mu = 2.0$ and 0.2 . The scaled results, following Eq. (9), are shown in Fig. 4 and are identical within simulational fluctuations to those for $P = 0$ of Fig. 2 provided that the latter are scaled by the common factor $x_\pm x_{\pm} = 1/4$.

3.3.2. Effect of external field One can modify the Hamiltonian Eq. (1) to add spin-dependent energies, e.g., by introducing an external magnetic field as done in [24] in a similar context. Analysis of level-spacing statistics has shown that, upon application of such field, the universality class of the problem changes from the Gaussian symplectic ensemble to that of the Gaussian unitary ensemble [24]. This is to be expected from symmetry considerations [28]. On the other hand, conservation of average polarisation is now not guaranteed since time-reversal symmetry has been broken by the magnetic field [18].

In this way, at energy $E$ there are more open propagation channels ($\varepsilon_i(\sigma) > E$) for one spin species than for the other. Again, at least two possible implementations can be suggested: (i) a field acting only on the left lead [24], or (ii) a spin-dependent chemical potential acting on every site of the sample. For simplicity here we stick to option (i).
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Figure 5. Probability distributions for total \((g)\) and partial \((g_{ab})\) conductances of system with \(M = N = 20\) sites for energy \(E = 0\), in the conducting phase with \(\mu = 2.0\), \(W = 3.0\), and \(\Delta = 3.75\). \(N_s = 10^5\) independent samples.

With \(\varepsilon_i^0\) being the self-energy of an orbital on the left lead in the absence of field, we establish our Zeeman-like energy origin such that \(\varepsilon_i(+) = \varepsilon_i^0\), \(\varepsilon_i(-) = \varepsilon_i^0 + \Delta (\Delta > 0)\), so propagation of plus spins is favored. As the unperturbed single-electron band spans the interval \(-4 \leq E \leq 4\) in the square-lattice geometry, we usually take \(1.0 \lesssim \Delta \lesssim 4.0\) so the incoming beam exhibits a significant spin imbalance.

In this Section we always take the incoming beams as fully spin-unpolarised, in the manner of Sec. 3.2 above. Thus any resulting polarisation is driven by the Zeeman-like gap \(\Delta\).

In what follows we specialize to the conducting phase, where the shape of conductance distributions is in general close to Gaussian [21, 26]. In this context the central estimates, denoted by \(\langle \cdots \rangle\), and error bars given for conductances and related quantities below correspond, respectively, to mean value and RMS deviation of the associated distributions.

We start by making \(\Delta = 3.75\). Figs. 5 and 6 show the distributions for total and partial conductances, and should be compared, respectively, with the rightmost and leftmost groups of Fig. 2 which both correspond to \(\Delta = 0\). For \(\mu = 2.0\) (Fig. 5) channel asymmetry is manifest in that there is a grouping of distributions by exiting channels, respectively for majority \([(+, +)\) and \((+, -)\)] and minority \([-,-) and (-, +)\] spins, while for \(\Delta = 0\) all four distributions coincide. Note that this is not the same pairing exhibited by the \(\mu = 0.2\) curves in Fig. 2 where one has \([(-, +)\) and \((-,-)\)] and \([(+, +)\) and \((-,-)\)]], both due to up-down symmetry.
Figure 6. Probability distributions for total ($g$) and partial ($g_{ab}$, with $a, b = \pm$) conductances of system with $M = N = 20$ sites for energy $E = 0$, in the conducting phase with $\mu = 0.2$, $W = 3.0$, and $\Delta = 3.75$. $N_s = 10^5$ independent samples.

For $\mu = 0.2$ (Fig. 6) all four channels are fully split, as up-down symmetry is now absent. However, a tendency towards the same grouping of Fig. 5 still holds.

The polarisation $P$ of the exiting current can be evaluated [25] as

$$P = \frac{g_{++} + g_{+-} - (g_{--} + g_{-+})}{g_{++} + g_{+-} + g_{--} + g_{-+}},$$

(10)

see Eq. (7).

In Fig. 7 the probability distributions for $P$ are shown, for systems with fixed width and varying aspect ratios $M/N$. The distributions broaden out as the system becomes more wire-like, and develop a more pronounced negative skew. On the other hand the position of their peak value remains essentially unchanged. So, despite the Hamiltonian not being invariant under time reversal, we see indications that polarisation of the beam is conserved in this case. We defer a more thorough discussion of this point to Sec. 4.

While Fig. 7 is for $\mu = 0.2$, we have found qualitatively very similar outcomes for larger $\mu$, including the stability of the peak location for $P(P)$ against varying $M$. Having this in mind, we kept $M = 10$ fixed and varied several other parameters. In this way we are reasonably sure to be retaining the main qualitative features of the quantities under study, while the spread of distributions is kept lower than for larger $M$.

Fig. 8 shows, for fixed $\Delta = 3.75$, the variation of the average exiting polarisation $\langle P \rangle$, and total conductance $\langle g \rangle$, against the intensity $\mu$ of SO coupling. The maximum exhibited in panel (a) for $\mu \approx 0.75$ illustrates the competition between single-channel conduction with species segregation (which dominates in the low-$\mu$ region) and processes...
including many SO-induced spin flips (characteristic of large $\mu$). The $\mu$-interval where neither process is the clear winner allows the emergence of a larger polarisation. Note however that the difference between minimum and maximum values of $\langle P \rangle$ is only some 30% of the largest, on account of the largish value of $\Delta$. On the other hand, panel (b) shows that $\langle g \rangle$ is monotonically increasing with $\mu$, that is, SO effects lead to higher total conductance for fixed $\Delta$.

The leftmost points of panel (a), (b) of Fig. 8 correspond to $\mu = 0.01$ which most probably is in the insulating phase; approximate calculations indicate that for $W = 3.0$ the metal-insulator boundary lies at $\mu \approx 0.06$. Even so, such point in $(W, \mu)$ space would have an associated localization length much larger than the current system’s size. Thus we believe it is justifiable to present data concerning this point together with those unequivocally belonging in the conducting phase.

Panel (a) of Fig. 9 shows the increase of $\langle P \rangle$ against increasing $\Delta$ (which is expected at least for $1 \leq \Delta \leq 4$, along which interval up- and down-spin subbands display significant overlap around $E = 0$), for $\mu = 0.01, 0.2$, and 2.0. In panel (b) of the same Figure, for $\mu = 0.01$ one has $g \approx g_{++} + g_{--}$. So the separation between the corresponding curve and those for larger $\mu$ indicates the strength of the contribution of SO interactions to conductance, when compared to that from single-channel processes. For $\mu = 2.0$ one sees that the former effect amounts to between 35% and 80% of the latter (respectively at $\Delta = 1.0$ and 4.0).
Figure 8. For $E = 0$ with $W = 3.0$, $\Delta = 3.75$, and varying $\mu$, panel (a) shows average exiting polarisation $\langle P \rangle$ at right end, and (b) gives average total conductance $\langle g \rangle$, of systems of fixed width $N = 20$, length $M = 10$ sites. All for $N_s = 10^5$ independent samples.

Figure 9. For $E = 0$ with $W = 3.0$, panel (a) shows average exiting polarisation $\langle P \rangle$ at right end, and (b) gives average total conductance $\langle g \rangle$, of systems of fixed width $N = 20$, length $M = 10$ sites against varying $\Delta$. Blue circles: $\mu = 0.01$; red squares: $\mu = 0.2$; black crosses: $\mu = 2.0$. All for $N_s = 10^5$ independent samples.
We now turn to cases in which the effects of site disorder are suppressed. Still with $E = 0$ and $\Delta = 3.75$ we took $W = 10^{-5}$. Since the only other significant parameter in Eq. (11) is $\mu$, which we considered to be 0.2 and 2.0, this value of $W$ is essentially zero for practical purposes here. We focused on the evolution of $P(P)$ for systems of width $N = 20$ sites across, and lengths $M = 10, 20,$ and 40. The picture for $\mu = 2.0$ was qualitatively and quantitatively very similar to that given in Fig. 7 for $W = 3.0, \mu = 0.2$: peak positions and RMS widths respectively $0.54 - 0.55$ and $0.04 - 0.06$ ($W = 10^{-5}, \mu = 2.0), 0.54 - 0.56$ and $0.08 - 0.12$ ($W = 3.0, \mu = 0.2$).

On the other hand, for weak SO couplings $\mu = 0.2$, as shown in Fig. 10, it is seen that for this combination of parameters the system can function as a spin filter [25], with the beam polarisation increasing as it propagates. Quantitatively, $\langle P \rangle (M = 40) = 0.774(14), \langle P \rangle (M = 10) = 0.741(8)$. So, although the error bars extend about halfway between the two averages, the trend against increasing $M$ is clear. Taking strong SO coupling $\mu = 2.0$, the spin-filter effect becomes essentially undiscernible: one gets $\langle P \rangle (M = 40) = 0.541(75), \langle P \rangle (M = 20) = 0.540(65), \langle P \rangle (M = 10) = 0.541(55).

In this region of parameter space it is easy to capture the decay of the spin-spin correlation function $F_{zz}(L)$

$$F_{zz}(L) = \langle \sigma^z(0) \sigma^z(L) \rangle,$$  

which is the conditional probability to find an electron with spin $\sigma^z$ at $x = L$, for an
incident electron at $x = 0$ with $\sigma^z = \pm 1$. In terms of the $g_{\sigma\sigma'}$ of Eq. (7), this is:

$$F_{zz} = \frac{1}{2} \left\langle \frac{g^{++} - g^{--}}{g^{++} + g^{--}} + \frac{g^{--} - g^{++}}{g^{--} + g^{++}} \right\rangle.$$  (12)

The spin relaxation length $\Lambda_s$ is defined by assuming an exponential decay for the correlation function, $F_{zz}(L) \propto \exp(-L/\Lambda_s)$. Fig. 11 displays data for $E = 0$, $\Delta = 3.75$, $W = 10^{-5}$, $\mu = 0.2$, from which a fit to the above expression gives $\Lambda_s = 22(2)$. Of course this is intended mostly for illustration, since here one has only three data points. Nevertheless, analysis of such semi-quantitative results can prove enlightening. For example, keeping the same set of parameters and system sizes but making $W = 3.0$ gives $\Lambda_s = 9.0(2)$; if one then keeps $W = 3.0$ and makes $1.0 \leq \Delta \leq 4.0$, $\Lambda_s$ remains within 10% of that. However, for strong SO coupling $\mu = 2.0$, spin relaxation takes place at very short distances even for very low site disorder. In this case, already for $M = 10$ the distributions of $F_{zz}(M)$ remain essentially centred around zero for all sets of physically plausible parameters used here.

4. Discussion and Conclusions

We have studied model tight-binding Hamiltonians for the description of electron transport in the presence of SO couplings, especially in connection with spin-dependent properties.
In Sec. 3.2 we established the properties of the spin-dependent (partial) conductances defined in Eq. (7), in the simple instance of unpolarised incident beams. We considered the cases of weak and strong SO interactions, respectively $\mu = 0.2$ and 2.0. Recalling that in the absence of SO coupling and in zero external field the spin-switching conductances $g_{+-}$, $g_{-+}$ would both vanish, we saw that the separation of spin-switching channels from the non-spin-switching ones $g_{++}$, $g_{--}$ is gradually erased as the magnitude of SO interactions is increased. This is illustrated in Fig. 2 by the contrasting behaviour of the $\mu = 0.2$ and $\mu = 2.0$ families of curves.

In Sec. 3.3 we examined two distinct procedures which are designed to produce spin-polarised incident beams. In Sec. 3.3.1 we imposed spin-dependent amplitudes on the wavefunctions inciding on the left boundary of the system, see Eq. (8). This corresponds to a straightforward generalization of well-known procedures used in variants of the classical problem of directed flow with exclusion, which include conditional allowance of site double-occupation (mimicking the Pauli principle) [5]. Overall, we found that the effect of using such constrained input vectors amounts to a modulation of the channel-specific conductances by the respective incoming and outgoing polarisations, the latter being predicted to equal the former on the basis of the time-reversal symmetry of the Hamiltonian [15]. Though numerical data are doubtless compatible with such conservation, compare Figs. 3 and 4 respectively with Figs. 1 and 2, it is not clear at this point how one might extract additional physical insight from the resulting picture.

We recall from [5] that the classical model studied there, where SO effects are mimicked by so-called ”spin-flipping” sites, always exhibits polarisation decay against distance. This would be in line with entropic interpretations of a spin-flipping agent contributing towards equalising spin populations in an initially spin-ordered beam. So one sees that the symmetries imbedded in the quantum-mechanical formulation used here are enough to counteract any such trend, even though the initial beams are prepared in as close a manner as possible in either case.

In Sec. 3.3.2 we included a Zeeman-like term in the Hamiltonian, acting only on the left lead [24], while keeping the incoming beams fully spin-unpolarised. This is the simplest way to induce an up-down spin asymmetry, and bears a qualitative resemblance to the procedure of Sec. 3.3.1 in that it is a local change limited to the incidence edge.

Removing up-down symmetry has the following effects on the $g_{ab}$ distributions. Firstly, for strong SO couplings ($\mu = 2.0$), the four sets of data which coincide for $\Delta = 0$, see the rightmost curves of Fig. 2, now split according to exiting channel. In Fig. 5 the coinciding distributions for $g_{-+}$ and $g_{--}$ are concentrated at low values of $g$, while those for $g_{++}$ and $g_{+-}$ have their peak for a higher $g$. This of course reflects the positive bias given by $\Delta$. Secondly, for the weak SO value $\mu = 0.2$ the partial split seen in the leftmost curves of Fig. 2 is now complete, and four distinct curves are seen in Fig. 6. In summary, weakening SO effects always tends to split channel-specific conductance distributions; only, with an applied field there is an additional splitting effect due to energetics.

On the other hand, the strength of SO couplings has a subtle effect on the exiting
polarisation $\langle P \rangle$, captured in panel (a) of Fig. 8. The maximum exhibited by $\langle P \rangle$ against varying $\mu$ shows that the optimum conditions for that are a mix of single-channel conduction with species segregation and processes involving many SO-induced spin flips (which dominate, respectively, for low and high $\mu$). It can be estimated from panel (b) of Fig. 8 that, for $\Delta = 3.75$ and $\mu = 2.0$, the contribution of SO effects to the conductance amounts to some 75% of that originating from single-channel processes. In the range $1 \leq \Delta \leq 4$ this varies between 35% and 80%, see panel (b) of Fig. 9.

Some further features can be unveiled when the limit of very low site disorder is considered, together with weak SO couplings. For $W = 10^{-5}$, $\mu = 0.2$, Fig. 10 shows that, for large $\Delta = 3.75$ the exiting polarisation actually increases the longer the system length $M$ is (at least for $10 \leq M \leq 40$ with width $N = 20$, which spans the aspect-ratio change from slablike to wirelike). Thus the system works as a spin filter [25]. On the other hand, keeping other parameters fixed and increasing the SO couplings to $\mu = 2.0$, the spin-filter effect becomes undetectable (see Sec. 3.3.2).

Still for $\mu = 0.2$ but with $W = 3.0$, as illustrated in Fig. 7 (i) the average values $\langle P \rangle$ fluctuate by some 2 – 3% with no systematic variation against $M$, and (ii) the error bars are larger than said fluctuations between averages (and much broader than the corresponding ones for $W = 10^{-5}$). So we conclude that in this case no evidence is discernible of a spin-filtering effect. As stated in Sec. 3.3.2 keeping $W = 3.0$ and making $\mu = 2.0$ the final result for polarisations is very similar to that for $\mu = 0.2$.

Recall that the spin-dependent, field-like, parameter $\Delta$ added to the Hamiltonian in Sec. 3.3.2 breaks time-reversal symmetry. So there is no guarantee that results pertaining to that Section should exhibit conservation of spin polarisation [18]. Nevertheless, we have found for moderately strong site disorder $W$, and for both weak and strong SO couplings, that the average spin polarisation is kept constant along significant distances within the system (though of course, variations associated with a very large characteristic length cannot be ruled out). Moreover, in the special case of low site disorder and weak SO interactions, we have evinced spin-filter behaviour (see Fig. 10), with spin polarisation increasing with distance from the injection edge. In contrast with the results for the classical model of [5], we have not found combinations of parameters which present spin polarisation decaying with distance.

By investigation of the spin-spin correlation function [8], as illustrated in Fig. 11 one can extract significant information on the characteristic length $\Lambda_s$, at least for low ($W = 10^{-5}$) and moderate ($W = 3.0$) site disorder, provided the SO coupling is weak. For strong SO interactions correlation decay takes place over short distances, comparable to the lattice spacing.

It would then appear that the polarisation results for the classical process studied in [5], and their always-decaying behaviour against distance, find a closer qualitative correspondence here with the properties of the correlation function, rather than those of its namesake.
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