Quantum Monte Carlo simulation for the spin-drag conductance of the Hubbard model

Kim Louis and Claudius Gros
Fakultät 7, Theoretische Physik, University of the Saarland, 66041 Saarbrücken, Germany
E-mail: louis@lusi.uni-sb.de

New Journal of Physics 6 (2004) 187
Received 27 July 2004
Published 6 December 2004
Online at http://www.njp.org/
doi:10.1088/1367-2630/6/1/187

Abstract. In the situation of two electrostatically coupled conductors, a current in one conductor may induce a current in the other one. We will study this phenomenon, called Coulomb drag, in the Hubbard chain where the two 'conductors' are given by fermions with different spin orientations. With the aid of a Monte Carlo approach, which we presented in a recent paper, we calculate the trans-conductance in different variants of the Hubbard chain (with/without impurity and additional (long-ranged) interactions) for different fillings.

Contents

1. Introduction 2
2. Definition of the spin drag in the Hubbard model 3
3. Description of the MC method 4
4. Numerical results 5
   4.1. Trans-conductance in the Hubbard model 5
   4.1.1. Comparison with the Hubbard model 5
   4.1.2. Numerical simulations 6
   4.2. Magnetic impurity 7
   4.3. Zig-zag chain 10
5. Conclusion 12
Appendix. Spin-dependent interaction—broken spin-rotational invariance 13
References 15
The Coulomb-drag effect describes how two conductors (only coupled by the Coulomb force) may influence each other. Since the Coulomb repulsion is relatively small, a sizeable effect will only arise when the two conductors are very close to each other. This condition may be met either in mesoscopic systems—where, with the advent of new technologies (e.g., carbon nanotubes), the problem of Coulomb drag has attracted considerable interest (see, e.g., [1]–[4])—or in the spin-drag problem. Instead of considering two conductors, one may look at drag effects between different fermion species, e.g., fermions with different spin orientations. Since fermions with different spins are not spatially separated, there is a large Coulomb force between them which can lead to all kinds of correlation effects, e.g., a drag effect. In the last few years, the interest in spin-dependent transport increased. One key problem is the generation of a spin-polarized current, i.e., a current where only fermions with one of the two spin orientations flow. In this context, it is important to keep in mind that the spin-polarized current may affect the fermions with the opposite spin orientation. Hence, the drag effect may play here a crucial role even though it is, experimentally, not directly accessible. (This is because the driving potentials are, in general, not spin-dependent.)

For this ‘spin-drag’ problem, the trans-resistivity of higher-dimensional systems has been investigated in previous publications, e.g., using the Boltzmann equation [5] or the random-phase approximation [6]. In this paper, we focus on trans-conductance for the Hubbard model. While most authors used a bosonization approach to compute the conductance [7, 8], we will use here, for the study of the trans-conductance, a Monte Carlo (MC) method we introduced in a recent paper [9]. The strategy we followed there was to map our fermion system via the Jordan–Wigner transformation to a spin system which can be analysed by efficient though standard MC techniques. We will now extend this method to the one-dimensional Hubbard model concentrating on the question how a spin-polarized current (driven by a voltage drop which is assumed to be spin-dependent) affects the fermions with opposite spin orientations.

In section 2, we present the model and give some central definitions for the spin-drag problem. Section 3 contains the technical details on the subject of MC simulations. The MC method of our choice [9, 10] was a variant of the stochastic series expansion (SSE) as introduced in [11]–[14]. This method allows an investigation of the one-dimensional Hubbard model [15, 16].

In section 4.1, we present our results for the standard Hubbard model and compare then with analytical predictions from bosonization theory. To obtain a spin-polarized current we add in section 4.2 an impurity to the system, which acts like the combination of a one-site chemical potential and a one-site magnetic field. We show that such a ‘magnetic’ impurity can produce the desired spin-polarized current.

The Hubbard model can also be mapped to a spinless-fermion ladder. Hence, our results may also describe that situation, but there one might argue that the very specific modelling of the Coulomb (on-site) interaction in the Hubbard model is unrealistic (and may differ from other approaches, e.g., [1]–[4]). We therefore discuss two variants (with additional interaction terms) of our model. Firstly, we will discuss in section 4.3 a situation where fermions with different spins live on different sites. The full system has the geometry of a zig-zag chain. Secondly, we show in the appendix that a spin-polarized interaction leads to equal cis- and trans-conductance. This is similar to the ‘absolute’ drag result found, e.g., in [3].
2. Definition of the spin drag in the Hubbard model

Our model Hamiltonian is the standard Hubbard model (with \( N \) sites or atoms)

\[
H_{\text{Hubb}} = t \sum_n \sum_{\sigma = \uparrow, \downarrow} \left( c_{n,\sigma}^\dagger c_{n+1,\sigma} + c_{n+1,\sigma}^\dagger c_{n,\sigma} \right) - \mu \sum_n n_{n,\sigma} + U \sum_n n_{n,\uparrow} n_{n,\downarrow},
\]

(1)

where \( n_{n,\sigma} \) is the occupation number of fermions with spin \( \sigma \) at site \( n \) and \( c_{n,\sigma}^\dagger \) is the corresponding annihilation (creation) operator. To perform our transport calculations, we will use the approach from [9]. Since the hopping term does not connect fermions with different spins, it is natural to consider current and potential operators for each spin orientation separately. Following [9], the potential operators then read (\( e \) being the charge unit and \( x \) the position of the voltage drop):

\[
P_{\downarrow}^\dagger = e \sum_{n > x} n_{n,\downarrow}, \quad P_{\uparrow}^\dagger = e \sum_{n > x} n_{n,\uparrow}.
\]

The conductance (of a spinless-fermion chain) is the linear response of one potential operator to another; therefore, the explicit form of the current operators is not needed here [9]. As we have two potentials, we can define four transport quantities (conductances) \( g_{ij} \) which describe the (linear) response of \( P^\dagger \) to \( P^\dagger \), where \( i, j \in \{ \uparrow, \downarrow \} \). Further details on how to evaluate the \( g_{ij} \)'s are to be found in section 3.

For the moment, we will discuss only symmetric models, i.e., we have spin-rotational invariance (the only asymmetric model that we will discuss appears in section 4.2); thus, we end up with only two distinct quantities. We call \( g_c := g_{\downarrow\downarrow} = g_{\uparrow\uparrow} \) the cis-conductance and \( g_t := g_{\downarrow\uparrow} = g_{\uparrow\downarrow} \) the trans-conductance.

The naming conventions come from physical interpretation of these coefficients, which is given below: if we switch on, at a certain time, a (supposedly) spin-polarized potential which acts only on spin-up fermions (i.e., we add a time-dependent perturbation of the form

\[
VP^\dagger \theta(t),
\]

where \( V \) is the voltage amplitude and \( \theta \) the Heavyside-step function), then we will find a current of spin-up fermions

\[
I^\dagger = g_c V.
\]

This is the \textit{drive} current governed by the cis-conductance, but there will also be a current of spin-down fermions

\[
I^\dagger = g_t V,
\]

the \textit{drag} current (governed by the trans-conductance). The latter may be non-zero, even though the spin-down fermions do not feel the applied potential.

The situation of a non-vanishing trans-conductance (or drag current) is called \textit{Coulomb drag}. This problem has been studied, e.g., for coupled spinless-fermion systems by bosonization in [1]–[3] and to second-order perturbation theory in [4].

Normally, (since spin-polarized potentials are not available) one is only interested in the (full) conductance of the Hubbard model, where both fermion species feel the same potential and the full current is the sum of the currents of the spin-up and spin-down fermions. It is straightforward to see that the cis- and trans-conductance directly give us the conductance of the Hubbard model through the relation

\[
g_{\text{Hubbard}} = 2(g_c + g_t).
\]

New Journal of Physics 6 (2004) 187 (http://www.njp.org/)
Figure 1. The model Hamiltonian that will be discussed in this paper. Thin solid lines indicate a full Heisenberg-like interaction between the sites and broken lines stand for sites coupled only by a $z-z$ term (Ising-like interaction). The upper part is for $U' = 0$ and the lower for $U' = U$ (other values of $U'$ are not considered). A plaquette as used in the MC scheme is indicated by thick lines.

3. Description of the MC method

Before starting with MC, we have to cast our Hamiltonian in a convenient form.

Using the Jordan–Wigner transform, the Hubbard model can be mapped to a spin ladder. To each occupation operator we introduce a spin operator, i.e., we perform replacements $n_{n, \uparrow} \rightarrow S_n^z + 1/2$ and $n_{n, \downarrow} \rightarrow S_n^z + 1/2$. If we express the Hubbard Hamiltonian with these new operators, we obtain the following spin ladder (with $2N$ sites):

$$
H = \sum_n \left[ J_x (S_n^- S_{n+2}^+ + S_n^+ S_{n+2}^-) / 2 + J_z S_n^z S_{n+1}^z + B S_n^z \right] + \sum_n \left[ U S_{2n}^z S_{2n+1}^z + U' S_{2n+1}^z S_{2n+2}^z \right],
$$

where the sites with even number represent spin-up fermions and the sites with odd numbers, spin-down fermions. (For the Hubbard model one has to put $J_z = 0 = U'$.) The parameters $J_z$ and $U'$ are used to model the spin-polarized interaction from the appendix and the zig-zag chain from section 4.3; see bottom half of figure 1. The sites $2n$ and $2n+1$ in the ladder therefore represent one atom of the Hubbard model and interact via an Ising interaction representing the Coulomb force (see figure 1). The hopping amplitudes satisfy $J_x = 2t$, and the strength of the magnetic field $B$ in equation (2) is obtained from the chemical potential through the relation $B = U/2 + U'/2 - \mu$. Half-filling corresponds therefore to $B = 0$. The two potential operators $P_{x, i}^\dagger$ introduced in the previous section can be related to potential operators for the two chains ($e$ being the charge unit)

$$
P_{x, i}^\dagger = e \sum_{n > x} S_{2n+1}^z, \quad P_{x}^\dagger = e \sum_{n > x} S_{2n}^z.
$$

Then, we may obtain the four conductances $g_{ij}$ introduced in the previous section by computing ($i, j \in \{\downarrow, \uparrow\}$)

$$
g_{ij}(\omega_M) = -\omega_M / \hbar \int_0^{\hbar \beta} \cos(\omega_M \tau) \langle P_{x, i}^\dagger P_{y, j}^\dagger(i\tau) \rangle \, d\tau
$$

at the Matsubara frequencies $\omega_M = 2\pi M(\beta \hbar)^{-1}$, $M \in \mathbb{N}$, and then extrapolating to $\omega = 0$. (The extrapolated value should not depend on $x$ or $y$ [9]. We chose $x = N/2 = y - 1$.) For

New Journal of Physics 6 (2004) 187 (http://www.njp.org/)
the extrapolation from \( g(\omega_M) \) to \( g(\omega = 0) \), we will use a quadratic fit from the first three Matsubara frequencies. (We will use open boundary conditions (OBCs) instead of periodic boundary conditions (PBCs).) Since the Hamiltonian contains Heisenberg-like interactions as well as Ising-like interactions, it is advantageous to use the stochastic cluster series expansion (SCSE) introduced in [10]. For the Hubbard model, the SCSE gives essentially the same update scheme as the one used in [16]. We will explain it now shortly.

Following [10], we split the Hamiltonian according to
\[
H = \sum_{\mathcal{h} \in \mathcal{h}} h(P),
\]
but this time into four-site clusters, called plaquettes (see figure 1). The following operators belong to the plaquette \( P \) (containing interactions between the sites \( 2n, 2n + 1, 2n + 2 \) and \( 2n + 3 \)):
\[
\begin{align*}
    h_{P}^{(1)} &= J_x S_{2n}^+ S_{2n+2}^- / 2, \\
    h_{P}^{(2)} &= J_x S_{2n}^- S_{2n+2}^+ / 2, \\
    h_{P}^{(3)} &= J_x S_{2n+1}^+ S_{2n+3}^- / 2, \\
    h_{P}^{(4)} &= J_x S_{2n+1}^- S_{2n+3}^+ / 2, \\
    h_{P}^{(5)} &= C + U/2 S_{2n}^z S_{2n+1}^z + U/2 S_{2n+2}^z S_{2n+3}^z + U' S_{2n+1}^z S_{2n+2}^z + J_z S_{2n+1}^z S_{2n+3}^z + J_z S_{2n}^z S_{2n+2}^z + B/2(S_{2n}^z + S_{2n+1}^z + S_{2n+2}^z + S_{2n+3}^z).
\end{align*}
\]
The set \( \mathcal{h} \) consists of all \( h_{P}^{(i)} \) for all plaquettes \( P \) and all \( i = 1, \ldots, 5 \).

The heart of the SCSE programme is the so-called loop update, where a spin flip of a subset (loop) of all spin variables is proposed. Since the sites with even and odd numbers form two chains, which are only coupled by a \( z-z \) interaction term, we find that the set of spin variables that will be flipped in the loop update belongs entirely to one of the chains. Therefore, we can view the new algorithm as making loop updates for each chain separately. During a loop update for one chain, the spin variables of the other chain remain fixed. The consequence of this is that, if we update, e.g., the even chain, then operators with superscript \( i = 3 \) or \( 4 \) can be neglected (as they are irrelevant for the loop construction), and the coupling terms (between the chains) reduce to magnetic field terms (for the even chain).

It is, however, advantageous to consider another variant of the loop update. The construction is similar to the first variant, but now we propose spin flips for both chains, i.e., spin variables belonging to sites \( 2n \) and \( 2n + 1 \) are flipped simultaneously. This may be viewed as a construction of two parallel loops—one for each chain. Since the two loops must be parallel, the number of possible transitions between different plaquette states is decreased. This may lead to a less efficient algorithm [13], but one should note that this parallel-loop update becomes deterministic for the case of \( B=0 \) and, hence, enhances the efficiency of the algorithm (at least for this situation) considerably.

4. Numerical results

4.1. Trans-conductance in the Hubbard model

4.1.1. Comparison with the Hubbard model. In bosonization theory, the Hubbard model is described by two boson fields \( \Phi_{\uparrow,\downarrow} \) representing the degrees of freedom of different spin orientations. The current operators for the spin sectors are then given by \( J_{\uparrow,\downarrow} \propto \partial_x \Phi_{\uparrow,\downarrow} \) [7]. The conductance can be written in the form of a current–current correlator [7] and may be evaluated in terms of the Luttinger-liquid parameters \( K_{\rho,\sigma} \) of the charge and spin field [8].

New Journal of Physics 6 (2004) 187 (http://www.njp.org/)
Figure 2. Cis- and trans-conductance (filled and open symbols) of the Hubbard model as a function of $U$ for two different $\mu$’s (200 sites, $T = 0.02t/k_B$, OBCs, $2 \times 10^5$ MC sweeps.) The (solid) arrow indicates the $U_T$ for which the charge gap (present at half-filling) satisfies $\Delta(U_T) = k_BT$. (The dotted arrow shows $U_{T/2}$ where $\Delta(U_{T/2}) = k_BT/2$ for comparison.)

$\Phi_{\rho/\sigma} = (\Phi_\uparrow \pm \Phi_\downarrow)/\sqrt{2}$. The result is (using the linearity of the correlator and the results from [17])

$$g_c = \frac{1}{2}(K_\rho + K_\sigma), \quad g_t = \frac{1}{2}(K_\rho - K_\sigma). \quad (4)$$

When $\mu = U/2$, we are at half-filling, where Umklapp processes are responsible for a gap in the system [18]. The (charge) gap $\Delta(U)$ depends on the Hubbard repulsion $U$ and is finite for all $U$.

4.1.2. Numerical simulations. We now present MC results for the trans-conductance in the Hubbard model equation (1) (or equation (2) for $U' = 0$).

We performed simulations for two different chemical potentials: Firstly, $\mu = U/2$, corresponding to half-filling and, secondly, $\mu = 0$. In the latter case, the system is no longer at half-filling, but has a $U$-dependent filling, which is shown in figure A.2 of the appendix (in the large-$U$ limit, the system reaches quarter-filling).

We show $g_c$ and $g_t$ as a function of $U$ for the two different $\mu$’s in figure 2. The figure shows that the Coulomb drag is very sensitive to a change in chemical potential.

Let us first look at the half-filled case (figure 2). If $U$ is very large, the Coulomb repulsion acts as an effective projection to those configurations satisfying $P^\dagger = -P^\dagger$. This implies that $g_c + g_t \to 0$ as $U \to \infty$. This contemplation is in accordance with figure 2. We should actually expect from equation (4) that, for $T = 0$, we have $g_c + g_t = K_\rho = 0$ because of the charge gap $\Delta(U) > 0$ for all $U > 0$ (cf [18]). This should lead to a discontinuous jump at $U = 0$, without the Coulomb force evidently $g_t = 0$ and $g_c$ is the conductance of uncoupled spinless-fermion chains from [17]. Here, we emphasize that our method is a finite-temperature method,
which means that the conductances calculated by us interpolate smoothly between the values for $U = 0$ and $\infty$. The crossover is expected to take place at that interaction value $U_T$ which satisfies $\Delta(U_T) = k_B T$. It is therefore interesting to see how $g_c, g_t$ scale with temperature. However, our method gives only access to the low-$T$ regime [9], such that we will compare here results only for two different temperatures, $k_B T = 0.01 t$ and $0.02 t$. In the two subsequent simulations for the cis-/trans-conductance, we did not find any difference at all. This implies only a weak temperature dependence (at low $T$) for the interaction $U_T$ which governs the crossover. Since $\Delta(U)$ is known from analytical results [19], we can calculate the two crossover interactions—defined by $\Delta(U_{0.02}) = 0.02 t$ and $\Delta(U_{0.01}) = 0.01 t$—finding that $U_{0.02} \approx 1.25 t$ and $U_{0.01} \approx 1.12 t$ do not differ much, as expected (they are also both indicated by arrows in figure 2).

Another important consequence of $g_c + g_t \to 0$ is that the signs of the cis- and trans-conductance are opposite or—in terms of the spin-up and spin-down currents—that the induced drag current flows in the opposite direction of the drive current [20].

Now, we will turn to the spin sector. We have $K_\rho = 1$ by spin-rotational invariance of the Hubbard model [18], implying (see equation (4)) $g_c - g_t = 1$ for all $U$, very well satisfied by figure 2.

Putting the two results for $g_c \pm g_t$ together, we obtain $g_c = 0.5 e^2/h = -g_t$ valid at high $U$. This large-$U$ limit of $g_c$ may also be computed in second-order perturbation theory. In this approximation, the Hubbard model can be mapped to a Heisenberg model. The operator (on the Hilbert space of the original Hamiltonian equation (1)) $P^\dagger_x$, which is effectively equal to $-P^\dagger_x$, is identified with the operator (on the Hilbert space of the effective Heisenberg model) $P_x = \sum_{n \geq 0} T_n^c \cdot (T_n^c = (n_{n,\uparrow} - n_{n,\downarrow})/2$ is the spin operator for fermions, here denoted by $T$ to avoid confusion with the spin operators appearing in section 3.) Applying the results from [9], computation of $g_c$ reduces then to computation of the spin conductance of the Heisenberg model, which equals $1/2$ in units of $e^2/h$.

In the case of zero $\mu$ (again figure 2) where the system is away from half-filling there is no charge gap. Hence, $K_\rho$ is finite, and so equation (4) tells us that $g_c + g_t = K_\rho$ does not decay with $U$. (Here we note that $g_c + g_t$ agrees (within error bars) with the values for $K_\rho$ available in [18].) We still have $K_\rho = 1$, which leads to $g_c - g_t = 1$ for all $U$ (again very well satisfied by the figure).

Finally, we consider the large-$U$ limit. Inserting $K_\rho(U = \infty) = 0.5$ and $K_\rho \equiv 1$ from [18] in equation (4) yields $g_c = 0.75$ and $g_t = -0.25$ (units $e^2/h$) [18]. These results are in accordance with the figure. (Note that the statistical error increases with $U$ such that we cannot compute $g(U)$ for sufficiently high $U$ in order to extract the large-$U$ limit accurately.)

4.2. Magnetic impurity

In this subsection, we will study the influence of an impurity. The modelling of the impurity follows [7], but for the spin-drag problem it is natural to consider a spin-dependent impurity, as we will do here. We extend therefore our Hamiltonian in the following way:

\[ H = H_{\text{Hubb}} + B_{\text{Imp}} H_{N/2,\uparrow}, \]

i.e., we introduce an (impurity) potential at exactly one central site (which acts only on one spin orientation, see figure 3).

Figure 4 shows cis- and trans-conductances as a function of the impurity potential $B_{\text{Imp}}$ at half-filling. (The example is chosen such that the trans-conductance in the unperturbed system
Figure 3. The model Hamiltonian with an impurity at site \( N/2 \) for \( N = 6 \) in the spin-ladder representation from the upper half of figure 1 (for \( U' = 0 \)). The site on which the impurity potential acts is encircled.

Figure 4. The cis- and trans-conductance (filled and empty symbols) as a function of the impurity strength \( B_{\text{Imp}} \) at half-filling. The impurity acts on spin-up fermions. Note that the cis-conductance for the spin-up fermions \( g_{\uparrow\uparrow} \) (▲) might differ from the one for the spin-down fermions \( g_{\downarrow\downarrow} \) (▼). The two trans-conductances are the same. The conductance of an \( xxx \) (Heisenberg) chain with one impurity (which should coincide with the large-\( U \) limit of the cis-conductance) is given for comparison. (\( \mu = U/2, U = 2t, N = 192 \) sites, \( T = 0.02t/k_B \)).

is relatively large.) The conductance of the Heisenberg chain with one impurity, which is the large-\( U \) limit of \( g_c \), is given for comparison.

Although the two cis-conductances, \( g_{\uparrow\uparrow} \) and \( g_{\downarrow\downarrow} \), could in principle differ (the model is now asymmetric) they do not in the case of half-filling at least within error bars. Both cis- and trans-conductance go—more or less linearly—to zero as the impurity strength increases.

We note that, within error bars, \( g_c = -g_t \) such that the full conductance of the system

\[
g = 2(g_c + g_t)
\]

remains zero after insertion of the impurity. Furthermore, experiments with our method at different temperatures find no sizeable \( T \)-dependence.

In the case of zero chemical potential, \( \mu = 0 \), we find a splitting of the two cis-conductances (see figure 5). This is particularly interesting since this finding implies a spin-polarized current.
Figure 5. The cis- and trans-conductance (filled and empty symbols) as a function of the impurity strength $B_{\text{Imp}}$ in the Hubbard model away from half-filling. The impurity acts on spin-up fermions. Note that the cis-conductance for the spin-up fermions $g_{\uparrow\uparrow}$ (▲) differs from the one of the spin-down fermions $g_{\downarrow\downarrow}$ (▼). The two trans-conductances are the same. ($\mu = 0$, $U = 4t$, $N = 192$ sites, $T = 0.02t/k_B$.)

If we assume a (spin-independent) driving potential of the form

$$V(P^\uparrow + P^\downarrow)$$

($V$ being the voltage amplitude), then the current is

$$I = I^\uparrow + I^\downarrow, \quad I^\uparrow = (g_{\uparrow\uparrow} + g_{\downarrow\uparrow})V, \quad I^\downarrow = (g_{\downarrow\uparrow} + g_{\uparrow\downarrow})V.$$

The average spin of a fermion in the current is therefore (using $g_{\downarrow\uparrow} = g_{\uparrow\downarrow} = g_t$)

$$S = \frac{I^\uparrow - I^\downarrow}{2I} = \frac{g_{\uparrow\uparrow} - g_{\downarrow\downarrow}}{2(g_{\uparrow\uparrow} + g_{\downarrow\downarrow} + 2g_t)},$$

different from zero (see figure 6).

An interesting problem is the question whether, for $\mu = 0$, the cis-conductance in the pure (spin-down) sector $g_{\downarrow\downarrow}$ survives or not when we increase $B_{\text{Imp}}$ to $\infty$. Note that a finite $g_{\downarrow\downarrow}$ would imply a total spin polarization, i.e., $S = -1/2$. The limit $B_{\text{Imp}} \to \infty$ of $g_{\downarrow\downarrow}$ cannot be taken directly (because of problems with the MC simulation), but here we note that there is another way to model the impurity. Instead of applying a local magnetic field on one site, one can introduce a weak link, i.e., decrease the hopping amplitude for spin-up fermions between the sites $N/2$ and $N/2 + 1$ from the initial value $t$ to $t_{\text{Imp}}^\uparrow$. These two variants of impurities behave similarly [7]. We computed the cis-conductance for the unaffected spin orientation for the model with $t_{\text{Imp}}^\uparrow = 0$ (corresponds to $B_{\text{Imp}} = \infty$) at $\mu = 0$, $U = 4t$, $N = 200$ sites. We find a value of about $(0.79 \pm 0.03) e^2 / h$. 

New Journal of Physics 6 (2004) 187 (http://www.njp.org/)
Figure 6. The negative average spin polarization ($-S$) of the induced current as a function of the impurity strength $B_{\text{Imp}}$ in the Hubbard model away from half-filling. The impurity acts on spin-up fermions. The broken curve is obtained by fitting $g_{\uparrow \uparrow}$, $g_{\downarrow \downarrow}$ and $g_{t}$ in figure 5 with an exponential ansatz and substituting these fits into the formula for $S$. ($\mu = 0$, $U = 4t$, $N = 192$ sites, $T = 0.02t/k_B$.)

The different behaviour of the cis-conductance in the (unaffected) spin-down sector at half-filling and away from half-filling may be explained as follows: Suppose $B_{\text{Imp}}$ and $U$ are large. The effect of the $B_{\text{Imp}}$ term on the fermions is that it forbids occupation of the impurity site for one of the two fermion species (in our case spin-up fermions). At half-filling, a spin-up fermion can hop from one site to another only by exchanging the site with a spin-down fermion (there are no empty sites), i.e., simultaneously with the spin-up a spin-down fermion must hop in the opposite direction and vice versa (implying $g_{c} = -g_{t}$). A fermion of a certain spin index can then only pass the impurity site if accompanied by a fermion of opposite spin (which moves in the opposite direction). Since the impurity site is forbidden for one of the two fermion species, no fermion can pass the impurity site, and both cis-conductances must go to zero.

Away from half-filling the hopping of a spin-up fermion does not necessarily require the hopping of a spin-down fermion (the spin-up fermion can hop to an empty site) and hence the impurity affects only one of the two cis-conductances.

4.3. Zig-zag chain

So far, we have dealt with a system of two fermion species, where the two species reside on the same set of sites. In contrast to this, the bosonization approaches considered mostly systems of two coupled spinless-fermion conductors. We can compare our results with that situation, if we interpret the Hubbard model as a spinless-fermion ladder. Here, one assumes that each fermion species lives on a different conductor (i.e., the two indices $(n, \uparrow)$ and $(n, \downarrow)$ are supposed to label (spatially) different sites; compare section 3 and upper half of figure 1). But one should note that, for this case, the parameter $U$ should be small (since the distance between separated conductors is large) and the Coulomb interaction should be long-ranged (not on-site as in the Hubbard model). Hence, we are led to the question how a variation in the interaction term modifies our results.
To address this question we add a new interaction term to the Hubbard model

\[ H = H_{\text{Hubb}} + U \sum_{n} n_{n,\downarrow} n_{n+1,\uparrow}. \]

This Hamiltonian corresponds to equation (2) with \( U' = U \). One can justify introducing this new interaction term if the fermion species live on different sites where each spin-down site \((n, \downarrow)\) lies between two spin-up sites, \((n, \uparrow)\) and \((n + 1, \uparrow)\). This model has therefore the geometry of a frustrated zig-zag chain as depicted in the lower half of figure 1.

One should note that this system has a total of \( 2N \) sites, \( N \) sites for each fermion species. (Although it would be useful to adopt the notion of a system with two coupled (spinless-fermion) chains, we will keep here the notation of a system of spinfull fermions.)

The results for the spin drag in this model are shown in figure 7. We discuss again two chemical potentials: one is \( \mu = U \) implying half-filling, the other is again \( \mu = 0 \). In the latter case the (mean) occupation number per site \( n_{\rho} \) is different from one half (the occupation at half-filling) and depends on \( U \). It is shown in figure 8.

One sees in figure 7 that \(|g_{c,\ell}|\) grow with the strength of the interaction. This may be explained as follows: firstly, the Coulomb interaction mediates an attractive nearest-neighbour interaction for fermions with equal spin orientation (this is a consequence of the frustration). Therefore, in a simple approximation the only effect of the Coulomb interaction is to renormalize the Luttinger-liquid parameters for the two spin sectors \( K^{\uparrow,\downarrow} \). Since the Luttinger parameter for a spinless-fermion chain increases with the strength of the attraction [8], we expect that \( K^{\uparrow,\downarrow} \) increases as \( U \) increases. Since \( K^{\uparrow,\downarrow} \) gives the conductance of one spin sector [17] (which is essentially the cis-conductance) we have that \( g_{c} \) increases with \( U \).

One may also infer from the figure that the dependence of \( g_{c,\ell} \) on a chemical-potential shift is weak. Within error bars \( g_{c} \) decreases only slightly upon shifting \( \mu \) away from half-filling.
One should note that in the limit $U = \infty$ the ground state is a spin-polarized configuration (see figure 9). For $\mu = U$ this means that all conductances are zero in the large-$U$ limit, for one spin sector is empty and the other, completely filled. In contrast to this, for $\mu = 0$ one of the two spin sectors may remain conducting. The crossover to the ordered state occurs at values of $U$ larger than $3t$ which may be seen by simulating and comparing the occupation number for different states. For $\mu = 0$, the difference in occupation (of the two spin sectors) $n_\sigma = \langle | \sum_n (n_{n,\uparrow} - n_{n,\downarrow}) | \rangle / (2N)$ is shown in figure 8; for $\mu = U$, it is zero within error bars as long as $U \leq 3t$. We conclude that, for the values of $U$ considered in figure 7, the two spin sectors have approximately the same filling.

5. Conclusion

In this paper, we discussed the spin drag for the Hubbard model at zero temperature. We found that the trans-conductance is negative—at half-filling, the Umklapp even enforces $g_c = -g_t$. In that respect, our situation is different from two coupled Tomonaga–Luttinger models as considered.
in [1]–[3] which do not incorporate Umklapp. The ‘absolute-drag’ result of the form \( g_c = g_t \) (e.g., from [3]) can only be recovered by introducing a spin-polarized interaction (see the appendix).

If we assume that a given potential is, in general, not spin-dependent, the only relevant quantity is the full conductance \( g = 2(g_c + g_t) \), which is only non-zero away from half-filling. Here, both spin orientations contribute equally to the current. However, the situation changes when we add a magnetic impurity. Even if the driving potential is still spin-independent, the resulting current will be (partially) spin-polarized, if we are away from half-filling. In the limit of a large impurity potential, the current will be fully spin-polarized.

### Appendix. Spin-dependent interaction—broken spin-rotational invariance

In the Hubbard model, cis- and trans-conductance have opposite sign, in sharp contrast to the bosonization results (for coupled spinless-fermion chains), where cis- and trans-conductance are both positive. The discrepancy may come from a different modelling of the interaction. In the bosonization approaches, each chain is given by an interacting system (i.e., the Luttinger-liquid parameter \( K \) may differ from unity), while, in the Hubbard model, each spin sector is represented by a non-interacting fermion system. In this appendix, we will show that a spin-polarized interaction leads to a positive trans-conductance as found in the bosonization approaches. To this end, we will now discuss the following variant of our Hamiltonian:

\[
H = H_{\text{Hubb}} + \sum_{n,\sigma} J_z \left( n_{n,\sigma} - \frac{1}{2} \right) \left( n_{n+1,\sigma} - \frac{1}{2} \right). \tag{A.1}
\]

Here, the new \( J_z \) term breaks the spin-rotational invariance. Hence, \( K_{\sigma} \) may now be different from unity.

Firstly, we consider the large-\( U \) limit at half-filling. The \( U \) term acts then as an effective projection to the configurations with exactly (because of half-filling) one fermion per site, i.e., \( n_{n,\uparrow} = 1 - n_{n,\downarrow} \). We now set up an effective (second-order perturbation theory) Hamiltonian. From the kinetic energy term we obtain again a Heisenberg model with exchange parameter \( 4t^2/U \). The \( J_z \) term of the Hamiltonian does not change the configuration (in the occupation-number basis) and gives therefore a direct energy contribution \( 2J_z \sum_n T_n^z \) to the effective Hamiltonian, where \( T_n^z = (n_{n,\uparrow} - n_{n,\downarrow})/2 \) denotes the spin of the fermion on site \( n \). The full effective Hamiltonian reads

\[
H_{\text{eff}} = \sum_n \left( 4t^2/U \right) \left( T_n^+ T_{n+1}^- + T_{n+1}^+ T_n^- \right) / 2 + \sum_n \left( 2J_z + 4t^2/U \right) T_n^z T_{n+1}^z,
\]

and is an \( xxz \) chain. If the anisotropy is larger than the hopping amplitude, i.e., if \( J_z > 0 \), this model is gapped (implying both a charge and a spin gap in the original model). We therefore expect that cis- and trans-conductance tend to zero, if we increase \( U \) and keep a finite \( J_z \).

Now we consider a zero chemical potential \( \mu = 0 \). We expect that this chemical potential shift away from half-filling closes the charge gap, but leaves the spin gap more or less unaffected. We consider again the large-\( U \) limit. In any configuration, the \( J_z \) term of the Hamiltonian gives the following contribution for two neighbouring sites:

- \( -J_z/2 \) if the two sites are occupied by anti-parallel spins,
- \( J_z/2 \) if the two sites are occupied by parallel spins or are both empty,
- \( 0 \) if one site is occupied and the other is not.
Figure A.1. The same as figure 2, but for $J_z = 0.8t$ (here $N = 140$). The simulations away from half-filling suffer from large autocorrelation times.

We assume that there is a spin gap and that the (degenerate) ground state configurations are those for which the spins of the particles are ordered antiferromagnetically. If only these configurations are allowed, the $J_z$ term can be represented as a one-site potential with a contribution $\pm J_z/2$ for empty/occupied sites. (One obtains the same energy contributions as from the $J_z$ term of the original Hamiltonian, if one keeps in mind that each site appears in precisely two pairs of neighbouring sites.) We can set up the following effective Hamiltonian (this is just the restriction of the original Hamiltonian to the assumed ground-state configurations, i.e., zeroth order in $U$)

$$\sum_n \left[ \left( R_n^+ R_{n+1}^- + R_{n+1}^+ R_n^- \right) / 2 + J_z R_n^z \right],$$

which is an $xx$ chain in magnetic field, where the ‘spin’ operator $R_n^z$ (in this case denoted by $R$ to avoid confusion with previous spin operators) is defined by $R_n^z = -1/2$ if there is a particle on site $n$ and by $R_n^z = +1/2$ if site $n$ is empty. Since the effective Hamiltonian describes the charge part of the Hamiltonian, the full conductance $2(g_c + g_t)$ for the original model should coincide with the conductance of the new Hamiltonian which is $e^2/h$ as the system is non-interacting \cite{8, 17}. Since we have $g_c = g_t$ by the assumption of a spin gap and equation (4), the relation $g = 2(g_c + g_t)$ yields $g_c = 0.25 e^2/h = g_t$.

In principle, the model equation (A.1) can also be analysed with the MC method developed in this paper, but we found that the simulation for this case is problematic: we measured large autocorrelation times for finite $J_z$ and $\mu$ (e.g., for the computation of the compressibility). We must therefore restrict ourselves to $J_z \leq 0.8t$.

For $J_z = 0.8t$, we present cis- and trans-conductance results in figure A.1. In the large-$U$ limit, we find good agreement with our prediction that $g_c = g_t = 0.25 e^2/h$, which gives credit to the simulation data despite the large autocorrelation times.

Here, we want to mention once again the remarkable fact that the sign of the trans-conductance (the direction of the induced current) changes when we switch on the magnetic field and switch on the spin-polarized interaction. (The trans-conductance is negative for all $U$ in figure 2, whereas in the present situation we expect $g_t = g_c = K_p/2 > 0$ for $T = 0, U = \infty$.)

\cite{8, 17}
Occupation in the ground state: since we identified the ground state of the Hamiltonian equation (A.1), \( H(\mu = 0) \), with the ground state of the \( xx \) chain in magnetic field, we can calculate the occupation per state of this Hamiltonian in the large-\( U \) limit, the result being

\[
\sum_{n,\sigma}(n_{n,\sigma})/N = 1 - \arccos(J_z/[2t])/\pi.
\]

This prediction was tested against an MC simulation and obtained good agreement (see figure A.2).

**References**

[1] Flensberg K 1998 *Phys. Rev. Lett.* **81** 184
[2] Komnik A and Egger R 2000 *EPJ Preprint* condmat/0007443
[3] Nazarov Yu D and Averin D 1998 *Phys. Rev. Lett.* **81** 653
[4] Mortensen N A, Flensberg K and Jauho A P 2001 *Phys. Rev. Lett.* **86** 1841
  Mortensen N A, Flensberg K and Jauho A P 2002 *Phys. Rev. B* **65** 085317
[5] Flensberg K, Jensen T S and Mortensen N A 2001 *Phys. Rev. B* **64** 245308
[6] d’Amico I and Vignale G 2003 *Phys. Rev. B* **68** 045307
  d’Amico I and Vignale G 2000 *Phys. Rev. B* **62** 4853
  Takahashi Y, Shizume K and Masuhara N 2001 *Physica E* **10** 22
[7] Kane C L and Fisher M P A 1992 *Phys. Rev. Lett.* **68** 1220
  Kane C L and Fisher M P A 1992 *Phys. Rev. B* **46** 15233
[8] Gogolin A, Nersesyan A and Tsvelik A 1998 *Bosonization and Strongly Correlated Systems* (Cambridge: Cambridge University Press)
[9] Louis K and Gros C 2003 *Phys. Rev. B* **68** 184424
[10] Louis K and Gros C 2003 *Phys. Rev. B* submitted (Preprint cond-mat/0310465)
[11] Dorneich A and Troyer M 2001 *Phys. Rev. E* **64** 066701

*New Journal of Physics* **6** (2004) 187 (http://www.njp.org/)
[12] Sandvik A W and Kurkijärvi J 1991 Phys. Rev. B 43 5950
Sandvik A W 1992 J. Phys. A: Math. Gen. 25 3667
[13] Syljuåsen O F and Sandvik A W 2002 Phys. Rev. E 66 046701
[14] Sandvik A W 1999 Phys. Rev. B 59 R14157
[15] Clay R T, Sandvik A W and Campbell D K 1999 Phys. Rev. B 59 4665
[16] Sengupta P, Sandvik A W and Campbell D K 2002 Phys. Rev. B 65 155113
[17] Apel W and Rice T M 1982 Phys. Rev. B 26 7063
[18] Schulz H J 1990 Phys. Rev. Lett. 64 2831
Schulz H J 1994 ‘The metal–insulator transition in one dimension’, Lecture given at Los Alamos Meeting on Strongly Correlated Electron Systems (December 1993) Preprint cond-mat/9412036
[19] Umeno Y, Shiroishi M and Klümper A 2003 Europhys. Lett. 62 284
[20] Schlottmann P 2004 Phys. Rev. B 69 035110