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2001 J. Phys.: Condens. Matter 13 5135

(http://iopscience.iop.org/0953-8984/13/22/310)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **13** (2001) 5135–5157 www.iop.org/Journals/cm PII: S0953-8984(01)21594-X

Charge and spin transport in the one-dimensional Hubbard model

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Received 1 February 2001, in final form 27 March 2001

Abstract

We study the charge and spin currents transported by the elementary excitations of the one-dimensional (1D) Hubbard model and derive the corresponding current spectra. We present results both for finite-size systems and in the thermodynamic limit. This includes finding the couplings of both the low-energy and finite-energy (string) excitations to external charge and spin probes. At zero magnetic field the general structure of the charge–spin separation survives at all energy scales and the effective charges of both the low-energy and finite-energy charge excitations are studied as functions of the on-site Coulomb interaction U, electronic density n, and applied magnetic field H. In some limits the effective charge of the low-energy excitations equals that of the electrons, whereas that of the finite-energy charge-string excitations of rapidity length γ is found to be 2γ times the electronic charge. At $U = \infty$ the spin excitations do not contribute to spin transport, whereas the low-energy charge excitations *feel* an effective flux given by $(\phi_\uparrow N_\uparrow - \phi_\downarrow N_\downarrow)/(N_\uparrow + N_\downarrow)$, where N_σ is the number of electrons of spin σ and ϕ_σ is a spin-dependent flux. This reveals that at zero magnetic field and $U = \infty$ there is no spin transport, while at finite magnetic field the low-energy charge excitations also carry spin. In the $U \gg t$ limit the spin is carried both by holons and spinons. Finally, we find that the charge- and spin-current spectra can be derived from a semi-classical approach.

1. Introduction

For more than twenty years the transport properties of strongly correlated electron systems have been a subject of experimental and theoretical interest. Low-dimensional conductors and Mott insulators show large deviations in their transport properties from the usual Fermi-liquid quasi-particle description. It is now understood that electronic correlations play an important role in these systems [1–8], even when these correlations are small [6]. Solvable one-dimensional (1D)

many-electron models such as the Hubbard chain [9, 10], the supersymmetric t–J model [11], and the spinless fermion model [12] are often used as starting models for the study of the electronic properties of quasi-one-dimensional conductors [13–15].

Although the Hubbard chain was diagonalized long ago [9, 10], the involved form of the Bethe-*ansatz* (BA) wave function has prevented the full calculation of dynamic response functions, these including the charge–charge and spin–spin response functions and their associated conductivity spectra.

However, in the last ten years many theoretical aspects of the Hubbard-model transport properties have been understood. Information on the low-energy behaviour of correlation functions can be obtained by combining the BA with conformal-field theory [16]. Several approaches using bosonization [17, 18], the pseudo-particle formalism [19], scaling methods [20], and spin-wave theory [21] have been used to investigate the low-energy transport properties of the model away from half-filling and at the metal–insulator transition [9]. Partial information on the optical conductivity of the Hubbard model at finite frequencies has been obtained by numerical methods [22–24]. Recently, exact results on the optical conductivity of the 1D Hubbard model have been obtained by the present authors [13] using the same BA representation as we use in this article, as well as by other groups using different methods [14, 15]. Also the transport properties of spin systems have attracted attention since the spin stiffness is a good probe of the nature of the spectrum [25, 26]. In mesoscopic physics, spin-polarized transport has become an important field of research, and a theory for spin transport in a Luttinger liquid was recently developed [27].

The study of charge transport at finite temperatures in integrable models, in particular in the 1D Hubbard model, has also been an active field of research. A series of comparative numerical and analytical studies have explored the differences in transport properties between integrable and non-integrable 1D models, including the Hubbard model [28–37]. Most of these studies have dealt with generalizations to finite temperature of Kohn's zero-temperature concepts and approach [38].

The pseudo-particle theory of reference [39] introduced new branches of pseudo-particles and generalized for all energy scales previous low-energy studies [40]. The new pseudo-particle branches are associated with *heavy pseudo-particles*. These are the quantum objects needed for the description of gapped branches of energy eigenstates relatively to the ground state. Recently, combination of that pseudo-particle theory with newly found symmetries has allowed the evaluation of analytical low-energy expressions for correlation functions associated with non-linear elementary-excitation bands [41]. Combining that non-linear theory with symmetries associated with the set of conservation laws of the model [42], one can derive expressions for finite-energy correlation functions, for example the absorption band edge of the frequency-dependent optical conductivity $\sigma(\omega)$ [13].

In this paper we study the charge and spin currents transported by the pseudo-particles which describe the elementary low- and finite-energy excitations of the 1D Hubbard model. We derive expressions for the charge- and spin-current spectra of these pseudo-particles. Similarly to the case for Fermi-liquid quasi-particles, as a result of correlations the pseudo-particle group velocity and current spectra are different quantities. When defined at the pseudo-Fermi momenta, the ratios of these charge and spin currents over the group velocity provide the pseudo-particle effective charge and spin, respectively, whose physical meaning we discuss in this paper.

The paper is organized as follows. In section 2 the BA equations with spin-dependent Peierls factors are presented. In section 3 the charge and spin spectra of the elementary excitations of finite but large systems are derived. We first motivate the general study by looking at the problem at large values of U. The charge and spin currents for $U = \infty$ and

$U \gg t$ are computed. In section 4 we derive the general equations valid in the thermodynamic limit for the charge and spin spectra and study the effective charge carried by the pseudo-particles. In section 5 we derive the same results as in section 4 by using a semi-classical approach. Finally, in section 6 we present the concluding remarks.

2. Bethe-*ansatz* equations

In this section we present the BA equation for a spin-dependent Peierls phase factor. The Hamiltonian for the Hubbard model is given by

$$\hat{H} = -t \sum_{j,\sigma} (c^{\dagger}_{j\sigma} c_{j+1\sigma} + \text{h.c.}) + U \sum_{j} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} \tag{1}$$

where $c^{\dagger}_{j\sigma}$ ($c_{j\sigma}$) creates (annihilates) an electron with spin projection σ (here and when used as an operator index, $\sigma = \uparrow, \downarrow$, and $\sigma = \pm 1$ otherwise), $\hat{n}_{j,\sigma} = c^{\dagger}_{j\sigma} c_{j\sigma}$ is the number operator at site j, and $c_{L+1\sigma} = c_{1\sigma}$. The charge ($\rho$) and spin ($\sigma_z$) current operators are given by

$$\hat{J}^{\rho} = -e\,\mathrm{i}t \sum_{\sigma} \sum_{j=1}^{N_a} (c^{\dagger}_{j\sigma} c_{j+1\sigma} - c^{\dagger}_{j+1\sigma} c_{j\sigma}) \tag{2}$$

and

$$\hat{J}^{\sigma_z} = -\frac{1}{2}\mathrm{i}t \sum_{\sigma} \sum_{j=1}^{N_a} \sigma\, (c^{\dagger}_{j\sigma} c_{j+1\sigma} - c^{\dagger}_{j+1\sigma} c_{j\sigma}) \tag{3}$$

respectively. Since neither $\hat{J}^{\rho}$ nor $\hat{J}^{\sigma_z}$ commutes with the Hamiltonian, the real part of the corresponding conductivities has in addition to a zero-frequency coherent peak a finite-frequency incoherent structure [13].

In the presence of a time-dependent vector potential $\mathcal{A}(t)$ the amplitude t for hopping between sites i and $i+1$ changes according to the well known Peierls substitution as follows:

$$\begin{aligned} &t_{i+1,i} \to t_{i+1,i}(\mathcal{A}(t)) \\ &t_{i+1,i}(\mathcal{A}(t)) = t_{i+1,i} \exp[-\mathrm{i}e(r_{i+1} - r_i)\mathcal{A}/\hbar c] \end{aligned} \tag{4}$$

where r_i is the position of the site i on the lattice. It has been possible to solve the Hamiltonian (1) with the additional hopping phase $\exp([-\mathrm{i}e(r_{i+1} - r_i)\mathcal{A}/\hbar c])$. For convenience we write $\mathcal{A} = \hbar c\phi/(aeL)$, where the lattice spacing a is given by $a = r_{i+1} - r_i$. More generally, a spin-dependent vector potential $\mathcal{A}_{\sigma}$ can be introduced and the model (1) can be solved by means of the coordinate BA either with twisted or toroidal boundary conditions, the two approaches giving essentially the same results [24, 25, 43]. One obtains the energy spectrum of the model parametrized by a set of rapidity numbers $\{k_j, \Lambda_{\delta}\}$ which are solutions of the BA interaction equations given by

$$\mathrm{e}^{\mathrm{i}k_j L} = \mathrm{e}^{\mathrm{i}\phi_{\uparrow}} \prod_{\delta=1}^{N_{\downarrow}} \frac{\sin k_j - \Lambda_{\delta} + \mathrm{i}U/4}{\sin k_j - \Lambda_{\delta} - \mathrm{i}U/4} \qquad (j = 1, \ldots, N) \tag{5}$$

and

$$\mathrm{e}^{-\mathrm{i}(\phi_{\downarrow} - \phi_{\uparrow})} \prod_{j=1}^{N} \frac{\sin k_j - \Lambda_{\delta} + \mathrm{i}U/4}{\sin k_j - \Lambda_{\delta} - \mathrm{i}U/4} = -\prod_{\beta=1}^{N_{\downarrow}} \frac{\Lambda_{\beta} - \Lambda_{\delta} + \mathrm{i}U/2}{\Lambda_{\beta} - \Lambda_{\delta} - \mathrm{i}U/2} \qquad (\delta = 1, \ldots, N_{\downarrow}). \tag{6}$$

The above equations have both real and complex solutions for the rapidities k_j and Λ_{β}. Some of the previous studies of the $\phi_{\sigma} \neq 0$ problem [25, 43] have only considered the real BA rapidities solutions of equations (5) and (6) which refer to the low-energy excitation spectra.

Using the string hypothesis, valid for a finite system of large size L, equations (5) and (6) lead to the following set of coupled algebraic equations [24,44]:

$$k_j L = 2\pi I_j^c + \phi_\uparrow - \sum_\gamma \sum_{j'=1}^{N_{s,\gamma}} 2\tan^{-1}\left(\frac{\sin k_j/u - R_{s,\gamma,j'}}{\gamma+1}\right) - \sum_{\gamma>0}\sum_{j'=1}^{N_{c,\gamma}} 2\tan^{-1}\left(\frac{\sin k_j/u - R_{c,\gamma,j'}}{\gamma}\right) \tag{7}$$

$$L\sin^{-1}\left(u\sqrt{\gamma^2+(R_{c,\gamma,j}+1/u)^2} - u\sqrt{\gamma^2+(R_{c,\gamma,j}-1/u)^2}\right) = 2\pi I_j^{c,\gamma} - \gamma(\phi_\uparrow+\phi_\downarrow) - \sum_{j'=1}^{N_c} 2\tan^{-1}\left(\frac{\sin k_{j'}/u - R_{c,\gamma,j}}{\gamma}\right) + \sum_{\gamma'>0}\sum_{j'=1}^{N_{c,\gamma'}} \Theta_{\gamma,\gamma'}(R_{c,\gamma,j} - R_{c,\gamma',j'}) \tag{8}$$

and

$$\sum_{j'=1}^{N_c} 2\tan^{-1}\left(\frac{R_{s,\gamma,j} - \sin k_{j'}/u}{1+\gamma}\right) = 2\pi I_j^{s,\gamma} + (\gamma+1)(\phi_\downarrow - \phi_\uparrow) + \sum_{\gamma'}\sum_{j'=1}^{N_{s,\gamma'}} \Theta_{\gamma+1,\gamma'+1}(R_{s,\gamma,j} - R_{s,\gamma',j'}). \tag{9}$$

In the above equations we have introduced $u = U/(4t)$. The functions $\Theta_{\gamma,\gamma'}(x)$ (and $\Theta_{\gamma+1,\gamma'+1}(x)$) of equations (7), (8), and (9) are defined in reference [39]. The following definitions for the real parts of the rapidities $\Lambda_\alpha^{n+1}/u = R_{s,\gamma,j}$ (with $n+1=\gamma$ and $\alpha = j$) and $\Lambda_\alpha^n/u = R_{c,\gamma,j}$ (with $n=\gamma$ and $\alpha = j$), where $\gamma = 1, 2, \ldots$ for the c,γ sums and $\gamma = 0, 1, 2, \ldots$ for the s,γ sums, allow us to recover Takahashi's formulae for $\phi_\sigma = 0$ [10]. Here and often below we use the notation $c \equiv c, 0$, which indicates that the c,γ sums run over $1, 2, \ldots$.

The relevant numbers I_j^c, $I_j^{c,\gamma}$, and $I_j^{s,\gamma}$ which appear in going from equations (5) and (6) to equations (7), (8), and (9) are the quantum numbers whose occupancies describe the energy eigenstates. In table 1 we give a classification of the type of excitations described by the associated quantum numbers, as well as the various nomenclatures existing in the literature. The I_j^c quantum numbers are associated with the low-energy charge excitations and play an

Table 1. Types of excitation associated with the quantum numbers (Q.N.) I_j^c and $I_j^{\alpha,\gamma}$, with $\alpha = c, s$. The spin-string excitations are gapped only for finite magnetic field H. At low energy, both the holon and spinon excitations can be described by bosonization methods. The smallest gap of the charge-string excitations occurs at half-filling and is the Mott–Hubbard gap Δ_{MH}. In the table, P.P. stands for pseudo-particle.

Q.N.	Type of excitation	Gap	Rapidity	P.P.
I_j^c	Holons	Gapless	k_j	$c, 0$
$I_j^{s,0}$	Spinons	Gapless	$R_{s,0,j}$	$s, 0$
$I_j^{c,\gamma>0}$	Charge strings	Gapped	$R_{c,\gamma,j}$	$c, \gamma \geqslant 1$
$I_j^{s,\gamma>0}$	Spin strings	Gapped ($H \neq 0$)	$R_{s,\gamma,j}$	$s, \gamma \geqslant 1$

important role in the metallic phase. At half-filling the system is a Mott insulator, and all the I_j^c quantum numbers are occupied in the ground state. In this case, charge excitations involve occupancy of the $I_j^{c,\gamma}$ quantum numbers. The energy eigenstates with occupied $I_j^{c,\gamma}$ numbers have a gap relatively to the ground state. The minimal energy required for a single occupancy of the $I_j^{c,1}$ quantum numbers equals, at half-filling, the Mott–Hubbard gap [13]. The $I_j^{s,\gamma}$ quantum numbers are associated with spin excitations of the system. In the ground state, at zero magnetic field, all $I_j^{s,0}$ quantum numbers are occupied. Excitations which change the $s, 0$ occupancies and keep the $s, \gamma > 0$ occupancies zero are spin-triplet or higher-order multiplet excitations. On the other hand, singlet excitations involve changes of both the $s, 0$ and $s, \gamma > 0$ occupancies.

The numbers I_j^c and $I_j^{\alpha,\gamma}$ are integers or half odd integers [10] when the numbers $\bar{N}_c$ and $\bar{N}_{\alpha,\gamma}$ are even or odd, respectively, where

$$\begin{aligned} &\bar{N}_c = \sum_{\gamma=0} N_{s,\gamma} + \sum_{\gamma=1} N_{c,\gamma} \\ &\bar{N}_{c,\gamma} = 1 + L - N + N_{c,\gamma} \qquad \bar{N}_{s,\gamma} = 1 + N - N_{s,\gamma} \end{aligned} \tag{10}$$

and $N_{\alpha,\gamma}$ stands for the number of occupied $I_j^{\alpha,\gamma}$ quantum numbers, with N the total number of electrons. The spacing between adjacent quantum numbers $I_j^{\alpha,\gamma}$ is always one, independently of the value of the on-site repulsion U. It is therefore natural to interpret $q_j^{\alpha,\gamma} = 2\pi I_j^{\alpha,\gamma}/L$ as a momentum [39], the rapidities $R_{\alpha,\gamma,j}$ and k_j being functions of $q_j^{\alpha,\gamma}$ and q_j^c, respectively. We call the occupied values of the I_j^c and $I_j^{\alpha,\gamma}$ numbers c and α, γ pseudo-particles, respectively. On the other hand, the holons and spinons referred to in table 1 correspond in the present representation to the non-occupied I_j^c and $I_j^{s,0}$ numbers, respectively. The connection of pseudo-particles with the SO(4) symmetry [45] of the Hubbard model was discussed by two of the present authors in a previous work [46].

The total number of electrons and the total number of down-spin electrons, $N_\downarrow$, obey the following sum rules:

$$N = N_c + 2A_c \tag{11}$$

and

$$N_\downarrow = A_c + A_s \tag{12}$$

respectively, where

$$A_c = \sum_{\gamma>0} \gamma N_{c,\gamma} \qquad A_s = \sum_{\gamma=0} (\gamma + 1) N_{s,\gamma}. \tag{13}$$

The numbers I_j^c, $I_j^{c,\gamma}$, and $I_j^{s,\gamma}$ belong to the intervals

$$\begin{aligned} &|I_j^c| < \frac{L}{2} \\ &|I_j^{c,\gamma}| < \frac{1}{2}(L - N + 2A_c - T_c^\gamma) \\ &|I_j^{s,\gamma}| < \frac{1}{2}(N - 2A_c - T_s^\gamma) \end{aligned} \tag{14}$$

where T_α^γ (with $\alpha = c, s$) is given by

$$T_c^\gamma = \sum_{\gamma'=1} t_{\gamma,\gamma'}^c N_{c,\gamma'} \qquad T_s^\gamma = \sum_{\gamma'=0} t_{\gamma,\gamma'}^s N_{s,\gamma'} \tag{15}$$

with $t_{\gamma,\gamma'}^c = 2\min(\gamma, \gamma') - \delta_{\gamma,\gamma'}$ and $t_{\gamma,\gamma'}^s = 2\min(\gamma + 1, \gamma' + 1) - \delta_{\gamma,\gamma'}$.

All energy eigenstates considered in the BA solution are described by different occupancies of the quantum numbers $I_j^{\alpha,\gamma}$. For example, the ground state [39] is described by a compact symmetric occupancy around the origin of the numbers I_j^c and $I_j^{s,0}$, and by zero occupancy for the numbers $I_j^{c,\gamma}$ and $I_j^{s,\gamma>0}$. The general classification of the excitations is summarized in table 2.

Table 2. The numbers $N_{\alpha,\gamma}$ of the different excitations. The notation is as follows: G.S., Ex_0, $\mathrm{Ex}_{c,\gamma}$, and $\mathrm{Ex}_{s,\gamma}$ stand for ground states, low-energy eigenstates (no-strings), eigenstates with c, γ charge strings of length γ, and eigenstates with s, γ spin strings of length γ, respectively.

State	N_c	$N_{s,0}$	$N_{c,\gamma>0}$	$N_{s,\gamma>0}$
G.S.	N	$N_\downarrow$	0	0
Ex_0	N	$N_\downarrow$	0	0
$\mathrm{Ex}_{c,\gamma}$	$N-\sum_{\gamma>0}2\gamma N_{c,\gamma}$	$N_\downarrow-\sum_{\gamma>0}\gamma N_{c,\gamma}$	$N_{c,\gamma}$	0
$\mathrm{Ex}_{s,\gamma}$	N	$N_\downarrow-\sum(\gamma+1)N_{s,\gamma}$	0	$N_{s,\gamma}$

The energy and momentum eigenvalues are given by [10, 39]

$$E(L,\phi,U,N_\sigma)=-2t\sum_{j=1}^{N_c}\cos k_j+4t\sum_{\gamma=1}\sum_{j=1}^{N_{c,\gamma}}\mathrm{Re}\sqrt{1-u^2[R_{c,\gamma,j}-\mathrm{i}\gamma]^2} \tag{16}$$

and

$$P=\sum_{j=1}^{N_c}\frac{2\pi}{L}I_j^c+\sum_{\gamma}\sum_{j=1}^{N_{s,\gamma}}\frac{2\pi}{L}I_j^{s,\gamma}-\sum_{\gamma}\sum_{j=1}^{N_{c,\gamma>0}}\frac{2\pi}{L}I_j^{c,\gamma}+\frac{N_\uparrow}{L}\phi_\uparrow+\frac{N_\downarrow}{L}\phi_\downarrow+\pi\sum_{\gamma>0}N_{c,\gamma} \tag{17}$$

respectively.

We stress that equations (7)–(9) are only valid in the limit of very large system size L, where Takahashi's string hypothesis becomes valid [10,47]. The general solution of equations (7)–(9) for large system size L, arbitrary electron numbers N_σ, and Coulomb interaction U is a very difficult problem. Below we solve the problem explicitly for the charge and spin currents of a large system of size L in the limits $U=\infty$ and $U\gg t$.

3. Currents transported by the elementary excitations

To gain some insight into the problem, we start by studying the charge and spin currents transported by the pseudo-particle excitations listed in table 1, in the limits $U=\infty$ and $U\gg t$. The charge- and spin-current operators $\hat{J}^\rho$ and $\hat{J}^{\sigma_z}$ associated with the 1D Hubbard model are given in equations (2) and (3), respectively. The current expectation values $J_m^\rho\equiv\langle m|\hat{J}^\rho|m\rangle$ and $J_m^{\sigma_z}\equiv\langle m|\hat{J}^{\sigma_z}|m\rangle$ relative to the energy eigenstate $|m\rangle$ are given by [25]

$$J_m^\rho=\frac{\mathrm{d}E_m}{\mathrm{d}(\phi/L)}\qquad\phi=\phi_\uparrow=\phi_\downarrow \tag{18}$$

and

$$J_m^{\sigma_z}=\frac{\mathrm{d}E_m}{\mathrm{d}(\phi/L)}\qquad\phi=\phi_\uparrow=-\phi_\downarrow \tag{19}$$

respectively, with $E_m=E_m(\phi)$ the corresponding energy eigenvalue. Below we write the currents J_m^ρ and $J_m^{\sigma_z}$ in units of the electron charge $(-e)$ and spin $(1/2)$, respectively.

3.1. The $U = \infty$ case

Let us consider first energy eigenstates with c and $s, 0$ occupancies only. In this case the number of electrons is related to N_c and A_s as follows:

$$N_\uparrow = N_c - A_s \qquad N_\downarrow = A_s \qquad N_c = N_\uparrow + N_\downarrow. \tag{20}$$

At $U = \infty$ the charge-string excitations have infinite energy relatively to the ground state and, therefore, drop out of the problem. In physical terms this means that states with finite double occupancy are not permitted. The rapidities $R_{s,\gamma,j}$ decouple from the charge degrees of freedom and all the spin excitations are degenerate [48–50], because the s, γ pseudo-particles have in this limit a flat dispersion relation. Equations (7)–(9) then reduce to

$$k_j^\infty L = 2\pi I_j^c + \phi_\uparrow + \sum_{j'=1}^{N_{s,0}} 2\tan^{-1}(R_{s,0,j'}^\infty) \tag{21}$$

and

$$N_c\, 2\tan^{-1}(R_{s,0,j}^\infty) = 2\pi I_j^{s,0} + (\phi_\downarrow - \phi_\uparrow) + \sum_{j'=1}^{N_{s,0}} \Theta_{1,1}(R_{s,0,j}^\infty - R_{s,0,j'}^\infty) \tag{22}$$

with $\Theta_{1,1}(x) = 2\tan^{-1}(x/2)$. We see from the structure of equations (21) and (22) that the Hubbard-model Hilbert space decouples, in this case, into a product of two Hilbert subspaces, each of them associated with a different effective Hamiltonian. These are a chain of length L and N_c spinless fermions and a Heisenberg spin-one-half chain of length N_c, as was first discussed by Ogata and Shiba [50]. This is, however, a very delicate decoupling as regards the finite-temperature properties. In fact, if U is very large but not infinity, in a given finite-temperature calculation N_c is not constant, implying that the length of the Heisenberg chain also varies.

The energy eigenvalues are given by

$$E_m(L, \phi, N_\sigma) = E_m^\infty = -2t \sum_{j=1}^{N_c = N} \cos k_j^\infty. \tag{23}$$

Equations similar to equations (21)–(23) have been derived for the ground state in the study of persistent currents in finite-size rings [51]. If we use equation (22) in equation (21) we obtain a solution for k_j^∞ in terms of the quantum numbers I_j^c and $I_j^{s,0}$ only. This solution reads

$$k_j^\infty = \frac{2\pi}{L} I_j^c + \frac{\phi_\uparrow(N_c - A_s) + \phi_\downarrow A_s}{LN_c} + \frac{2\pi}{LN_c} \sum_{j=1}^{N_{s,0}} I_j^{s,0}. \tag{24}$$

Equation (24) shows that in the present case of $U = \infty$ the spin degrees of freedom are still coupled to the charge excitations through the quantum numbers $I_j^{s,0}$. These act as a fictitious flux piercing the ring of spinless fermions. Furthermore, the flux dependence of k_j can be defined in terms of an effective flux Φ_{eff} given by

$$\Phi_{eff} = \frac{\phi_\uparrow N_\uparrow + \phi_\downarrow N_\downarrow}{LN_c}. \tag{25}$$

The value of Φ_{eff} depends on whether we are computing the charge or the spin currents. We therefore have a flux Φ_{eff}^ρ for charge and a flux $\Phi_{eff}^{\sigma_z}$ for spin given by

$$\Phi_{eff}^\rho = \frac{\phi}{L} \qquad \Phi_{eff}^{\sigma_z} = \frac{\phi}{L} \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \tag{26}$$

respectively. These equations together with equations (18) and (19) give

$$J_m^{\rho} = +2t \sum_{j=1}^{N_c} \sin k_j \tag{27}$$

and

$$J_m^{\sigma_z} = 2t \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} \sum_{j=1}^{N_c} \sin k_j. \tag{28}$$

Equation (27) shows that the charge c pseudo-particle current is that of spinless fermions, in agreement with the well known factorization of the Hubbard model in spinless fermions and an antiferromagnetic Heisenberg chain [50]. The charge-current spectrum of the c pseudo-particles is $2t \sin k_j$ and equals, in this case, the corresponding group velocity. This implies that the effective charge transported by the c pseudo-particle is 1, equalling the electronic charge. The fact that k_j depends on the statistical flux term ϕ_s^{stat}:

$$\phi_s^{stat} = \frac{2\pi}{LN_c} \sum_{j=1}^{N_{s,0}} I_j^{s,0} \tag{29}$$

shows that the charge transport is affected by the background configuration of the spins. The effect of ϕ_s^{stat} on the finite-size finite-temperature charge stiffness was studied in reference [37]. Equation (28) is also interesting, since it reveals that we can only have spin currents in the system provided that a magnetic field is applied, which introduces an asymmetry between the $N_\uparrow$ and $N_\downarrow$ electron populations. If the system is half-filled the sum $\sum_{j=1}^{N_c} \sin k_j$ is zero in the thermodynamic limit for the ground state and transport is blocked for both charge and spin. Since for $U = \infty$ the energy does not depend on the rapidities $R_{s,\gamma,j}$, we have in this limit that the $s, 0$ and $s, \gamma \geqslant 1$ pseudo-particles do not transport either charge or spin, whereas the c pseudo-particles can transport both charge and spin if we apply a magnetic field to the system. This means that the charge–spin separation considered in bosonization refers only to zero magnetic field.

3.2. The $U \gg t$ case

If U is finite but t^2/U corrections are neglected, the energy eigenvalues are given by

$$E_m = -2t \sum_{j=1}^{N_c} \cos k_j + U \sum_{\gamma>0} \gamma N_{c,\gamma}. \tag{30}$$

Proceeding as before we obtain that the c pseudo-particles feel an effective charge flux

$$\Phi_{eff}^{\rho} = \frac{\phi}{L} \frac{N_h - N_d}{N_h + N_d} \tag{31}$$

where N_h is the number of empty lattice sites and N_d is the number of doubly occupied sites. If we are in the metallic phase the energy eigenstates described by finite occupancy of c, γ pseudo-particles have no important role for charge transport. On the other hand, in the insulating phase, only the above energy eigenstates are relevant for zero-frequency charge transport at finite temperature. That is, the finite-temperature charge-transport properties of the Mott–Hubbard insulating phase are controlled by the charge-string excitations. In this case, however, $\Phi_{eff}^{\rho} = 0$, and both charge and spin transport are blocked. This implies that at large U and at half-filling, charge and spin zero-frequency transport is controlled by t^2/U corrections to the energy.

Let us now compute the charge and spin currents up to order t^2/U. We first consider the case of energy eigenstates with c and $s,0$ occupancy only. We start by writing $k_j = k_j^\infty + \delta k_j$ and $R_{s,0,j} = R_{s,0,j}^\infty + \delta R_{s,0,j}$, where δk_j and $\delta R_{s,0,j}$ represent the t/U correction to the rapidities k_j and $R_{s,0,j}$, respectively. Introducing k_j and $R_{s,0,j}$, written as before, in equations (7)–(9) and expanding the resulting equations up to first order in t/U we obtain

$$\delta k_j = -\frac{8t B_m^s}{LU} \sin k_j^\infty + \frac{8t}{LUN_c} B_m^s A_m^c \tag{32}$$

where

$$B_m^s = \sum_{j=1}^{N_\downarrow} \frac{1}{1+(R_{s,0,j}^\infty)^2} \qquad A_m^c = \sum_{j=1}^{N_c} \sin k_j^\infty. \tag{33}$$

We can identify $-B_m^s$ with the energy of Heisenberg-chain eigenstates with no $s,\gamma > 1$ occupancy. For zero magnetic field there is only one such state and therefore $-B_m^s$ corresponds to the ground-state energy of a Heisenberg chain of size N_c. The energy of the Hubbard chain is in this limit given by

$$E(L,\phi,N_\sigma,U) = E_m^\infty + 2t \sum_{j=1}^{N_c} \delta k_j \sin k_j \tag{34}$$

and the charge and spin currents can be computed using equations (18) and (19), as before. Note that the flux dependence of $R_{s,0,j}^\infty$ must now be taken into account for the calculation of the spin current. The charge current J_m^ρ is basically given by equation (27) with a small correction of the order of t^2/U, coming from the second term in equation (34). The main difference refers to the spin current which has in general a finite value. However, for zero magnetic field, $J_m^{\sigma_z}$ is given by

$$J_m^{\sigma_z} = 2t \sum_{j=1}^{N_c} \sin k_j^\infty \frac{\mathrm{d}\,\delta k_j}{\mathrm{d}(\phi/L)} \propto \frac{\mathrm{d}B_m^s}{\mathrm{d}(\phi/L)} = 0. \tag{35}$$

For the zero-magnetization ground state, $j = 1,\ldots,N_{s,0}$ for the $s,0$ band and, therefore, the number of available $I_j^{s,0}$ quantum numbers equals the $N_{s,0}$ occupancies, leading to zero value for the derivative of B_m^s with respect to the flux, as can be seen from figure 1, and therefore $J_m^{\sigma_z}$ is zero.

Let us now consider that a spin-singlet excitation is created and find the corresponding spin current. For simplicity we consider the ground-state distribution of the I_j^c quantum numbers. We also consider the case of zero magnetic field, since in this case the spin is transported by the s,γ pseudo-particles only. This corresponds to the following variations of the pseudo-particle numbers:

$$\Delta N_{s,0} = -2 \qquad \Delta N_{s,1} = 1. \tag{36}$$

Let us consider the case for which N is even and $N_\uparrow = N_\downarrow$ are odd. In this case the I_j^c quantum numbers are half-odd integers and $I_j^{s,0}$ quantum numbers are integers in the ground state:

$$I_j^c = -\frac{L-1}{2}, -\frac{L-3}{2}, \ldots, -\frac{1}{2}, \frac{1}{2}, \ldots, \frac{L-3}{2}, \frac{L-1}{2}$$

$$I_j^{s,0} = -\frac{N_\uparrow - 1}{2}, -\frac{N_\uparrow - 3}{2}, \ldots, 0, \ldots, \frac{N_\uparrow - 3}{2}, \frac{N_\uparrow - 1}{2}.$$

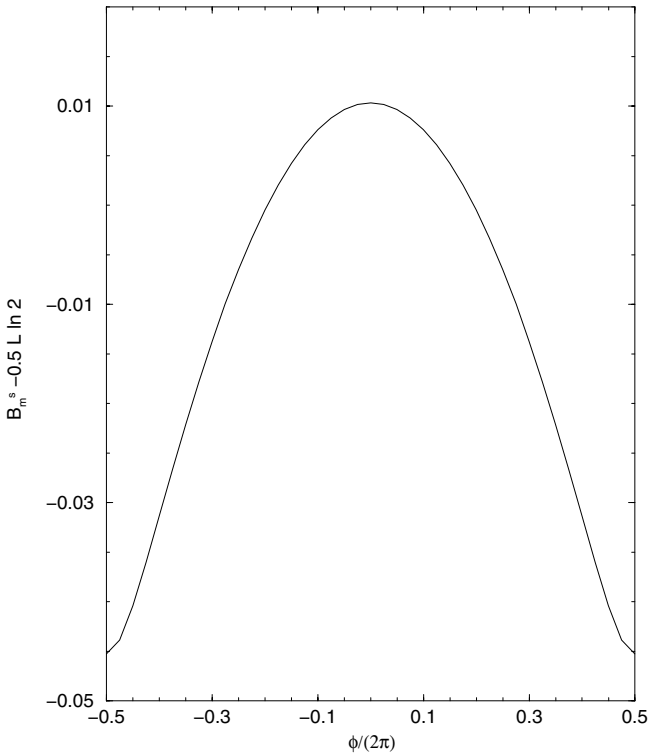

Figure 1. The $B_m^s - 0.5L \ln 2$ term as a function of the flux $\phi/(2\pi)$, for $L = 40 = 2N_\downarrow$. It is clear that $\mathrm{d}B_m^s/\mathrm{d}\phi$ is zero at $\phi = 0$. Therefore the corresponding current expectation value $J_m^{\sigma_z}$ is zero.

When an s, 1 pseudo-particle is created, the $I_j^{s,0}$ numbers remain unchanged but the I_j^c quantum numbers change to integers. This collective excitation of the c pseudo-particles contributes to the excitation momentum, which is given by

$$q = \sum_{j=1}^{N_c} \frac{2\pi}{L} I_j^c + \sum_{j=1}^{N_\downarrow - 2} \frac{2\pi}{L} I_j^{s,0} = \pi \frac{N_c}{L} + \sum_{j=1}^{N_\downarrow - 2} \frac{2\pi}{L} I_j^{s,0} \tag{37}$$

and $I_j^{s,1}$ only has the occupied $j = 0$ value $I_0^{s,1} = 0$. Note that at half-filling the contribution of the $c, 0$ pseudo-particles to q equals π. For the class of energy eigenstates that we are considering, the BA equations (7) and (9) are written as

$$k_j L = 2\pi I_j^c + \phi_\uparrow - \sum_{j'=1}^{N_{s,0}} 2\tan^{-1}(\sin k_j/u - R_{s,0,j'}) - 2\tan^{-1}\left(\frac{\sin k_j/u - R_{s,1}}{2}\right) \tag{38}$$

$$\sum_{j'=1}^{N_c} 2\tan^{-1}\left(\frac{R_{s,1} - \sin k_{j'}/u}{2}\right) = 2\pi I^{s,1} + 2(\phi_\downarrow - \phi_\uparrow) + \sum_{j'=1}^{N_{s,0}} \Theta_{2,1}(R_{s,1} - R_{s,0,j'}) \tag{39}$$

$$\sum_{j'=1}^{N_c} 2\tan^{-1}(R_{s,0,j} - \sin k_{j'}/u)$$

$$= 2\pi I_j^{s,0} + (\phi_\downarrow - \phi_\uparrow) + \sum_{j'=1}^{N_{s,0}} \Theta_{1,1}(R_{s,0,j} - R_{s,0,j'}) + \Theta_{1,2}(R_{s,0,j} - R_{s,1}) \tag{40}$$

with

$$\Theta_{1,2}(x) = \Theta_{2,1}(x) = 2\tan^{-1}(x) + 2\tan^{-1}(x/3). \tag{41}$$

Proceeding as before, we can compute δk_j for a spin-singlet excitation (sse), obtaining

$$\delta k_j^{sse} = \delta k_j - \frac{8t}{LU}\frac{2\sin k_j^{\infty}}{4+(R_{s,1}^{\infty})^2} + \frac{8t}{LUN_c}\frac{2A_m^c}{4+(R_{s,1}^{\infty})^2} \tag{42}$$

where δk_j is given by equation (32), but $N_{s,0}$ has diminished by two. The spin current is given by

$$J_m^{\sigma_z} = \frac{8t^2}{U}\left(\frac{N_c}{L} - \cos(2\phi_s^{stat})\frac{\sin(2\pi N_c/L)}{L\sin(2\pi/L)}\right)\frac{\mathrm{d}B_{sse}}{\mathrm{d}(\phi/L)} \tag{43}$$

where B_{sse} reads

$$B_{sse} = -\frac{2}{4+(R_{s,1}^{\infty})^2} - \sum_{j=1}^{N_{\downarrow}-2}\frac{1}{1+(R_{s,0,j}^{\infty})^2} \tag{44}$$

and is a function of the excitation momentum q given by equation (37), which in this case reads

$$q = \frac{2\pi}{L}I_1^{s,0} + \frac{2\pi}{L}I_2^{s,0} + \pi\frac{N_c}{L}.$$

In the limit $L\to\infty$, $N_c\to\infty$ and $n_c = N_c/L$ finite, the spin current is given by

$$J_m^{\sigma_z} = \frac{8t^2}{U}\left(n_c - \frac{\sin(2\pi n_c)}{2\pi}\right)\frac{\mathrm{d}B_{sse}}{\mathrm{d}(\phi/L)}. \tag{45}$$

The fact that $\mathrm{d}B_m^s/\mathrm{d}(\phi/L)$ is zero for states with no s, 1 occupancy implies that the spin current is transported by the two holes created in the s, 0 band; that is, the spin current is transported by the two spinons.

These have an excitation spectrum determined by

$$E(q) = \frac{8t^2}{U}\left(n_c - \frac{\sin(2\pi n_c)}{2\pi}\right)(B_{sse} + B_m^s)$$

where q is the excitation momentum given in equation (37). The number of two-spinon spin-singlet excitations with the same c pseudo-particle occupancy is $N_{\downarrow}(N_{\downarrow}-1)/2$. The excitation energy $E(q)$ of these eigenstates is represented in figure 2. It is clear that E is a two-parameter excitation spectrum, which is controlled by the two-spinon momenta $2\pi I_{1,2}^{s,0}/L$.

The group velocity $v(q)$ and the spin-current spectrum $J^{\sigma_z}(q)$ are given by

$$v(q) = \frac{\mathrm{d}E(q)}{\mathrm{d}q} \qquad J^{\sigma_z}(q) = \frac{\mathrm{d}E(q)}{\mathrm{d}(\phi/L)} \tag{46}$$

respectively, and are represented in figure 3 for the case $n_c = 1$. In this figure only the group velocity and the spin-current spectrum associated with the envelope curves of $E(q)$ are shown.

From figure 3 it is clear, as for a Fermi liquid, that $v(q)$ and $J^{\sigma_z}(q)$ are not in general the same function, in contrast to the case for spin transport by independent electrons. In figure 3 the solid line corresponds to states in which the two spinons travel together, whereas the dashed lines represent the states in which one spinon is fixed at the (pseudo-) Fermi points $I_j^{s,0} = \pm(N_{\uparrow}-1)/2$. Also from figure 3 and for the solid and dashed lines (the envelope curves of all these two-parameter excitations) we see that the spin current is zero when the two spinons occupy the $I_j^{s,0} = \pm 1/2$ and the $I_j^{s,0} = \pm(N_{\uparrow}-1)/2$ quantum numbers. Obviously when the two spinons occupy two symmetric $I_j^{s,0}$ numbers the spin current is zero. Note that, when the two spinons travel together, $v(q)$ and $J^{\sigma_z}(q)$ are given by the same function, apart from a numerical constant. Otherwise, $v(q)$ and $J^{\sigma_z}(q)$ do not coincide. These results show the importance of correlations in charge and spin transport.

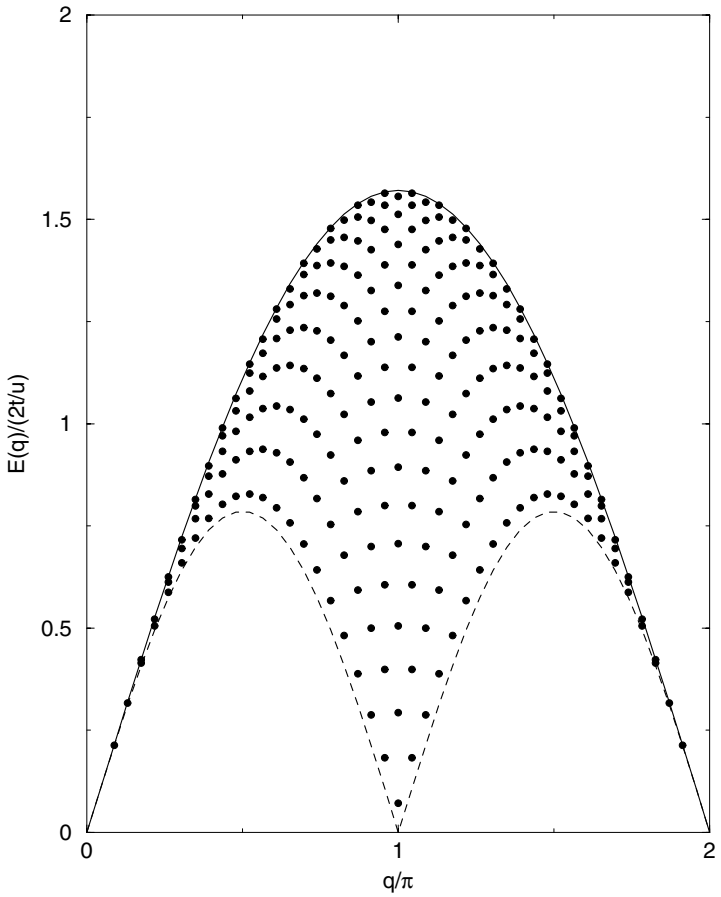

Figure 2. The spectrum of a spin-singlet excitation associated with two spinons at half-filling for $U \gg t$ up to order t^2/U, obtained by numerical solution of the BA equations. We consider the case $n = 1$ and $N_\uparrow = N_\downarrow$ here. The circles represent the excitation energies of a system with $L = 46$ and $N_\uparrow = N_\downarrow = 23$. The solid and dashed lines represent the thermodynamic limit solutions $E(q)/(2t/u) = (\pi/2)|\sin(q/2)|$ and $E(q)/(2t/u) = (\pi/4)|\sin q|$, respectively.

4. Charge-current spectrum

The discussion on charge and spin transport for large U of the previous section can be generalized to all finite values of the on-site repulsion U. As follows from the analysis of that section, the discussion of spin transport becomes more transparent if we describe the low-energy excitations in terms of spinons rather than $s, 0$ pseudo-particles. In this section we restrict consideration to the pseudo-particle charge transport and we will discuss the general formulation of spin transport in terms of spinons elsewhere [53].

Our goal is to compute the charge-current spectrum $J^{\rho}_{\alpha,\gamma}(q)$ of the 1D-Hubbard-model α, γ pseudo-particles for all values of U and electronic densities n, in the thermodynamic limit. In a previous work we considered the finite-frequency charge conductivity of the Hubbard model [13]. Here we study the current expectation value in any energy eigenstate, extending the work presented in references [19, 37, 54] for states with $c, \gamma > 0$ occupancies. In this section we find, as in the case of the quasi-particles of a Fermi liquid, that the spectrum $J^{\rho}_{\alpha\gamma}(q)$

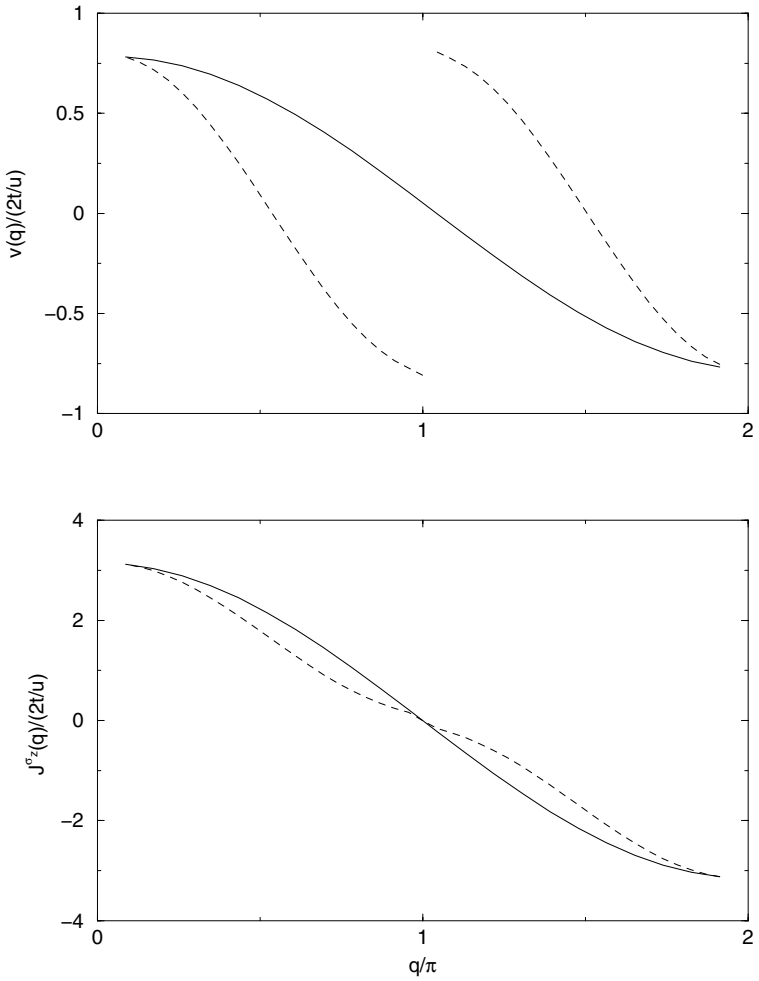

Figure 3. The group velocity and spin-current spectrum of a spin-singlet excitation involving the creation of a s, 1 pseudo-particle at half-filling and for $U \gg t$. Both $v(q)$ and $J(q)$ are presented in units of $2t/u$. The solid and dashed lines are associated with the corresponding envelope curves in figure 2, represented using the same symbols.

does not equal to the group velocity defined as

$$v_{\alpha,\gamma}(q) = \frac{\mathrm{d}\epsilon_{\alpha,\gamma}(q)}{\mathrm{d}q} \tag{47}$$

where $\epsilon_{\alpha,\gamma}(q)$ is the dispersion of the α, γ pseudo-particles.

For states generated from the ground state by small changes of the $I_j^{\alpha,\gamma}$ occupancies, the energy eigenvalues (16) can be written as

$$E_m = E_0 + \sum_{\alpha,\gamma,j} \delta N_{\alpha,\gamma}(q_j^{\alpha,\gamma})\epsilon_{\alpha,\gamma}(q_j^{\alpha,\gamma}) + \text{h.o.} \tag{48}$$

where $\delta N_{\alpha,\gamma}(q_j^{\alpha,\gamma})$ represents the occupancy deviations in the momenta $q_j^{\alpha,\gamma}$ relatively to the ground state and h.o. stands for higher-order terms [39]. The next-higher-order term represents the two-pseudo-particle interaction. For many physical properties and quantities, such as

the thermodynamics and the charge and spin currents, only the terms of order zero and one are relevant, whereas in some cases the third- and higher-order terms also play an important role [41]. The dispersions $\epsilon_{\alpha,\gamma}(q)$ can be experimentally probed by scattering experiments [5,7] and are defined in the appendix.

The computation of the charge current (18) involves the expansion of equations (7)–(9) and (16) up to first order in the flux ϕ. This gives

$$J^{\rho} = -2t\sum_{j} N_c(q_j^{c,0})k^{\phi}(q_j^{c,0})\sin[k(q_j^{c,0})] + \sum_{\gamma>0} 4t\sum_{j} N_{c,\gamma}(q_j^{c,\gamma})\,\mathrm{Re}\,\frac{u^2[R_{c,\gamma}(q_j^{c,\gamma})-\mathrm{i}\gamma]}{\sqrt{1-u^2[R_{c,\gamma}(q_j^{c,\gamma})-\mathrm{i}\gamma]^2}}R^{\phi}_{c,\gamma}(q_j^{c,\gamma}) \tag{49}$$

where $N_{c,\gamma}(q_j^{c,\gamma})$ is the distribution of occupied quantum numbers $I_j^{c,\gamma}$ in a given energy eigenstate. The functions $W^{\phi}(q)$ (with $W = k$, $R_{s,\gamma}$, and $R_{c,\gamma}$) are the derivatives of the rapidities defined by equations (7)–(9) with respect to the flux ϕ at $\phi = 0$. These obey a new set of equations that can be easily obtained from equations (7)–(9).

To obtain the charge current α, γ pseudo-particle spectrum we write equation (49) in the form

$$J^{\rho}_{m} = J^{\rho}_{0} + \sum_{\alpha,\gamma,j}\delta N_{\alpha,\gamma}(q_j^{\alpha,\gamma})J^{\rho}_{\alpha,\gamma}(q_j^{\alpha,\gamma}) \tag{50}$$

where J^{ρ}_{0} is the ground-state current, which we can choose to be zero. Moreover, we expand all of the rapidities $W(q)$ and the functions $W^{\phi}(q)$ in terms of $\delta N_{\alpha,\gamma}(q_j^{\alpha,\gamma})$. Using the same procedure as reference [39], we obtain [55]

$$J^{\rho}_{\alpha,\gamma}(q) = \sum_{\alpha'}\sum_{\gamma'}\theta(N_{\alpha',\gamma'})\mathcal{C}^{\rho}_{\alpha',\gamma'}\left[v_{\alpha,\gamma}(q)\delta_{\alpha,\alpha'}\delta_{\gamma,\gamma'} + F^{1}_{\alpha,\gamma;\alpha',\gamma'}(q)\right]. \tag{51}$$

Here the function $\theta(N_{\alpha',\gamma'})$ restricts the sums to the occupied branches of $I_j^{\alpha,\gamma}$ numbers characterizing a given energy eigenstate and

$$F^{1}_{\alpha,\gamma;\alpha',\gamma'}(q) = \frac{1}{2\pi}\sum_{j=\pm 1} jf_{\alpha,\gamma;\alpha',\gamma'}(q,\, jq_{F\alpha',\gamma'}). \tag{52}$$

The f-function $f_{\alpha,\gamma;\alpha',\gamma'}(q,q')$ is defined in the appendix and $\mathcal{C}^{\rho}_{\alpha,\gamma}$ are the coupling constants for the coupling of pseudo-particles to charge given in table 3.

Table 3. Charge couplings $\mathcal{C}^{\rho}_{\alpha,\gamma}$ of the α, γ pseudo-particles to external probes.

Type of excitation	$\mathcal{C}^{\rho}_{\alpha,\gamma}$
$c, 0$	1
$c, \gamma \geqslant 1$	2γ
s, γ	0

As in a Fermi liquid [56,57], the expressions for the elementary currents (51) involve the group velocities $v_{\alpha,\gamma}(q)$ and the interactions (or f-functions) $f_{\alpha,\gamma;\alpha',\gamma'}(q,q')$. However, in contrast to the case for the Fermi-liquid quasi-particles, the pseudo-particle charge-coupling constants listed in table 3 are different from the corresponding electronic couplings.

The coupling constants of table 3 play an important role in the description of charge transport in the many-body system and are a generalization for $\gamma > 0$ occupancy of the couplings introduced in reference [19]. In the case of a Hilbert subspace spanned by states with c and $s, 0$ occupancy only, equation (51) leads to the expressions already obtained in

reference [19]. When $\mathcal{C}^{\rho}_{\alpha,\gamma} = 0$ the corresponding α, γ pseudo-particle does not couple to charge. Note that the s, γ pseudo-particles do not directly couple to charge, in agreement with our $U \gg t$ analysis. Here we found that this result holds for arbitrary finite values of U.

In a Fermi liquid the effective charge transported by the quasi-particles is defined as the ratio of the charge-current spectrum over the group velocity, taken at the Fermi momentum [56, 57]. In the Hubbard model the quantum numbers I^{c}_{j} and $I^{s,0}_{j}$ are compactly distributed around the origin for the ground state. It is therefore sensible to define (pseudo-) Fermi points as $q^{\alpha,\gamma}_{F} = 2\pi I^{\alpha,\gamma}_{F}/L$, where $I^{\alpha,\gamma}_{F}$ is the largest quantum number occupied in the ground state. As in a Fermi liquid, the low-temperature transport properties are controlled by the excitations close to the (pseudo-) Fermi points. The ratio of the charge-current spectrum over the group velocity provides a measure of the effective charge carried by the pseudo-particles. The effective charges e_{c} and $e_{c,\gamma}$ are defined as [19]

$$e_{c} = -e\frac{J^{\rho}_{c}(q^{c}_{F})}{v_{c}(q^{c}_{F})} \qquad e_{c,\gamma} = -e\frac{J^{\rho}_{c,\gamma}(q^{c,\gamma}_{F})}{v_{c,\gamma}(q^{c,\gamma}_{F})} \tag{53}$$

respectively ($-e$ is the electronic charge).

Analytical expressions for $e_{\alpha,\gamma}$ can be derived in some limits and are given in table 4. In general we have that $e_{c,0}$ tends to $-e$ for $n \to 0$ and $n \to 1$, and for $H \to H_{c}$ for all values of U, as can be seen in figures 4 and 5. Here H_{c} is the critical magnetic field for fully polarized ferromagnetism. For intermediate densities the effective charge of the $c, 0$ pseudo-particle excitation is larger than the electron charge. The $n = 0$ and $n = 1$ limiting value of $e_{c,0}$ is simple to understand. For very low densities there is barely any interaction among the electrons and therefore the charge of the elementary excitations tends to that of the electrons. For n close to 1 the chain is almost half-filled and there are very few holes in the system—which are responsible for the charge transport. As in the low-density case, these holes do not interact very much and the effective charge of the excitations is again that of the electrons. At other fillings the effective charge is larger than the electronic charge. This may be due to a cooperative effect (in bosonization the c pseudo-particle–pseudo-hole excitations are represented by a charge-density wave). The effective charge $e_{c,0} \to 1$ as $U \to \infty$, as can be seen from figure 5. This is because in this limit the $c, 0$ pseudo-particles transform into spinless fermions.

Table 4. The effective charge carried by the pseudo-particles. The function η_{γ} is defined as $\eta_{\gamma} = 2/(\pi)\tan^{-1}[(\sin(n\pi))/(u[\gamma+1])]$. The parameter $\xi^{1}_{\alpha,\gamma;\alpha',0}$ is defined in the appendix and the parameter ξ_{0} is defined in reference [16].

	$H \to H_{c}$	$H \to 0$	$n \to 1$
$e_{c,\gamma\geqslant 1}$	$-e(2\gamma - \eta_{\gamma-1})$	$-e(2\gamma + \xi^{1}_{c,\gamma;c,0})$	$-e\,2\gamma$
$e_{c,0}$	$-e$	$-e(\xi_{0})^{2}$	$-e$

At $n = 1$ the minimal energy gap between the ground state and an energy eigenstate with one $c, 1$ pseudo-particle is the Mott–Hubbard gap Δ_{MH}, such that for $U \gg t$ we have $\Delta_{MH} = U - 4t$. The average number of doubly occupied sites is given by

$$D = \left\langle \sum_{j} \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow} \right\rangle$$

which for $U \gg t$ reads $D = \sum_{\gamma>0} \gamma N_{c,\gamma}$ [37]. This means that for $U \gg t$ one $c, 1$ pseudo-particle can be identified with the creation of a single doubly occupied site in the system. We expect, therefore, that $e_{c,1} = -2e$ in this limit. This is, in fact, confirmed by figure 6. As

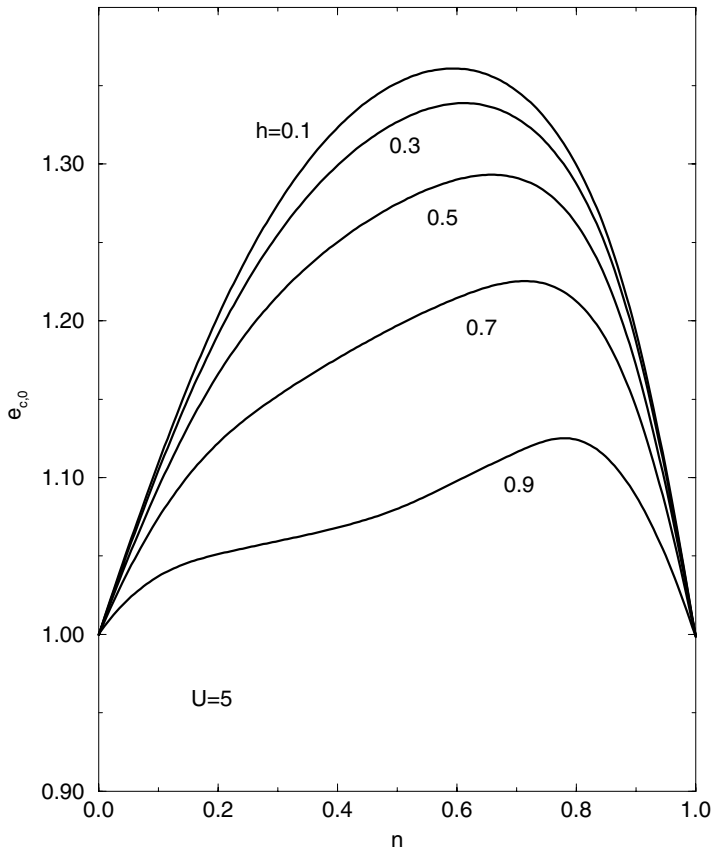

Figure 4. The effective charge $e_{c,0}$ (in units of $-e$) as a function of the electronic density n and for values of the magnetic field $h = H/H_c = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. The on-site repulsion is $U = 5$ in units of t.

U decreases the creation of c, γ pseudo-particles is not directly associated with the creation of doubly occupied sites and therefore we expect the modulus of the effective charge to be smaller than $|-2e|$, as is confirmed by figure 6. For $n \to 1$ and $n \to 0$ the large-U physics extends to all finite U-values and c, 1 pseudo-particles carry charge $-2e$ in these limits, as can be seen from figure 7 and as discussed above.

5. Semi-classical approach

The results of section 4 were obtained directly from the solution of the BA equations. We now show that the same results can be derived from a semi-classical approach.

The pseudo-particle interactions are described by the f-functions and due to the integrability of the model are of pure zero-momentum forward-scattering character. This means that the pseudo-particle collisions do not lead to momentum and energy transfer, the only result of these events being shifts in the pseudo-particle phases. As in the case of reference [19] which referred to c and s, 0 occupancy only, let us consider a semi-classical approach and assume that we perturb the system in such a way that the pseudo-particle distribution functions $N_{\alpha,\gamma}(q)$

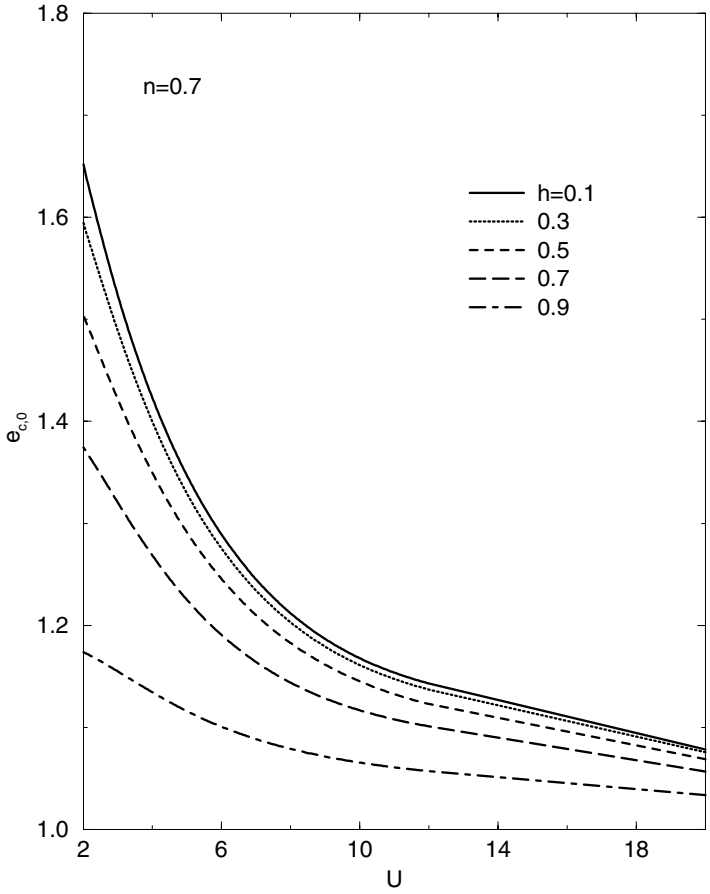

Figure 5. The effective charge (in units of $-e$) $e_{c,0}$ as a function of U (in units of t) at electronic density $n = 0.7$ and for values of the magnetic field $h = H/H_c = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. For other electronic densities the plots follow the same trends as for $n = 0.7$.

become spatially inhomogeneous and time dependent; that is,

$$N_{\alpha,\gamma}(q,x,t) = N^0_{\alpha,\gamma}(q) + \delta N_{\alpha,\gamma}(q,x,t) \tag{54}$$

where $N^0_{\alpha,\gamma}(q)$ is the initial homogeneous distribution. For example, in the ground state

$$N^0_c = \theta(q^c_F - |q|) \qquad N^0_{s,0} = \theta(q^{s,0}_F - |q|) \qquad N^0_{\alpha,\gamma>1} = 0 \tag{55}$$

where $\theta(x)$ is the step function. In a previous study, reference [39], we have computed the energy spectra of the pseudo-particle excitations. Both as in a Fermi liquid and in the case of reference [19], if the distribution functions are now spatially inhomogeneous and time dependent, the renormalized energy band of the α, γ pseudo-particle is given by

$$\breve{\varepsilon}_{\alpha,\gamma}(q,x,t) = \epsilon_{\alpha,\gamma}(q) + \frac{1}{2\pi}\sum_{\alpha',\gamma'}\int_{-q^{\alpha',\gamma'}}^{q^{\alpha',\gamma'}} \mathrm{d}q'\, \delta N_{\alpha',\gamma'}(q',x,t)\, f_{\alpha,\gamma;\alpha',\gamma'}(q,q') \tag{56}$$

where $q^{\alpha,\gamma} = 2\pi I^{\alpha,\gamma}/L$ is the limit of the pseudo-Brillouin zone and $I^{\alpha,\gamma}$ is the highest possible value of the available $I^{\alpha,\gamma}_j$ quantum numbers. Let us introduce the total charge

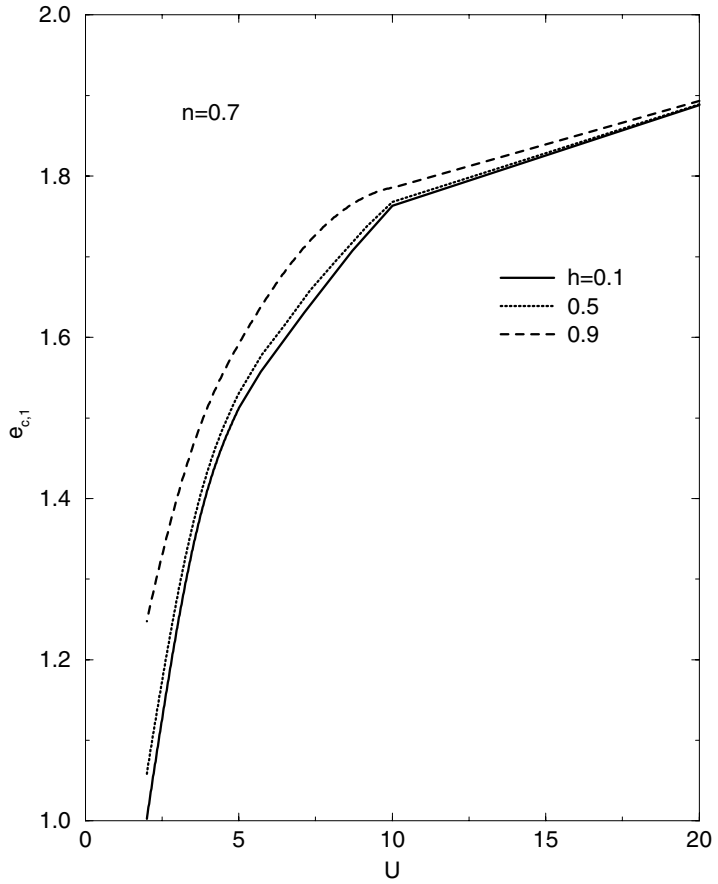

Figure 6. The effective charge $e_{c,1}$ (in units of $-e$) as a function of U (in units of t) at electronic density $n = 0.7$ and for values of the magnetic field $h = H/H_c = 0.1$ (full line), $h = 0.5$ (dotted line), and $h = 0.9$ (dashed line). For other electronic densities, the plots follow the same trends as for $n = 0.7$.

$-eN = -e(N_c + 2A_c) = \mathcal{A}^\rho$. In the case where we are considering the spatial inhomogeneity of the system, this implies that the mean total charge at point x and time t are given by

$$\langle \mathcal{A}^\rho(x,t)\rangle = \langle \mathcal{A}^\rho\rangle_0 - e\frac{L}{2\pi}\int_{-q^{c,0}}^{q^{c,0}} \mathrm{d}q\ \delta N_{c,0}(q,x,t) - e\sum_\gamma 2\gamma\frac{L}{2\pi}\int_{-q^{c,\gamma}}^{q^{c,\gamma}} \mathrm{d}q\ \delta N_{c,\gamma}(q,x,t). \tag{57}$$

The physical origin of the coupling constants listed in table 3 is clear from equation (57).

Within the semi-classical approach, the response to a scalar field, $V^\rho(x,t)$, is proportional to the conserved quantity $\mathcal{A}^\rho$. As for the case with only c and $s, 0$ occupancy [19], in the presence of the inhomogeneous potential the force $\mathcal{F}^\rho(x,t)_{\alpha,\gamma}$ that acts upon the α, γ pseudo-particle is given by

$$\mathcal{F}^\rho_{\alpha,\gamma}(x,t) = -[\partial V^\rho(x,t)/\partial x]\mathcal{C}^\rho_{\alpha,\gamma} \times (-e).$$

The deviations $\delta N_{\alpha,\gamma}(q,x,t)$ are determined from the solution of the system of kinetic

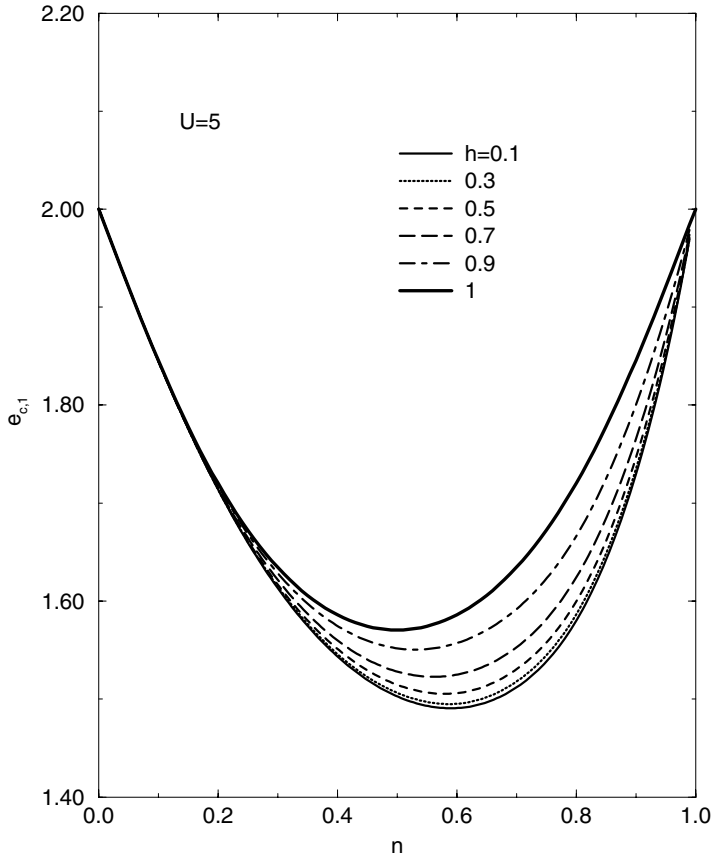

Figure 7. The effective charge $e_{c,1}$ (in units of $-e$) as a function of the electronic density n for values of the magnetic field $h = H/H_c = 0.1$, $h = 0.3$, $h = 0.5$, $h = 0.7$, and $h = 0.9$. The on-site Coulomb interaction is $U = 5$ in units of t.

equations (one equation for each occupied α, γ branch) given by

$$0 = \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial t} + \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial x}\frac{\partial \check{\varepsilon}_{\alpha,\gamma}(q,x,t)}{\partial q} - \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial q}\frac{\partial \check{\varepsilon}_{\alpha,\gamma}(q,x,t)}{\partial x} - \frac{\partial N_{\alpha,\gamma}(q,x,t)}{\partial q}\frac{\partial V^{\rho}(x,t)}{\partial x}\mathcal{C}^{\rho}_{\alpha,\gamma} \times (-e). \tag{58}$$

Introducing equation (54) in equation (58), expanding to first order in $\delta N_{\alpha,\gamma}(q,x,t)$, and using equation (56), we obtain the following set of linearized kinetic equations:

$$0 = \frac{\partial\, \delta N_{\alpha,\gamma}(q,x,t)}{\partial t} + v_{\alpha,\gamma}(q)\frac{\partial\, \delta N_{\alpha,\gamma}(q,x,t)}{\partial x} - \frac{\partial\, \delta N_{\alpha,\gamma}(q,x,t)}{\partial q}\frac{\partial V^{\rho}(x,t)}{\partial x}\mathcal{C}^{\rho}_{\alpha,\gamma}(-e) - \frac{\partial N^{0}_{\alpha,\gamma}(q,x,t)}{\partial q}\sum_{\alpha',\gamma'}\frac{1}{2\pi}\int_{-q_{\alpha',\gamma'}}^{q_{\alpha',\gamma'}} \mathrm{d}q'\, \frac{\partial\, \delta N_{\alpha',\gamma'}(q',x,t)}{\partial x} f_{\alpha,\gamma;\alpha',\gamma'}(q,q'). \tag{59}$$

Since $\langle \mathcal{A}^{\rho}(x,t)\rangle$ is a conserved quantity, the corresponding current $\langle \mathcal{J}^{\rho}(x,t)\rangle$ is given by

$$\frac{\partial \langle \mathcal{A}^{\rho}(x,t)\rangle}{\partial t} + \frac{\partial \langle \mathcal{J}^{\rho}(x,t)\rangle}{\partial x} = 0. \tag{60}$$

In order to derive $\langle \mathcal{J}^{\rho}(x,t)\rangle$, let us multiply equation (59) by $\mathcal{C}^{\rho}_{\alpha,\gamma} \times (-e)$, sum over α and γ, and integrate over q, obtaining (for $V^{\rho}(x,t) = 0$)

$$0 = \frac{\partial \langle \mathcal{A}^{\rho}(x,t)\rangle}{\partial t} + \frac{\partial}{\partial x}\left[\frac{L}{2\pi}\int \mathrm{d}q \sum_{\alpha,\gamma}(-e)\mathcal{C}^{\rho}_{\alpha,\gamma} v_{\alpha,\gamma}(q)\,\delta N_{\alpha,\gamma}(q,x,t) + \sum_{j=\pm 1}\sum_{\alpha,\gamma}(-e)\mathcal{C}^{\rho}_{\alpha,\gamma}\frac{L}{(2\pi)^2}\int \mathrm{d}q' \sum_{\alpha',\gamma'} j f_{\alpha,\gamma;\alpha',\gamma'}(jq_F^{\alpha,\gamma}, q')\,\delta N_{\alpha,\gamma}(q,x,t)\right]. \tag{61}$$

We than see that the conserved current can be written as

$$\langle \mathcal{J}^{\rho}(x,t)\rangle = -e\frac{L}{2\pi}\int \mathrm{d}q \sum_{\alpha,\gamma} J^{\rho}_{\alpha,\gamma}(q)\,\delta N_{\alpha,\gamma}(q,x,t) \tag{62}$$

with $J^{\rho}_{\alpha,\gamma}(q)$ given by

$$J^{\rho}_{\alpha,\gamma}(q) = \mathcal{C}^{\rho}_{\alpha,\gamma} v_{\alpha,\gamma}(q) + \frac{1}{2\pi}\sum_{j=\pm 1}\sum_{\alpha',\gamma'} j\mathcal{C}^{\rho}_{\alpha',\gamma'} f_{\alpha',\gamma';\alpha,\gamma}(jq_F^{\alpha',\gamma'}, q) \tag{63}$$

which, by symmetry, equals equation (51), derived from the solution of the BA equations using units of $-e = 1$. In the above discussion it was assumed that the sums over α, γ are restricted to the pseudo-particle branches with occupied $I_j^{\alpha,\gamma}$ quantum numbers.

Let us now use equation (62) in a simple application and compute the zero-temperature charge stiffness [19, 25]. This quantity is defined as [25, 38]

$$D = \frac{1}{2}\frac{\mathrm{d}^2(E_0/L)}{\mathrm{d}^2(\phi/L)}\bigg|_{\phi/L=0} = \frac{1}{2}\frac{\mathrm{d}(J_0^{\rho}/L)}{\mathrm{d}(\phi/L)}\bigg|_{\phi/L=0} \tag{64}$$

where E_0 and J_0^{ρ} stand for the ground-state energy and charge current in the presence of a small flux ϕ/L, respectively. That is, the charge stiffness can be determined by perturbing the ground-state charge current with a small flux ϕ/L:

$$\langle \mathcal{J}^{\rho}(x,t)\rangle = -e\frac{L}{2\pi}\int \mathrm{d}q\; J_c^{\rho}(q)\,\delta N_c(q,x,t). \tag{65}$$

The smallest perturbation on the J_0^{ρ} induced by ϕ/L corresponds the following asymmetric occupancy of the I_j^c numbers (for N even and N_{σ} odd):

$$I_j^c = -\frac{N-3}{2}, -\frac{L-3}{2}, \ldots, -\frac{1}{2}, \frac{1}{2}, \ldots, \frac{L-3}{2}, \frac{N-1}{2}, \frac{N+1}{2}. \tag{66}$$

This implies that $\delta N_c(q,x,t)$ corresponds to

$$\delta N_c(q,x,t) = \frac{2\pi}{L}\delta\left(q_1^c - \frac{\pi(N-1)}{L}\right) + \frac{2\pi}{L}\delta\left(q_2^c - \frac{\pi(N+1)}{L}\right) \tag{67}$$

leading in the thermodynamic limit (in units $-e = 1$) to

$$D = \frac{J_c^{\rho}(q_F^c)}{2\pi} \tag{68}$$

in agreement with references [19, 25]. In a similar manner we can derive the spin current, and from it the spin stiffness.

6. Concluding remarks

In this paper we have derived the current spectra and effective charges carried by the pseudo-particles of the 1D Hubbard model. Alternatively to the c and s, 0 pseudo-particles, the present results can be re-expressed in terms of holons and spinons, which can be identified with the c and s, 0 pseudo-holes. Moreover, for $\gamma > 0$, the c, γ and s, γ pseudo-particles can be shown to be associated with 'bound states' of 2γ holons and spinons, respectively.

In the case $U = \infty$ we have shown that the s, 0 pseudo-particle excitations do not carry spin. This is so because in this limit the energy dispersions of the s, γ pseudo-particles are flat. Nevertheless, the c, 0 pseudo-particle does transport spin if a finite magnetic field is applied to the system and $n < 1$. In the limit $U \to \infty$, we have shown that the spin is transported by the spinons when a spin-singlet excitation is created. We have also shown that spinons do not couple directly to charge probes. Again, for finite magnetic field the spin current has a contribution from the c pseudo-particle excitations, except at half-filling. When $n = 1$ we are in the insulating regime and charge transport in possible by means of exciting c, γ pseudo-particles across the Mott–Hubbard gap.

The pseudo-particles (or holons and spinons) play in the 1D Hubbard model the same role as the quasi-particles in Fermi-liquid theory. However, while the quasi-particles are labelled by the same quantum numbers as the electrons, only their energies being renormalized, the pseudo-particles (or holons and spinons) refer to different quantum numbers. For instance, while the Fermi-liquid quasi-particles have the same couplings to charge as the electrons, the pseudo-particle charge couplings given in table 3 differ from those of the electrons.

Since in the present model the electronic degrees of freedom couple to external charge and spin probes through the pseudo-particles (or holons and spinons), these exotic elementary particles are the transport carriers. For instance, the charge conductivity is fully determined by the coupling of these carriers to charge, as was shown in references [13, 37]. Furthermore, the results of reference [13] suggest that the unusual spectral properties detected in quasi-one-dimensional materials are successfully described by the pseudo-particle (and holon) transport.

Acknowledgment

This research was supported by the Portuguese Program PRAXIS XXI under grant number 2/2.1/FIS/302/94.

Appendix A. Excitation dispersions and f-functions

The pseudo-particle energy bands $\epsilon_{\alpha,\gamma}(q)$ are given by

$$\epsilon_c(q) = -2t\cos k^{(0)}(q) + 2t\int_{-Q}^{Q} \mathrm{d}k\ \widetilde{\Phi}_{c,0;c,0}(k, k^{(0)}(q))\sin k \tag{A.1}$$

$$\epsilon_{c,\gamma}(q) = 4t\,\mathrm{Re}\sqrt{1 - u^2[R^0_{c,\gamma}(q) - \mathrm{i}\gamma]^2} + 2t\int_{-Q}^{Q} \mathrm{d}k\ \widetilde{\Phi}_{c,0;c,\gamma}(k, R^{(0)}_{c,\gamma}(q))\sin k \tag{A.2}$$

$$\epsilon_{s,\gamma}(q) = 2t\int_{-Q}^{Q} \mathrm{d}k\ \widetilde{\Phi}_{c,0;s,\gamma}(k, R^{(0)}_{s,\gamma}(q))\sin k \tag{A.3}$$

where $Q = k^{(0)}(q_F^{\alpha,\gamma})$, $q_F^{c,0} = 2\pi I_F^{c,0}/L$, and the superscript (0) on $k(q)$ and $R^{\alpha,\gamma}$ indicates that these functions are computed in the ground state.

The functions $\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q')$ are the two-pseudo-particle phase shifts [39]. (In the case of the phase shifts and associated functions, we use the notation $c,0=c$.) The f-functions can be expressed in terms of the phase shifts and read

$$\frac{1}{2\pi}f_{\alpha,\gamma;\alpha',\gamma'}(q,q') = v_{\alpha,\gamma}(q)\Phi_{\alpha,\gamma;\alpha',\gamma'}(q,q') + v_{\alpha',\gamma'}(q')\Phi_{\alpha',\gamma';\alpha,\gamma}(q',q) + \sum_{j=\pm 1}\sum_{\alpha''}\sum_{\gamma''}\theta(N_{\alpha'',\gamma''})v_{\alpha'',\gamma''}\Phi_{\alpha'',\gamma'';\alpha,\gamma}(jq_{F\alpha'',\gamma''},q) \times \Phi_{\alpha'',\gamma'';\alpha',\gamma'}(jq_{F\alpha'',\gamma''},q'). \quad (A.4)$$

Finally, the parameters $\xi^1_{\alpha,\gamma;\alpha',\gamma'}$ of table 4 are combinations of these phase shifts given by

$$\xi^1_{\alpha,\gamma;\alpha',\gamma'} = \delta_{\alpha,\alpha'}\delta_{\gamma,\gamma'} + \sum_{j=\pm 1} j\Phi_{\alpha,\gamma;\alpha',\gamma'}(q_F^{\alpha,\gamma};jq_F^{\alpha',\gamma'}). \quad (A.5)$$

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