Charge currents of spin excitations in one-dimensional Hubbard model

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The current-carrying states in a one-dimensional system of interacting electrons are considered. The new exact results for the Hubbard model and for the bosonization method are used. Away from half filling both spin and charge excitations were found to carry currents which are proportional to their momenta for most cases. Being in a qualitative agreement with a single-particle picture of the noninteracting 1D Fermi gas, this result contradicts the spin-charge separation concept, since it is usually derived, e.g., from the bosonization approach or in strong repulsion picture. The paradox can be resolved by taking into account the spectrum parabolicity and re-examining the structure of the current operator within the bosonization approach.

It is commonly accepted that in repulsive one-dimensional Fermi liquids (see Refs. 1 and 2 for reviews) the spin and charge are "deconfined." The elementary excitations are *spinons* (which carry spin and no charge) and *holons* (which carry charge and no spin).[3] A hole in the Fermi sea splits spontaneously into a spinon-holon pair, while a spin-flip triplet excitation decays into two spinons. Such a deconfinement is apparent in at least two limits:

• *Weak coupling*, in which the problem may be bosonized.[4,5] The spectrum close to the Fermi level is assumed to be linear. Spin and charge fluctuations propagate at different velocities and an initially localized perturbation splits.

• *Strong-coupling* Hubbard model, which in leading order leads to spinless free fermions, with a residual Heisenberg interaction between spins (disregarding holes). Spinons appear as Bloch walls in the underlying local antiferromagnetic order, while holons are holes which do not disrupt the spin alternation along the lattice. The problem can be solved exactly in the Hubbard model using the Bethe ansatz solutions, for arbitrary interaction strength U and band filling ρ.[3,6–8] Such an analysis confirms the existence of spinons and holons. The corresponding spectra $\varepsilon_s(q)$ and $\varepsilon_h(q)$, as well as the allowed ranges of q are known.

In practice, spin-charge deconfinement raises a number of problems, even in 1D. In the weak-coupling limit, for instance, the spinon and holon spectra are found to be

$$\varepsilon_h(q)=4t(\cos q/2-\cos k_F), \quad |q|<\pi, \tag{1}$$

$$\varepsilon_s(q)=2t(\cos q-\cos k_F), \quad |q|<k_F. \tag{2}$$

It is straightforward to construct the continuum of hole states $\varepsilon(p)=\varepsilon_s(q)+\varepsilon_h(p-q)$ and to look for its lower bound $\varepsilon_{\min}$. The free hole energy is found to be $\varepsilon=2t\cos p<\varepsilon_{\min}(p)$. Thus the hole appears as a bound state of the spinon-holon pair! Very close to the Fermi level the two energies become equal, and the hole is indeed at the bottom of the continuum. There is therefore a marginal deconfinement. This is not true away from the Fermi level. (Marginal deconfinement actually occurs in holons and several spinons.) Such a bound state may disappear for larger U: this is not, however, manifestly clear!

Even if spin and charge are deconfined, the issue of the currents associated with each of these excitations arises. In a bosonization approximation[4,5] the answer is simple: a spin excitation carries no charge current whatsoever (decoupling is complete). Reasonable as it may seem, *this is actually wrong*—for reasons that are rather fundamental. Once again, this conclusion is obvious in two limits which shed light on the underlying physics.

• In a free Fermi gas ($U=0$), the elementary spin excitation is a spin flip (implying two spinons) in which a particle $k\uparrow$ below the Fermi level is moved to $(k+q)\downarrow$ above. The corresponding charge current is clearly

$$j=v_{k+q}-v_k, \tag{3}$$

where $v_k=\partial\varepsilon_k$ is the group velocity. Spin does not matter, and current is clearly related to the curvature of the spectrum $\partial v_k/\partial k$. The failure of the bosonization methods in getting j is then obvious: one assumes a linear spectrum with no curvature.

• In the opposite limit of strong coupling, $U\to\infty$, the Bethe ansatz (BA) solution simplifies considerably. It is expressed in terms of N_a orbital momenta k_i and M spin rapidities λ_a that satisfy the set of equations[3]

$$N_a k_j-\sum_{\beta=1}^{M}\theta(2\sin k_j-2\lambda_\beta)=2\pi I_j=N_a q_j \quad j=1,\dots N, \tag{4}$$

$$\sum_{j=1}^{N}\theta(2\sin k_j-2\lambda_\alpha)+\sum_{\beta=1}^{M}\theta(\lambda_\alpha-\lambda_\beta)=2\pi J_\alpha=N_a p_\alpha, \quad \alpha=1,\dots M, \tag{5}$$

where $\theta(x)=-2\arctan(2x/u)$, $u=U/t$, $N=\rho N_a$ is the number of particles, M is the number of spins "down," N_a is the number of chain sites, $\{I_j\}$, $\{J_\alpha\}$ are sets of integer or half-integer values, U is the value of the Hubbard onsite repulsion, and t is the hope integral between the nearest sites.

The total energy, momentum, and current are[3,9]

$$E=-2t\sum_t \cos k_i, \quad p=\sum_i k_i=\sum_i q_i+\sum_\alpha p_\alpha, \quad j=2t\sum_i \sin k_i. \tag{6}$$

In leading order in $1/U$ the rapidities are on the order of U. Equations (4) and (5) reduce to

$$k_i=q_i+\delta k, \quad -N\theta(2\lambda_\alpha)+\sum_\beta \theta(\lambda_\alpha-\lambda_\beta)=N_a p_\alpha. \tag{7}$$

Each k_i is shifted by a constant $\delta k = -(1/Na)\,\Sigma\,\theta(2\lambda_\alpha) = (1/N)\,\Sigma\,p_\alpha = p_s/N$, where p_s is the total momentum of spin excitations. (The calculation can be easily extended to first order in $1/U$, thereby generating the Heisenberg exchange). The total charge current is

$$j = J_0 - E_0 p_s/N_a, \quad J_0 = 2t \sum_i \sin q_i, \quad E_0 = -2t \sum_i \cos q_i. \tag{8}$$

The presence of spin excitations thus generates a charge current proportional to p_s. The spin and charge are decoupled, but the spin degrees of freedom modify the boundary conditions, thereby shifting the momenta slightly (they occupy part of the phase space), which accounts for the charge current.

These simple limits clearly demonstrate the existence of the effect and its physical origin. The charge current associated with spin is due to the curvature of the kinetic energy (the dispersion of the velocity). In the Hubbard model the curvature vanishes in the case of half filling, for which $E_0 = 0$: the spin-mediated current will then be zero, as expected. The physics is thus clear and consistent.

In practice, a much more general approach, with full BA solution, can be used. The rest of this article explores some of these generalizations, as well as the physical implications of that result.

The charge currents have been already evaluated explicitly for the strong-interaction limit.[9] Our recent studies for the weak-coupling limit and the calculations for a finite magnetic flux have shed more light and sharpened the above-mentioned contradiction. The following types of excitations have been considered: spin triplet and singlet pairs, hole and particle states, added particles, and gap states at half-filling history $\rho = 1$. All details will be published elsewhere.[10] Here we will concentrate mostly on the spin triplet states.

Consider the Hubbard model for $N = \rho N_a$ particles on the ring of N_a atoms in the presence of a magnetic flux Φ through it. The ground state and excitations are described by the BA equations (4) and (5), in which the following substitution should be made[11,12] $N_a k_j \to N_a(k_j - \nu)$, leaving $\sin k_j$ unchanged. Here, $\nu = (2\pi/N_a)(\Phi/\Phi_0)$, $\Phi_0 = hc/e$ is the unit magnetic flux.

Spin excitations were studied basically in Refs. 7, 8, 13, and 14. By analogy with the 1D Heisenberg model, the elementary spin excitations of the 1D Hubbard model are spin doublets ($s = 1/2$), which have an even number. Two spinons can form a spin singlet or a spin triplet excitation.

The excited states can be easily described[9] by the function $\tilde{\rho}(k_j) = N_a \rho_0(k_j)\delta k_j$, $\rho_0(k_j) = 1/[N_a(k^0_{j+1} - k^0_j)]$, where ρ_0 is a known function for the ground state,[3] and δk_j is the shift of the wave number $k_j - \nu$ due to the excitation.

For the spin triplet excitation the function $\tilde{\rho}(k) = f(\sin k)$ obeys the equation

$$f(t) = \nu/\pi + \sum_{i=1,2} 1/\pi \arctan(\exp 2\pi(t - \lambda_i)/u) + \int_{-\sin Q}^{\sin Q} f(t')K(t - t')dt', \tag{9}$$

where K is the standard BA kernel: the Fourier transform of $[\exp(|\omega|u/2)+1]^{-1}$, and $[-Q,Q]$ is the interval of k_j distribution for the ground state.[3] The momentum, the energy, and the current of excitations are expressed[9] in terms of $\tilde{\rho}(k)$ as follows:

$$p=\int_{-Q+\nu}^{Q+\nu}\tilde{\rho}(k)dk,\quad \epsilon=2\int_{-Q+\nu}^{Q+\nu}\tilde{\rho}(k)\sin kdk,\quad j=2\int_{-Q+\nu}^{Q+\nu}\tilde{\rho}(k)\cos kdk. \tag{10}$$

Alternatively, the current can be obtained as $j=-N_a\delta\epsilon/\delta\Phi$. There are two modifications due to the magnetic field: the new term ν/π in (9) and the shifts of the integration limits in (10).

All values are 2π periodic functions of Φ/Φ_0. To find the contribution of a single excitation, we must assume Φ to be an intensive variable in the mesoscopic sense, so that $\nu\sim 1/N_a$. In first two orders in Φ/Φ_0 we find for $u\gg 1$

$$\epsilon=v_s|p_s|+2\frac{\sin\pi\rho}{\pi}\nu^2N_a+2p_s\frac{\sin\pi\rho}{\pi\rho}\nu, \tag{11}$$

$$j=-8(\Phi/\Phi_0)\sin(\pi\rho)+2p_s\sin(\pi\rho)/\pi\rho,\quad p=p_s+2\pi\rho\Phi/\Phi_0. \tag{12}$$

Here p and p_s are the momentum and its value at $\nu=0$, so that the variation in ν should occur at the given p_s which is quantized by integral BA numbers. The first term in (12) is the diamagnetic ground-state contribution, and the second term is the *paramagnetic orbital spin wave current.* A more detailed information is provided by direct calculations of currents at zero flux $\Phi=0$.

The eigenvalues of the triplet excitations are decomposed additively to the corresponding values of the two spinons: $p=p_1+p_2$, $\epsilon=\epsilon_1+\epsilon_2$, $j=j_1+j_2$. For example, at small $u/\sin\pi\rho\ll 1$ we obtain (1)–(3) with $q=\pi\rho/2-p_i$ and $k_F=\pi\rho/2$: $j(p_i)=2[\sin(\pi\rho/2)-\sin(\pi\rho/2-p_i)]$. At a small momentum $p\ll 1$ we find that in the limits of weak and strong interactions the charge current of a spinon is

$$u\ll 1:\quad j\approx 2p\cos(\pi\rho/2);\quad u\gg 1:\quad j\approx 2p\sin\pi\rho/(\pi\rho),$$

in accordance with (2), (3), and (8). We have confirmed that at $\rho\neq 1$ the spin triplet waves carry the electric current which is proportional to the momentum.

The *spin singlet states*[8,13] are described by an additional pair of complex numbers $\lambda_0=\Lambda\pm i\Gamma$ and after bulky calculations[10] we obtain the same equation as the one [Eq. (9)] for the triplet case. Consequently, the energy and the current coincide for the singlet and the triplet states.

The hole states are the gapless charge excitations.[3,7] They are determined by a hole in the k distribution. The equation[10] for $\tilde{\rho}(k)$, the energy,[7] and the current[9] were found for $u\gg 1$. At the opposite limit $u\ll 1$ we find[10] the same results as for the triplet states. For large values of u the results are different: for the hole state the current is $j\approx 2p\cos(\pi\rho/2)$ in comparison with that at $u\gg 1$.

The states with one added particle are described by similar expressions for the energy and for the current at both limits, $u\gg 1$, (Ref. 9) and $u\ll 1$ (Ref. 10), [(1) and (3)] as $\epsilon\approx -2\cos p$, $j\approx\sin p$, $|p|>Q$.

We conclude that not only the charge excitations (hole and particle states, states with added particles) but also the spin states (spin triplet and singlet excitations) carry the electric current, $j\propto p$, at small p. Next we will consider this problem in the framework of the bosonization approach.

The bosonization procedure[4,5] relies upon a decomposition of the Fermi operator into right and left moving parts $\Psi_{\sigma,\pm}$, on the spectrum linearization in the vicinity of $\pm k_F$, and on a conceptually inconsistent interpretation of a two-parametric, low-energy cusp of particle-hole excitations [(1) and (2)] as a single spectrum of zero-sound like bosons. We introduce the Bose field φ_σ and the conjugated momentum π_σ with an appropriate "momentum cutoff" regularization. In these variables the Hamiltonian acquires a separable form $H\Rightarrow H(\varphi)+H(\sigma)$, where $\varphi=(\varphi_\uparrow+\varphi_\downarrow)/2$ and $\sigma=(\varphi_\uparrow-\varphi_\downarrow)/2$ are the charge and the spin polarization fields. For the forward scattering (the Tomanaga-Luttinger model) or, asymptotically, for the repulsive Hubbard model at $\rho\neq 1$ the Hamiltonians describe the sounds

$$H(\varphi)\propto(\partial_x\varphi)^2+\pi_\varphi^2;\quad H(\sigma)\propto(\partial_x\sigma)^2+\pi_\sigma^2. \tag{13}$$

The charge density n and the current j operators are expressed as $n\sim\partial_x\varphi$, $j=\Psi^\dagger\sigma_z\Psi\propto-\pi_\varphi\propto-\partial_t\varphi$, so that they contain the charge field operators only. Consequently, the eigenstates of the spin Hamiltonian $H(\sigma)$ should carry no current and should not interact with the electric field.

This general conclusion is in apparent disagreement with the exact results for the Hubbard model and for the noninteracting limit, as we have indicated above. In order to resolve the discrepancy, we will take into account the spectrum curvature (the Fermi velocity dispersion) Γ, which should obviously mix the degrees of freedom. The Hamiltonian and the current will then have the additional parts $H\to H+\delta H$, $\delta H=-\Gamma\Psi^\dagger\partial_x\Psi$, $\Gamma\approx\cos\pi\rho/2$; $j\Rightarrow j+\delta j$. Here the value Γ is given for the Hubbard model. Finally, we obtain

$$\delta n=0,\quad \delta j=\Gamma\Psi^\dagger(-i\partial_x)\Psi\sim-\Gamma(\partial_x\varphi\pi_\varphi+\partial_x\sigma\pi_\sigma),\quad \Gamma\approx\cos\pi\rho/2, \tag{14}$$

$$\delta H\sim(\partial_x\varphi)^3+3\partial_x\varphi[(\partial_x\sigma)^2+\pi_\varphi^2+\pi_\sigma^2]+6\pi_\varphi\pi_\sigma\partial_x\sigma. \tag{15}$$

Remarkably, the operator's relations $n\sim\partial_x\varphi$ and $j\sim-\partial_t\varphi$ have not been affected; what has been changed, however, is the equation of motion $\partial_t\varphi\sim\pi_\varphi$, which is now destroyed due to (15).

Let us now consider the effects of these modifications.

a) *Spin excitation currents.* The lowest excitations (magnons) of the spin Hamiltonian can be obtained by quantizing H_σ at $\Gamma=0$. It follows from (13) that

$$H_\sigma=\sum_k|k|a_k^\dagger a_k,\quad |\Omega>\rangle=a_k^\dagger|0\rangle,\quad \langle\Omega|j|\Omega\rangle=\Gamma k, \tag{16}$$

where $a_k\dagger$ and a_k are the creation and the annihilation magnon operators. The current is therefore proportional to the momentum; the ratio is independent of the weak interaction, in agreement with the exact results.

b) *Charge excitation currents.* For excitations of the charge Hamiltonian $H(\sigma)$ we find similarly to (16), in contrast with the spin case, that the current operator now has two contributions:

$$\langle\Omega|j|\Omega\rangle=\langle\Omega|\pi_\varphi|\Omega\rangle+\Gamma\langle\Omega|\pi_\varphi\partial\varphi/\partial x|\Omega\rangle. \tag{17}$$

The first term in (17) vanishes due to the nondiagonal nature of π_φ, so that the average value of the current remains the same, $\approx\Gamma k$, as for the spin excitation.

The mean value of $\langle\pi_\varphi\rangle$ can become nonzero and the contribution linear in the boson operators appears only for those states which are not eigenstates of the charge sound Hamiltonian. This occurs at the macroscopic current-carrying ground state. The magnetic flux is the current-controlling conjugated variable, when the number of sound bosons is not conserved due to the presence of the term $j\Phi\sim\Phi\pi_\varphi$ in the Hamiltonian.

Conclusions. For the Hubbard model with arbitrary filling ρ, both the charge (hole and particle) and the spin (singlet and triplet) gapless excitations carry a current, $j\propto p$ at $p\ll 1$. At the half filling $\rho=1$, only the states with one added particle are charged. In the bosonization approach for a linearized bare electronic spectrum neither spin nor charge sound excitations carry a current. The current arises only for macroscopic coherent states, when the number of charge sound bosons is not conserved, for example, in the presence of a magnetic flux. Allowance for the spectrum parabolicity leads to nonzero currents ($j\propto p$) for the charge and spin boson excitations, in agreement with the exact results for the Hubbard model and with the free fermion picture.

The appearance of the spin-wave charge current is both unexpected and natural. Remarkably, the spin-wave spectra and the whole BA construction evolve gradually, unlike other excitations, from the Heisenberg chain, which is equivalent at $\rho=1$ and $u\neq 0$ to arbitrary ρ. This is why it is tempting to view them as spin waves even in the presence of holes, $\rho\neq 1$. At the same time, for $\rho\neq 1$ there is a continuous evolution of spin excitations toward $u=0$, when they should become triplet electron-hole pairs. As such the triplet excitations evidently carry the current due to the electron-hole asymmetry caused by the Fermi velocity dispersion at $\rho\neq 1$. The bosonization tends to ignore this feature, as well as all effects of sound decomposition into a band of doublets. When u is not small, the currents cannot be interpreted anymore in terms of the spectrum curvature. The BA solution provides us with a more general point of view: the distributions of the holon quantum numbers are shifted in the presence of a spinon.

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