

CHARGE CURRENTS OF SPIN EXCITATIONS IN ONE DIMENSIONAL HUBBARD MODEL

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Submitted 21 October 1993

We consider current carrying states in a one dimensional system of interacting electrons. The new exact results for the Hubbard model and for the bosonization method are exploited. We find that away from half filling both spin and charge excitations 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 to the spin-charge separation concept as it is usually derived e.g. from the bosonization approach or in a strong repulsion pictures. The paradox is resolved by taking into account the spectrum parabolicity and reexamining the structure of the current operator within the bosonization approach.

It is commonly accepted that in repulsive one dimensional Fermi liquids (see [1, 2] for a reviews) spin and charge are "deconfined". Elementary excitations are *spinons* (that carry spin and no charge) and *holons* (that carry charge and no spin) [3]. A hole in the Fermi sea is supposed to split spontaneously into a spinon-holon pair, while a spin flip triplet excitations 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 that do not disrupt the spin alternation along the lattice. The problem can be solved exactly in the Hubbard model using 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 $\epsilon_s(q)$ and $\epsilon_h(q)$ are known, as well as the allowed ranges of q .

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

$$\epsilon_h(q) = 4t(\cos q/2 - \cos k_F), \quad |q| < \pi, \quad (1)$$

$$\epsilon_s(q) = 2t(\cos q - \cos k_F), \quad |q| < k_F. \quad (2)$$

It is straightforward to construct the continuum of hole states $\epsilon(p) = \epsilon_s(q) + \epsilon_h(p-q)$ and to look for its lower bound ϵ_{min} . One finds that the free hole energy: $\epsilon = 2t \cos p < \epsilon_{min}(p)$. 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 - hence there is a marginal deconfinement. This is not true away from Fermi level. (Marginal deconfinement actually occurs into holons and several spinons). Such a bound state may disappear for larger U : it is not obvious!

Even if spin and charge are really deconfined, the issue arises of the currents associated to each of these excitations. Within a bosonization approximation [4, 5] the answer is simple: a spin excitation carries no charge current whatsoever (decoupling is complete). Reasonable as it may look, *this is actually wrong* - for reasons that are rather fundamental. Once again, that conclusion is obvious in two limits that 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 Fermi level is shipped to $(k + q) \downarrow$ above. The corresponding charge current is clearly

$$j = v_{k+q} - v_k \quad (3)$$

where $v_k = \partial \varepsilon_k / \partial k$ 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, $U \rightarrow \infty$, the Bethe Ansatz (BA) solution simplifies considerably. It is expressed in terms of N_a orbital momenta k_j and M spin rapidities λ_α that satisfy the set of equations [3]

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

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

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 halfinteger values, U is the value of Hubbard onsite repulsion, t is the hopping integral between the nearest sites.

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

$$E = -2t \sum_i \cos k_i, \quad p = \sum_i k_i = \sum_i q_i + \sum_\alpha p_\alpha, \quad j = 2t \sum_i \sin k_i \quad (6)$$

In leading order in $1/U$ the rapidities are of order U . The above equations (4,5) reduce to

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

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

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

The presence of spin excitations thus generates a charge current proportional to p_s . Spin and charge are indeed decoupled, but the spin degrees of freedom modify

the boundary conditions, thereby shifting momenta somewhat (they occupy part of phase space) - hence a charge current.

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

In practice one may be much more general using the full BA solution. The rest of this note explores some of these generalizations, as well as the physical implications of that result.

The charge currents have been already evaluated explicitly for a strong interaction limit [9]. Our recent studies for a weak coupling limit and the calculations for a finite magnetic flux have given 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, gap states at half filling history $\rho = 1$. All details will be published elsewhere [10]. Here we will concentrate mostly on 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), (5), in which one should change [11, 12] $N_a k_j \rightarrow N_a(k_j - \nu)$, leaving $\sin k_j$ unchanged. There $\nu = (2\pi/N_a)(\Phi/\Phi_0)$, $\Phi_0 = hc/e$ is the unit magnetic flux.

Spin excitations were studied basically in [7, 8, 13, 14]. Similarly to the 1d Heisenberg model, elementary spin excitations of the 1d Hubbard model are spin doublets ($s = 1/2$), their number being even. Two spinons can form a spin singlet or a spin triplet excitation.

Excited states are conveniently described [9] by the function $\tilde{\rho}(k_j) = N_a \rho_0(k_j) \delta k_j$, $\rho_0(k_j) = 1/(N_a(k_{j+1}^0 - k_j^0))$, where ρ_0 is a known function for the ground state [3], δk_j is the shift of a wave number $k_j - \nu$ due to the excitation.

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

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

where K is the standard BA kernel: the Fourier transform of $[\exp(|\omega|u/2) + 1]^{-1}$, $[-Q, Q]$ 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:

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

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 integration limits in (10).

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

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

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

Here p and p_s are the momentum and its value at $\nu = 0$ so that the variation in ν should be taken at given p_s , which is quantized by integral BA numbers. The first term in (12) is the diamagnetic ground state contribution, the second one 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 a triplet excitations are decomposed additively to corresponding values of the two spinons: $p = p_1 + p_2$, $\epsilon = \epsilon_1 + \epsilon_2$, $j = j_1 + j_2$. E.g. at small $u/\sin \pi\rho \ll 1$ we arrive at (1)–(3) with $q = \pi\rho/2 - p_i$, $k_F = \pi\rho/2$: $j(p_i) = 2(\sin(\pi\rho/2) - \sin(\pi\rho/2 - p_i))$. At small momentum $p \ll 1$ we find for both limits of weak and strong interactions the charge current of a spinon as

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

in accordance with (2), (3), (8). We have confirmed that at $\rho \neq 1$ spin triplet waves carry the electric current 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 (9) for the triplet case. Consequently the energy and the current coincide for the singlet and for 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 for $\tilde{\rho}(k)$ [10], 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 triplet states. At large u results are different: for the hole state the current is $j \approx 2p \cos(\pi\rho/2)$ in compar to at $u \gg 1$.

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

We conclude that not only charge excitations (hole and particle states, states with added particles) but also 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 $\Psi_{\sigma,\pm}$ and 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), (2) as a single spectrum of zero sound like bosons. One introduces 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 case (the Tomanaga - Luttinger model) or asymptotically for the repulsive Hubbard model at $\rho \neq 1$ the Hamiltonians describe the sounds

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

The charge density n and 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 $H(\sigma)$, would carry no current and they would not interact with electric field.

This common conclusion is in apparent disagreement with both exact results for the Hubbard model and for the noninteracting limit as we have discussed 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. Then the Hamiltonian and the current acquire additional parts $H \rightarrow H + \delta H$, $\delta H = -\Gamma \Psi^\dagger \partial_x \Psi$, $\Gamma \approx \cos \pi \rho / 2$; $j \Rightarrow j + \delta j$. here the value Γ is given for the Hubbard model. Finally we obtain

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

$$\delta H \sim (\partial_x \varphi)^3 + 3 \partial_x \varphi \left[(\partial_x \sigma)^2 + \pi_\varphi^2 + \pi_\sigma^2 \right] + 6 \pi_\varphi \pi_\sigma \partial_x \sigma. \quad (15)$$

Remarkably the operator's relations $n \sim \partial_x \varphi$ and $j \sim -\partial_t \varphi$ are not effected, but what is changed is the equation of motion $\partial_t \varphi \sim \pi_\varphi$, which is now destroyed due to (15).

Consider now effects of these modifications.

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

$$H_\sigma = \sum_k |k| a_k^\dagger a_k, \quad |\Omega\rangle = a_k^\dagger |0\rangle, \quad \langle \Omega | j | \Omega \rangle = \Gamma k \quad (16)$$

where a_k^\dagger, a_k are the creation and the annihilation magnon operators. So the current value is proportional to the momentum, the ratio being independent of the value of a weak interaction which is in agreement with exact results.

b) *Charge excitations currents.* For excitations of the charge Hamiltonian $H(\varphi)$ we find similarly to (16), unlike the spin case, the current operator has now two contributions

$$\langle \Omega | j | \Omega \rangle = \langle \Omega | \pi_\varphi | \Omega \rangle + \Gamma \langle \Omega | \pi_\varphi \partial \varphi / \partial x | \Omega \rangle. \quad (17)$$

The first term in (17) vanishes due to nondiagonality 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 linear in boson operators contribution will appear only for those states which are not the eigenstates of the charge sound Hamiltonian. It happens at the macroscopic current carrying ground state, the magnetic flux being a current controlling conjugated variable, when the number of sounds 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 at arbitrary filling ρ both charge (hole and particle) and spin (singlet and triplet) gapless excitations carry a current, $j \propto p$ at $p \ll 1$. At the half filling $\rho = 1$ only states with one added particle are charged. Within 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, at the presence of a magnetic flux. The account of the spectrum parabolicity leads to nonzero currents ($j \propto p$) for both charge and spin boson excitations, which is in agreement with exact results for the Hubbard model as well as with a free fermion picture.

An appearance of the spin wave charge current is both unexpected and natural. Remarkably the spin waves the spectra and the whole BA construction evolve gradually, unlike other excitations, from the Heisenberg chain equivalent at $\rho = 1, u \neq 0$ to arbitrary ρ . This is why it is tempting to consider them as spin waves even at the presence of holes, $\rho \neq 1$. At the same time for $\rho \neq 1$ there is a continuous evolution of spin excitations towards $u = 0$ when they should become nothing but triplet electron-hole pairs. As such the triplet excitations will evidently carry the current due to electron-hole nonsymmetry caused by the Fermi velocity dispersion at $\rho \neq 1$. The bosonization tends to ignore the feature as well as all effects of sound decomposition into a band of doublets. When u is not small the currents can not 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 at the presence of a spinon.

The author S.B. was supported by the CNRS fellowship and by the Laue-Langevin Institute during the ac. year of 92/93. The author S.M. acknowledges the hospitality of the ILL in winter 93.

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