Charge-spin separation and the spectral properties of Luttinger liquids

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We compute the spectral function $\rho(q,\omega)$ of the one-dimensional Luttinger model. Charge-spin separation gives spectral weight at frequencies between the charge and spin-fluctuation dispersions while spectral weight above $v_\rho q$ and below $-v_\rho q$ is related to the anomalous dimensions of the fermion operators. The generalization of these results to many-particle correlations is discussed as well as the possibilities for their experimental verification in quasi-one-dimensional conductors.

The notion of a Luttinger liquid was coined by Haldane[1] to describe the universal low-energy phenomenology of gapless one-dimensional (1D) quantum systems. It is based on the exactly solvable Luttinger model[2] whose ground state can be viewed as a gas of noninteracting bosons, and postulates that this picture remains true, at least in terms of renormalized bosons and up to perturbative corrections, for the asymptotic low-energy properties of a much wider variety of 1D models of correlated fermions (or bosons), provided their low-energy excitations are gapless. There is thus an analogy to the Fermi-gas and Fermi-liquid pictures in higher dimensions, and the Luttinger liquid can be regarded as an effective theory for the 1D Fermi surface.

The distinctive properties of the Luttinger model are the absence of fermionic quasiparticles, anomalous dimensions of operators leading to power-law decay of the respective correlation functions, and charge-spin separation manifest in different velocities for the collective charge and spin fluctuations. This phenomenology has now been verified for several 1D lattice models.[3] Moreover, based on x-ray, nuclear-magnetic-resonance, and optical experiments,[4] it can be concluded that the normal state of some organic conductors and superconductors is, in fact, a Luttinger liquid. However, both the experimental and theoretical interest have been turned mainly toward the ground-state properties and the nonuniversal exponents characterizing the correlation functions. Charge-spin separation has received comparatively less attention, and its consequences as well as possible experimental verification have only been discussed in an approximate manner in the literature.[5]

Renewed interest for the properties of Luttinger liquids was stirred up by Anderson's proposal that the normal-state properties of the high-T_c superconductors could be described by a hypothetical "tomographic" Luttinger liquid in 2D.[5,6] Much of this discussion has been based on the spectral properties of the high-T_c materials measured in photoemission;[7] the spectral properties of the Luttinger liquid and, in particular, the signatures of charge-spin separation there, are, however, only poorly understood.

The present paper reports on a calculation of the spectral function

$$\rho(q,\omega)=-\pi^{-1}\mathrm{Im}G^R(k,\omega+\mu) \tag{1}$$

(G^R is the retarded fermion Green's function, μ is the chemical potential of the electrons) for the Luttinger liquid which can be measured by photoemission. Particular attention will be paid to the separate effects of charge-spin separation and of the anomalous dimensions of the fermion operators by comparing to two simplified versions of the model containing one feature but not the other. We shall also discuss qualitatively to what extent similar and complementary effects can be seen in many-particle correlation functions which are probed by different experiments.

The Luttinger Hamiltonian for spin-$\frac{1}{2}$ fermions can be written as the sum of the following terms:

$$H_0=\frac{\pi v_F}{L}\sum_{\nu=\rho,\sigma}\sum_p[\nu_+(p)\nu_+(-p)+\nu_-(-p)\nu_-(p)] \tag{2}$$

describes free charge and spin density fluctuations ($\nu=\rho,\sigma$) with the Fermi velocity v_F about the two Fermi points $\pm k_F$. The operators for charge and spin fluctuations

$$\nu_r(p)=\frac{1}{\sqrt{2}}\sum_k(c^\dagger_{rk_F+k+p\uparrow}c_{rk_F+k\uparrow}\pm c^\dagger_{rk_F+k+p\downarrow}c_{rk_F+k\downarrow}) \tag{3}$$

obey boson commutation relations. $c_{k,s}$ are the fermion operators. H_0 is the boson representation[2] of the free fermion Hamiltonian $H_0=v_F\sum_{k,s,r}(rk-k_F)c^\dagger_{k,s,r}c_{k,s,r}$, where the dispersion extends to infinity and all the negative-energy states are filled. It is remarkable that the model can be solved exactly in presence of the interactions

$$H_4=\frac{1}{L}\sum_{\nu=\rho,\sigma}\sum_p g_{4\nu}(p)[\nu_+(p)\nu_+(-p)+\nu_-(-p)\nu_-(p)]\ , \tag{4}$$

the forward scattering of fluctuations on the same branch of the spectrum; its effect is a renormalization of the Fermi velocities $v_F\to v_F+g_{4\nu}/\pi$ of charge and spin fluctuations which, in general, now will differ.

$$H_2=\frac{2}{L}\sum_{\nu=\rho,\sigma}\sum_p g_{2\nu}(p)\nu_+(p)\nu_-(-p)\ , \tag{5}$$

the forward scattering between particles on different sides of the Fermi surface, hybridizes density fluctuations on both branches. The effective interactions for charge and spin,

$$g_{i\rho}=\tfrac{1}{2}(g_{i\parallel}+g_{i\perp}),\quad g_{i\sigma}=\tfrac{1}{2}(g_{i\parallel}-g_{i\perp})\ , \tag{6}$$

are linear combinations of the fermions' coupling constants for parallel and antiparallel spins. The model is diagonalized by a Bogoliubov transformation;[2] the emerging gas of noninteracting bosons can be described completely by two nonuniversal parameters per degree of freedom, an exponent K_ν, determining the power-law decay of correlation functions, and v_ν, the renormalized velocities of the collective modes:

$$K_\nu=\left[\frac{\pi v_F+g_{4\nu}-g_{2\nu}}{\pi v_F+g_{4\nu}+g_{2\nu}}\right]^{1/2},$$
$$v_\nu=\left[\left[v_F+\frac{g_{4\nu}}{\pi}\right]^2-\left[\frac{g_{2\nu}}{\pi}\right]^2\right]^{1/2}. \tag{7}$$

Two important simplifications are possible: (i) spinless fermions, thus involving only charge degrees of freedom (this limit is formally obtained by setting $g_{i\perp}=0$ in the calculations). Here $g_2\neq 0$ introduces a nontrivial power-law decay of the correlation functions described by an exponent $K\neq 1$. (ii) $g_2=0$ but $g_{4\perp}\neq 0$, yielding $v_\rho\neq v_\sigma$ but $K_\nu=1$. This is a minimal model for charge-spin separation where the correlation exponents K_ν are the same as for free fermions but the velocities of charge and spin excitations differ. The two branches are now independent and we have a "one-branch Luttinger liquid." Even such a simplified model has physical relevance, e.g., for the edge excitations of the quantum Hall effect where the strong magnetic field gives a definite chirality to the particles, and where the spin degrees of freedom survive under certain circumstances.[8] For more complicated (and realistic) models possessing a Luttinger-liquid fixed point, the effective parameters K_ν ($K_\sigma=1$ for spin-rotation invariance) and v_ν can be calculated by a variety of methods.[3]

The retarded Green's function for a fermion $\Psi_{s,r}$ with spin s on the branch r of the dispersion,

$$G_r^R(x,t)=-i\Theta(t)\langle\{\Psi_{r,s}(x,t),\Psi_{r,s}^\dagger(0,0)\}\rangle\ , \tag{8}$$

where $\{\ldots,\ldots\}$ is the anticommutator, is evaluated via Haldane's bosonization identity,[1,9] yielding

$$G_r^R(x,t)=-\frac{\Theta(t)}{2\pi}e^{irk_Fx}\left\{\prod_{\nu=\rho,\sigma}\frac{1}{\sqrt{v_\nu t-rx}}\left[\frac{\Lambda^2}{(\Lambda+iv_\nu t)^2+x^2}\right]^{\gamma_\nu}+(x\to -x,t\to -t)\right\}. \tag{9}$$

Λ is a momentum transfer cutoff in the interactions $g_i(p)=g_i\exp(-\Lambda|p|)$ and $\gamma_\nu=(K_\nu+K_\nu^{-1}-2)/8>0$. For the Hubbard model, e.g., there is a restriction $\frac{1}{2}<K_\rho\leq 1$, implying $\gamma_\rho<\frac{1}{16}$, and $\gamma_\sigma=0$ for spin-rotation invariance.

We have not yet been able to Fourier transform this expression exactly, mainly due to difficulties in evaluating $\mathrm{Re}G(k,\omega)$. However, for the spectral properties $\mathrm{Im}G(k,\omega)$ is sufficient, and one can derive an integral representation for the full spin-$\frac{1}{2}$ fermion problem which can be evaluated asymptotically, and closed expressions for the two toy problems defined above. Let us start with the latter.

The spectral function for spinless fermions is [here $\gamma_0=(K+K^{-1}-2)/4$]

$$\rho_r(q_r,\omega)=\frac{1}{2\Gamma(\gamma_0)}\Theta(\omega+vrq_r)\gamma\left[\gamma_0,\frac{(\omega+vrq_r)\Lambda}{2v}\right]$$
$$\times\left\{(1-\delta_{\gamma_0,0})\Theta(\omega-vrq_r)\frac{\Lambda}{\Gamma(\gamma_0)v}\left[\frac{(\omega-vrq_r)\Lambda}{2v}\right]^{\gamma_0-1}\exp\left[-\frac{(\omega-vrq_r)\Lambda}{2v}\right]+\delta_{\gamma_0,0}\delta(\omega-vrq_r)\right\}$$
$$+(\omega\to-\omega,q_r\to -q_r)\ . \tag{10}$$

$q_r=k-rk_F$ measures the distance from the Fermi level. $\Gamma(\gamma_0)$ is the gamma function and $\gamma(\gamma_0,x)$ the incomplete gamma function. Equation (10) is plotted for the positive branch in Fig. 1. Spectral weight appears above the renormalized single-particle energy vq with a power-law divergence (for $\gamma_0<1$) as $\omega\to vq$, but also as a cusp singularity at negative energies below $-vq$. In between, the spectral weight vanishes. The positive-energy feature corresponds to the creation of particles above the Fermi sea while the negative-energy feature describes the annihilation of particles *above* the Fermi sea, present already in the ground state as a consequence of the g_2 interaction. This possibility is most easily seen by considering the momentum distribution function[10]

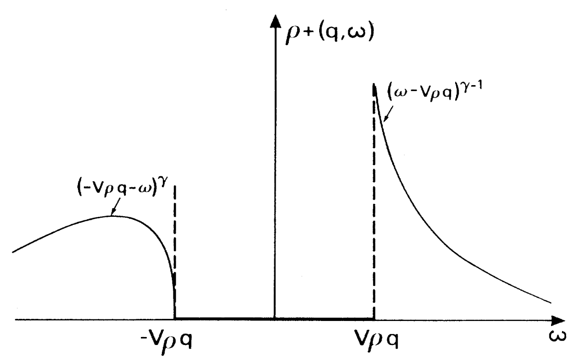

FIG. 1. Spectral function $\rho_+(q,\omega)$ for spinless fermions for $q>0$.

$$n(k_F+q)\approx\tfrac{1}{2}-C_1\,\mathrm{sgn}(q)|q|^{\alpha}-C_2 q\ . \tag{11}$$

Here, $\alpha=2\gamma_0$ and $n(k_F+q)$ is finite for $q>0$. The origin of the asymmetry in frequency is related to the small amount of particles excited above k_F in the ground state while the number of holes is of order 1. In a three-body approximation where the emission of only a single particle-hole pair is permitted, spectral weight appears at positive energy but vanishes at negative energy.[12] The spread of spectral weight is a consequence of the g_2 interaction, which allows an incoming particle (hole) to evaporate an arbitrary number of particle-hole pairs on the opposite branch (as in the x-ray edge problem). Exactly at k_F, the exponent of the divergence changes, and the spectral function behaves as $\rho_r(rk_F,\omega)\sim|\omega|^{2\gamma_0-1}$, i.e., is infinite for the parameters where $n(k)$ has an infinite derivative at k_F and is zero when $n(k)$ goes linearly through k_F. There is an earlier approximate calculation by Luther and Peschel.[13] The regions of nonvanishing spectral weight and the exponents of the singularities agree with their results after correction of some misprints. Unlike Luther and Peschel, at high frequencies we find an exponential decay of the spectral function.

The second toy problem is the one-branch spin-$\frac{1}{2}$ Luttinger liquid, $g_2=0$. This model exhibits charge-spin separation but the correlation exponents $K_\nu=1$ are those of free fermions. The spectral function is

$$\rho_r(q_r,\omega)=\frac{\Theta(\omega-v_\sigma rq_r)\Theta(v_\rho rq_r-\omega)+\Theta(v_\sigma rq_r-\omega)\Theta(\omega-v_\rho rq_r)}{\pi\sqrt{|\omega-v_\sigma rq_r||\omega-v_\rho rq_r|}}\ , \tag{12}$$

as is shown in Fig. 2 for the case $v_\rho>v_\sigma$ applying to repulsive interactions (for attractive interactions, the role of v_ρ and v_σ is just reversed). At k_F, the spectral function reduces to $\delta(\omega)$ and the momentum distribution is a step function with a unity jump at k_F, in agreement with Luttinger's theorem.[11] Although this seems to imply a Fermi liquid, it is clear that the physical picture is quite different and that the notion of a quasiparticle does not make sense since the δ-function weight does not survive the slightest displacement from the Fermi surface and instead deforms into (12). The incident electron decays into multiple particle-hole-like charge and spin fluctuations, which all live on the same branch as the incoming fermion. There is no spectral weight at negative energies. It is immediately apparent that $n(k)$ and, more generally, any quantity depending on k or ω alone, will not exhibit qualitatively new effects due to charge-spin separation. These can be manifest *only* in quantities depending on *both* q and ω.

Let us now turn to the spectral properties of the spinful Luttinger liquid. An analytic calculation is possible in the spin-rotation invariant case ($\gamma_\sigma=0$) in terms of integrals over Whittaker (i.e., confluent hypergeometric) functions, and the complete (lengthy) expression will be given elsewhere. It can, however, be evaluated asymptotically for $\omega\to\pm v_\nu rq_r$, and a sketch of the result is given in Fig. 3 for the ($r=+$) branch. Both the effects of charge-spin separation and of the anomalous exponents are obvious. Despite its appearance, the spectrum is not a simple addition of the spinless (g_2 finite) and the one-branch cases, and subtle transfers of spectral weight take place. Specifically, at positive energies there is a singularity

$$\rho_r(q_r,\omega)\sim|\omega-v_\rho rq_r|^{\gamma_\rho-1/2}\quad \text{as } \omega\to v_\rho rq_r \tag{13}$$

both from above and below. Compared to the one-branch case, the divergence from below is slower here at finite γ_ρ. Coming from above, the exponent is half of the one for spinless fermions. There is another singularity at the spin-fluctuation frequency:

$$\rho_r(q_r,\omega)\sim\Theta(\omega-v_\sigma rq_r)(\omega-v_\sigma rq_r)^{2\gamma_\rho-1/2}\quad \text{as } \omega\to v_\sigma rq_r\ . \tag{14}$$

Finite γ_ρ weakens the divergence with respect to the one-branch model. At negative energies, we obtain a cusp:

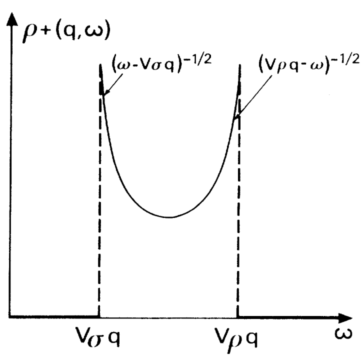

FIG. 2. Spectral function $\rho_+(q,\omega)$ for the one-branch Luttinger liquid for $q>0$.

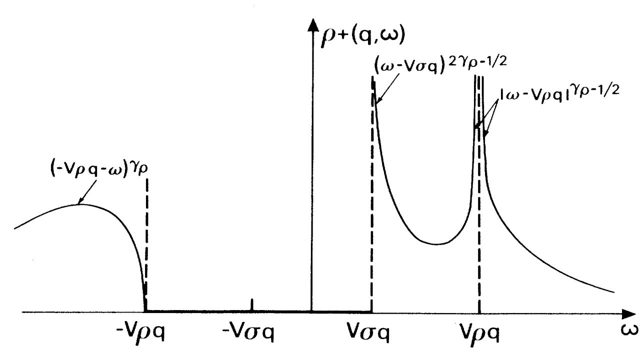

FIG. 3. Spectral function $\rho_+(q,\omega)$ for the spin-$\frac{1}{2}$ Luttinger liquid for $q>0$.

$$\rho_r(q_r,\omega) \sim \Theta(-\omega - v_\rho r q_r)(-\omega - v_\rho r q_r)^{\gamma_\rho} \quad \text{as } \omega \to -v_\rho r q_r \ . \qquad (15)$$

This is again similar to the spinless case though the exponent is only half. The spectral weight vanishes between $v_\sigma r q_r$ and $-v_\rho r q_r$. These features differ from a previous conjecture.[5] Although an explicit calculation was not possible for broken spin-rotation invariance ($\gamma_\sigma > 0$), from the implied hybridization of the two branches of the dispersion of the spin fluctuations it is clear that spectral weight will appear, presumably with a cusp singularity, already below $-v_\sigma r q_r$. Finally, the momentum distribution function $n(k)$ follows Eq. (11) with the appropriate exponent $\alpha = 2\sum_\nu \gamma_\nu$.

All features of $\rho(q,\omega)$ can, in principle, be measured with angle-resolved photoemission. It would be interesting to perform such experiments on low-dimensional conductors whose "normal" state is believed to be a Luttinger liquid.[4] There have been recent angle-integrated experiments,[14] measuring the energy-dependent density of states $N(\omega)$ ($\sim |\omega|^\alpha$ predicted for the Luttinger liquid) which do find an intriguing absence of spectral weight at the Fermi surface. To what extent this can be related to the Luttinger-liquid picture described here is not yet clear.

All many-particle correlation functions of the Luttinger model can be computed exactly and, generically, will exhibit structure similar to the single-particle Green's function above though with different correlation exponents.[9] All two-particle (such as density, spin-density, or superconducting) correlation functions have charge and spin contributions and are thus sensitive both to charge-spin separation and the anomalous exponents—but can yield complementary information. The exponents γ_ν depend only on the strength of the interactions but not on their sign—the exponents for the two-particle correlation functions are sign dependent. The singularities in the dynamical charge or spin structure factors, $S(2k_F+q,\omega)$ and $\chi(2k_F+q,\omega)$, measured in neutron scattering, are governed by an exponent $\alpha_{\mathrm{CDW/SDW}} = K_\rho + K_\sigma - 2$ (negative for repulsive and positive for attractive interaction) and are expected to occur at $\omega = \pm v_\rho q$ and $+v_\sigma q$ in analogy to the above. On the other hand, one can construct four-particle correlation functions describing, e.g., $4k_F$ charge-density waves, that involve only charge (or spin) degrees of freedom; they will be similar to Fig. 1 even for the spinful model, and $\alpha_{4k_F} = 4K_\rho - 2$. Different aspects of the effective interactions at the 1D Fermi surface are therefore probed by different experiments. The many-particle correlation functions are useful also for studying charge-spin separation and anomalous dimensions with quantum Monte Carlo simulations where some algorithms have severe problems with an accurate determination of single-particle properties.

Related work has been published recently. For one hole doped into a half-filled $U = \infty$ Hubbard model, square-root divergences are found at $\omega = \pm 2\sin(k)$.[15] Moreover, it has been pointed out that the spectral properties of the Luttinger liquid do influence the Fermi-edge singularities in semiconductor heterostructures in the 1D quantum limit.[16]

Note added. After submission of this paper, I have been informed by K. Schönhammer that V. Meden and he have independently obtained similar results.[17]

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