Spectral Properties of One Dimensional Insulators and Superconductors

S. Sorella
Interuniversitario di Fisica della Meteria and International School for Advanced Study, Via Beirut 4, 34013 Trieste, Italy

A. Parola
Interuniversitario di Fisica della Meteria and Istituto di Scienze Fisiche, Universitá di Milano, Via Lucini 3, Como, Italy
(Received 5 February 1996)

Conformal field theory and Bethe ansatz are used to investigate the low energy features of the spectral function in one dimensional models which exhibit a gap in the spin or in the charge excitation spectrum. Exotic behavior is found in the superconducting case, where the Green function displays momentum dependent Tomonaga-Luttinger liquid exponents. The predictions of the formalism are confirmed by Lanczos diagonalizations in the t-J model up to 32 sites. These results may be relevant in connection to photoemission experiments in quasi-one-dimensional insulators or superconductors. [S0031-9007(96)00426-7]

PACS numbers: 75.10.Jm, 71.27.+a, 74.25.Gz

In the last few years direct and inverse photoemission experiments have considerably improved, allowing for the accurate determination of momentum dependent energy spectra in low dimensional systems [1–3]. A first principles interpretation of this class of experiments requires a deep understanding of the effects of correlations on the electron (or hole) spectral function. One dimensional (1D) metals [4] have been the subject of an intense theoretical effort which led to a complete characterization of the long wavelength, low energy properties of electron dynamics and to the actual calculation of the correlation exponents which appear in the electron Green function [5,6]. However, some doubt has been cast on the relevance of these calculations for photoemission experiments because most of the quasi-1D systems are close to density wave or superconducting instabilities which open a gap in the charge or spin spectrum [3]. If the excitation spectrum is *fully gapped*, the Green function takes a free-particle-like form in every dimension. Instead, the effects of *a single branch* of gapless excitations (either spin or charge) have not been addressed in detail before, probably because the prejudice prevailed that a system with a gap should display exponentially decaying correlation functions in both space and time.

In this Letter, we develop a microscopic theory for determining the low energy properties of the spectral function in one dimensional correlated electron models with a gap either in the charge or in the spin channel. The main result of this work is that the presence of gapless excitations induces anomalous exponents in the Green function, by a nontrivial interaction with the extra electron (or hole) injected into the system. As a consequence, we generally find a spectral function with singularities along lines in the (k, ω) plane. These singularities are characterized by critical exponents which possibly depend on the *momentum* k of the electron: Numerical diagonalizations in the t-J model at $J = 2t$ fully confirm this picture providing quantitative agreement with predictions based on conformal field theory and Bethe ansatz techniques.

Spin and charge gaps are treated on the same footing in this Letter because they are believed to give rise to the same kind of singularities in the spectral function, despite the quite distinct physical nature of the state. In fact, it is possible to build specific models where the two regimes are mapped one onto the other: A well known example is the negative U Hubbard model at zero magnetization which is the prototype of one dimensional "superconductors," i.e., 1D models with spin gap and quasi off diagonal long range order. This model, via a particle-hole transformation, is mapped into the half filled, positive U system with *nonvanishing magnetization* which, on the contrary, is a Mott insulator characterized by a charge gap. The full Green function remains unaltered by particle-hole transformation leading to the same photoemission spectra in the two cases. In the following, we will explicitly deal only with the repulsive, half filled case, at arbitrary magnetization. The results will, however, hold for both one dimensional insulators and superconductors, being related only to the presence of a branch of gapless excitations in the spectrum.

The quantity which we are going to investigate is the hole Green function,

$$G(p,t) = i \langle \Psi_0 | \, c^{\dagger}_{p,\sigma} \, e^{-it(H-E_0-i\delta)} \, c_{p,\sigma} \, | \Psi_0 \rangle \, \theta(t), \quad (1)$$

where $|\Psi_0\rangle$ (E_0) is the ground state (energy) of the system with no holes and $\theta(t)$ is the step function. Because of spin-charge decoupling, the total energy E and momentum p are naturally written as a sum of a holon term $\epsilon_h(k)$ and a spinon contribution $\epsilon_s(Q)$ with $p = k + Q$. At long wavelengths it is known that holons and spinons behave as independent particles whose dynamics is governed by two commuting Hamiltonians: H_c and H_s, respectively. By substituting this decomposition $H = H_c + H_s$ into Eq. (1) and taking momentum conservation into account, we find that the hole Green function can be

 0031-9007/96/76(24)/4604(4)$10.00

written as a sort of convolution between a holon (G_h) and a spinon (Z) term,

$$G(p,t) = \int \frac{dQ}{2\pi} G_h(p - Q,t) Z_p(Q,t), \quad (2)$$

where $G_h(k,t)$ is just a free propagator: $\mathrm{Im}\, G_h(k,\omega) = \pi\,\delta(\omega - \epsilon_h(k))$. This simple form of the holon Green function is due to the presence of a gap in the charge excitation spectrum of the model which confines the low energy processes in the single holon sector. Instead, the spinon contribution Z is highly nontrivial due to the presence of gapless excitations and exhibits anomalous exponents at particular momenta Q_ν. As a result, the most relevant singularity in the full spectral function occurs at frequencies determined by the hole dispersion,

$$A(p,\omega) = \frac{1}{\pi} \mathrm{Im}\, G(p,\omega) \propto [\omega - \epsilon_h(p - Q_\nu)]^{2X_\nu(p)-1}. \quad (3)$$

Here $X_\nu(p)$ is a *momentum dependent* critical exponent determined by the low energy properties of the spinon dynamics, while $Q_\nu = (2\nu + 1)Q_F$ is an odd multiple of the spinon Fermi momentum $Q_F = \pi(1/2 - m)$, m being the magnetization per site. Equation (2) generalizes the exact form found in the $U \rightarrow \infty$ limit of the half filled Hubbard model [7] where $Z_p(Q,t)$ was explicitly calculated and turned out to be independent of p and t. In this limit, the hole dispersion is $\epsilon_h(k) = -2\cos k$ and the critical exponent takes the value $X_0 = X_{-1} = 1/4$.

In the following, we will analyze the long wavelength behavior of $Z_p(Q,t)$ which leads to Eq. (3) in the particular case of single (spin down) hole in the t-J model at arbitrary magnetization m. The case $m = 0$ gives information about the Mott insulator while the $m > 0$ ($m < 0$) choice refers to photoemission (inverse photoemission) experiments in "superconductors" via spin-up (spin-down) particle-hole transformation in the less than half filled attractive Hubbard model. Because of the universality underlying the behavior of one dimensional physics, we expect that these results will be qualitatively valid for generic 1D electron systems displaying a gap in the excitation spectrum. In fact, it is well known [8] that in this case the renormalization group flow drives the model towards the Luther-Emery fixed point irrespective of the details of the microscopic Hamiltonian. On the other hand, the t-J model allows for a direct comparison with Lanczos diagonalizations which can be pushed to fairly large lattice size in such a system.

The single hole problem in the t-J model can be reduced to a pure spin problem by a Galileo transformation [9] which fixes the hole at the origin O of the L-site lattice (L is chosen to be even). In this way, the charge degree of freedom can be exactly traced out leaving the problem of an effective momentum dependent spin Hamiltonian,

$$H_p^{\mathrm{eff}} = -[e^{ip}T + e^{-ip}T^\dagger] + J \sum_{i=1}^{L-2} \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (4)$$

Here p is the total lattice momentum of the one hole state and T is the translation operator along the squeezed chain with $l = L - 1$ sites, i.e., without the origin O. The Hamiltonian H^{eff} is written as the sum of two physically different contributions: The magnetic term is the standard Heisenberg model with *open* boundary conditions because no spin is present at the origin, while the kinetic of the hole manifests itself via the action of the translation operator T.

This mapping of the hole problem into a spin Hamiltonian is exact for every J and allows one to interpret the presence of the hole as the inclusion of a special type of *boundary operator* in the bulk spin Hamiltonian. An insight to the general features of the energy spectrum of this Hamiltonian can be obtained by examining the $J \rightarrow 0$ limit, where all the spin configurations on the squeezed chain which are eigenstates of the translation operator $T|\psi_Q\rangle = e^{iQ}|\psi_Q\rangle$ are degenerate provided they correspond to the same (spinon) momentum Q. This degeneracy is lifted by the magnetic term, which, at first order in J, selects the lowest energy state of the Heisenberg ring with the given spinon momentum Q. The corresponding hole energy is $E = \epsilon_h(p - Q) + \epsilon_s(Q)$, where the holon band is $\epsilon_h(k) = -2\cos k$ and the $O(J)$ spinon dispersion $\epsilon_s(Q)$ only depends on the bulk properties of the Heisenberg model. In this limit, the effects of spin-charge decoupling on the energy spectrum come out rather naturally as well as the role of the hole kinetic contribution in modifying the boundary conditions of the Heisenberg model, from open to periodic. Because of the peculiar form of the hole boundary operator in Eq. (4), the long wavelength behavior of H^{eff} is associated with a new class of fixed points different from those found in the framework of the *static* impurity problem [10].

After a standard Jordan-Wigner transformation the spin Hamiltonian maps onto a system of interacting spinless fermions at density $\rho = \frac{1}{2} - m$. At low energy, the relevant degrees of freedom are the momenta close to the Fermi points $\pm Q_F$. It is then possible to take the continuum limit of the model defining two independent fermionic fields $\psi_R(x)$ and $\psi_L(x)$ [6] for the right $k \sim Q_F$ and left $k \sim -Q_F$ movers on the squeezed chain with $0 < x < l$. The long wavelength limit of the translation operator can be written in terms of a well defined spinon momentum operator $\hat{P}$, $T = e^{i\hat{P}}$ where

$$\hat{P} = Q_F \int_0^l dx\,\{[\psi_R^\dagger(x)\psi_R(x) - \psi_L^\dagger(x)\psi_L(x)] + i[\psi_R^\dagger(x)\partial_x\psi_R(x) + \psi_L^\dagger(x)\partial_x\psi_L(x)]\}. \quad (5)$$

As anticipated, the competition between the hole kinetic term and the magnetic interaction in H^{eff} selects a particular effective boundary condition for the interacting fermion gas which simulates the presence of a scattering potential at the boundary together with a magnetic flux across the ring. This gives rise to independent boundary conditions for the right and left movers defined by two phase shifts,

$$\begin{aligned} \psi_R^\dagger(x + l) &= e^{i\delta_R}\psi_R^\dagger(x), \\ \psi_L^\dagger(x + l) &= e^{i\delta_L}\psi_L^\dagger(x). \end{aligned} \tag{6}$$

The long wavelength analysis proceeds by noting that, due to spin-charge decoupling, the effective Hamiltonian splits into the sum of two *commuting* terms

$$H^{\text{eff}} = \epsilon_h(p - \hat{P}) + H_J \tag{7}$$

governing charge and spin dynamics, respectively. Here H_J is the usual long wavelength form of the Heisenberg Hamiltonian in terms of the fermionic fields (ψ_L, ψ_R) [6] with the particular boundary conditions (6). It is known that the interacting Hamiltonian (7) can be turned into a free Fermi problem by a canonical transformation [6] which further modifies the boundary conditions (6). The bulk Tomonaga-Luttinger liquid properties of H_J are described by the dressed charge K_ρ shown in the inset of Fig. 1 [5].

Having characterized the long wavelength physics of the effective hole Hamiltonian (4) in terms of the dressed charge and the two phase shifts, let us move to the analysis of the spectral properties of the hole motion. As a first step, we fix our attention on the *overlap* ζ_p between the pure Heisenberg ground state on L sites $|\Psi_0\rangle$ and the one hole ground state $|\Psi_p\rangle$ at fixed momentum p,

$$\zeta_p = |\langle\Psi_p|c_{p,\downarrow}|\Psi_0\rangle|^2 \propto L^{-2X_\nu(p)}. \tag{8}$$

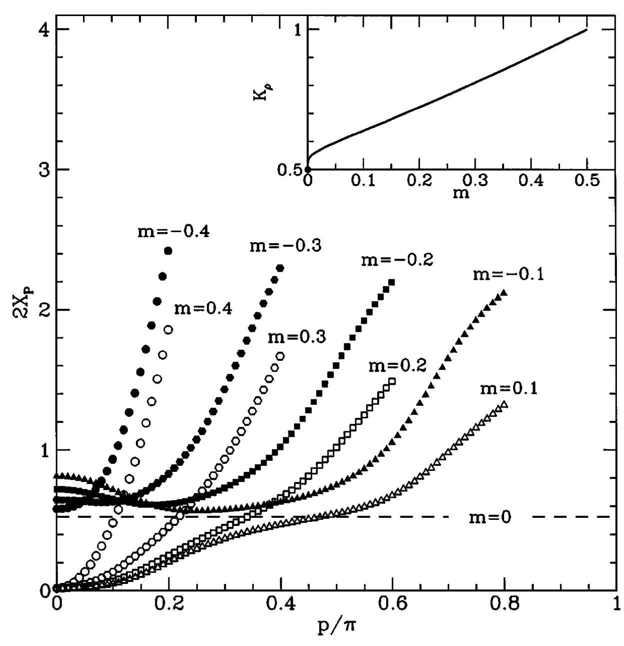

FIG. 1. Lowest critical exponent $X_\nu(p)$ as a function of the total momentum p of the spin down hole in the t-J model at $J = 2$ with several magnetizations m. Results are obtained by numerical solution of the set of integral equations defining the correction to scaling of the one hole ground state energy [15]. In the inset: Correlation exponent (or dressed charge) K_ρ for the Heisenberg model as a function of magnetization obtained by numerical solution of the integral equation for ξ_{22} of Ref. [5].

This quantity naturally enters the calculation of the hole spectral function as can be immediately checked by use of the Lehmann representation. As indicated in Eq. (8), the overlap ζ_p vanishes in the thermodynamic limit with a critical exponent which can be explicitly evaluated in terms of the previously introduced phase shifts,

$$X_\nu(p) = K_\rho\left(\frac{\delta_R + \delta_L}{2\pi} + \nu\right)^2 + \frac{1}{4K_\rho}\left(\frac{\delta_R - \delta_L}{2\pi}\right)^2. \tag{9}$$

The calculation parallels the known derivation of the orthogonality catastrophe in the impurity problem [11]. Here, the integer number ν defines the total spinon momentum of the one hole states $Q_\nu = (2\nu + 1)Q_F$ corresponding to an odd number of low energy spinons.

The phase shifts (6) are nonuniversal depending on the short wavelength properties of the model; however, it is possible to relate them to the form of the energy spectrum $E(p)$ of one hole at fixed momentum p which, according to Eq. (7), can be written as a sum of a charge and a spin contribution. In fact, we expect that low energy spinon dynamics is governed by some effective conformal field theory which should reflect the structure of the size corrections to the *spinon contribution* to the ground state energy, $E(p) - L\,\epsilon_\infty(p) = [\Delta E_c(p) + \Delta E_s(p)]/L$ with

$$\Delta E_s(p) = -v_s\frac{\pi}{6} + 2\pi v_s X_\nu(p). \tag{10}$$

Here v_s is the spinon velocity: $v_s = d\epsilon_s(Q)/dQ$ evaluated at Q_F and $X_\nu(p)$ coincides with the critical exponent (9).

In order to determine the unknown phase shifts δ_R and δ_L, we have analyzed the size corrections to the ground state energy (at fixed momentum p) in the Bethe ansatz soluble models: The Hubbard model at $U > 0$ [12] and the t-J model at $J = 2$ [13] with one hole and arbitrary magnetization. By suitably generalizing the pioneering work of Woynarovich [14] to the single hole case, we found exactly the form (10) of the energy size corrections, with quantitative predictions for the phase shifts which, in fact, explicitly depend on the total momentum p at every nonzero magnetization m. For $m = 0$, i.e., for the Mott insulator case, instead, we always find that only one of the two phase shifts is different from zero and takes the value π, both in the Hubbard and in the t-J model. Another analytic limit is the $J \to 0$ at arbitrary magnetization m where again the phase shifts are independent of p but are functions of the magnetization, $\delta_R = \pi(1 - m)$ and $\delta_L = \pi m$. Figure 1 shows the exponent $X_0(p)$ as a function of the total momentum p for the Bethe ansatz solvable limit of the t-J model ($J = 2$) at several magnetizations. A comparison with the value of the overlap exponent obtained by the use of Eq. (8) through Lanczos diagonalization of the model with magnetization $m = \pm 0.25$ is shown in Fig. 2. Lattice sizes ranging from 16 up to 32 sites have been used to fit the exponent $2X_\nu(p)$ in Eq. (8) leading to a quite good agreement between analytical and numerical results. This comparison gives confidence on the interpretation of the Bethe ansatz results for the single hole size correction in the framework of conformal field theory.

Now we are ready to use the previous analysis for the evaluation of the hole spectral function. In fact, the spinon contribution to the Green function $Z_p(Q,t)$ appearing in (1) can be calculated within the described formalism leading to the expression

$$Z_p(R,t) = \langle \Psi_0 | e^{i(\hat{P}R - H_J t + E_0 t)} | \Psi_0 \rangle. \tag{11}$$

The dependence on the total momentum p occurs only through the phase shifts (6) defining the boundary condition to H_J. The asymptotic behavior of $Z_p(R,t)$ can be analytically evaluated as

$$Z_p(R,t) \sim \frac{e^{iQ_\nu R}}{(R - v_s t)^{X_\nu(p)+\Delta}(R + v_s t)^{X_\nu(p)-\Delta}}, \tag{12}$$

showing that singularities characterized by different exponents (9) occur at wave vectors $Q_\nu = (2\nu + 1)Q_F$. The additional critical exponent Δ can be expressed in terms of the phase shifts: $\Delta = (\delta_R + \delta_L + 2\pi\nu)(\delta_R - \delta_L)/(2\pi)^2$. When the Fourier transform of Eq. (12) is substituted into the asymptotic form of the Green function (2) we obtain the anticipated expression (3) which constitutes the main result of this Letter together with the analytical evaluation of the critical exponent $X_\nu(p)$ in Bethe ansatz soluble models. Because of the allowed values for ν in (9) singularities at $Q_\nu = (2\nu + 1)Q_F$ are predicted, determining "shadow bands" in the spectral function.

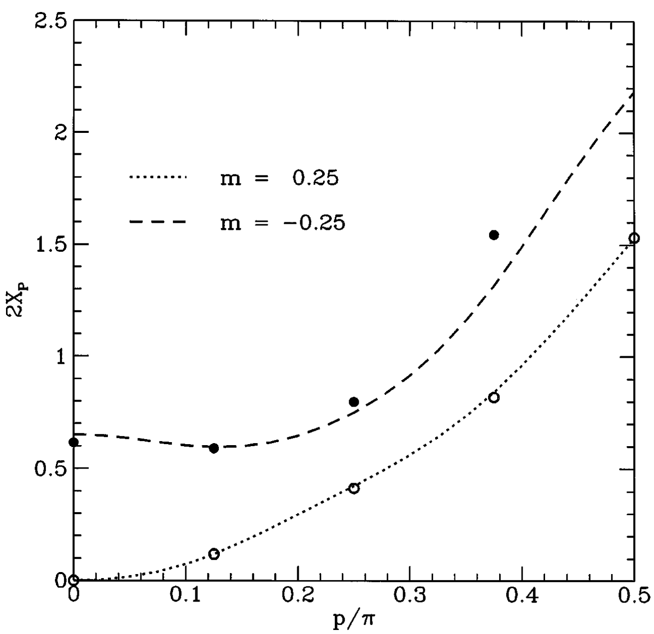

FIG. 2. Comparison between the analytical results of Fig. 1 for $m = \pm 0.25$ and Lanczos diagonalization. In the latter case, the exponent $X_\nu(p)$ is obtained by a size scaling of the numerical evaluation of the overlap ζ_p as defined by Eq. (8). Lines: analytical results, open dots: Lanczos data for $m = 0.25$, full dots: Lanczos data for $m = -0.25$.

From a physical point of view, our results show that the spectral function of Mott insulators and superconductors is characterized by branch cut singularities with exponents depending, in the latter case, on the momentum p of the injected particle. This feature is shared by all the models we have investigated: The Bethe ansatz solvable Hubbard and t-J models and the $J \to 0$ limit of the tJ_{XY} model [15]. We believe that it is a general feature of hole motion in 1D correlated systems thereby providing definite predictions for the analysis of photoemission experiments in quasi-one-dimensional systems characterized by a gap either in the charge or in the spin spectrum.

It is a pleasure to thank M. Fabrizio for extensive discussions and to acknowledge the kind hospitality at SISSA (A. P.), Cantoblanco University (S. S.), and ISI foundation (EU Contract No. ERBCHRX-CT920020).

[1] B. O. Wells *et al.*, Phys. Rev. Lett. **74**, 964 (1995); Z.-X. Shen *et al.*, Science **267**, 343 (1995).
[2] P. Aebi *et al.*, Phys. Rev. Lett. **72**, 2757 (1994).
[3] B. Dardel *et al.*, Phys. Rev. Lett. **67**, 3144 (1991).
[4] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981).
[5] H. Frahm and V. E. Korepin, Phys. Rev. B **42**, 10 533 (1990); **43**, 5653 (1991); N. Kawakami and S. K. Yang, Phys. Lett. A **148**, 359 (1990).
[6] I. Affleck, in *Field Strings and Critical Phenomena*, edited by E. Brézin and J. Zinn-Justin (North-Holland, Amsterdam, 1990), p. 563.
[7] S. Sorella and A. Parola, J. Phys. Condens. Matter **4**, 3589 (1992); K. Penc *et al.*, Phys. Rev. Lett. **75**, 894 (1995).
[8] J. Solyom, Adv. Phys. **28**, 201 (1979).
[9] Q. F. Zhong and S. Sorella, Phys. Rev. B **51**, 16 135 (1995).
[10] S. Eggert and I. Affleck, Phys. Rev. B **46**, 10 866 (1992); C. L. Kane and M. P. A. Fisher, Phys. Rev. B **46**, 15 233 (1992).
[11] P. W. Anderson, Phys. Rev. **164**, 352 (1967).
[12] E. M. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1455 (1968).
[13] P. A. Bares *et al.*, Phys. Rev. B **44**, 130 (1991).
[14] F. Woynarovich, J. Phys. A **22**, 4243 (1989).
[15] A. Parola and S. Sorella (to be published).