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Dynamical correlation functions of one-dimensional superconductors and Peierls and Mott insulators*

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Abstract. I construct the spectral function of the Luther-Emery model which describes one-dimensional fermions with one gapless and one gapped degree of freedom, *i.e.* superconductors and Peierls and Mott insulators, by using symmetries, relations to other models, and known limits. Depending on the relative magnitudes of the charge and spin velocities, and on whether a charge or a spin gap is present, I find spectral functions differing in the number of singularities and presence or absence of anomalous dimensions of fermion operators. I find, for a Peierls system, one singularity with anomalous dimension and one finite maximum; for a superconductor two singularities with anomalous dimensions; and for a Mott insulator one or two singularities without anomalous dimension. In addition, there are strong shadow bands. I generalize the construction to arbitrary dynamical multi-particle correlation functions. The main aspects of this work are in agreement with numerical and Bethe Ansatz calculations by others. I also discuss the application to photoemission experiments on 1D Mott insulators and on the normal state of 1D Peierls systems, and propose the Luther-Emery model as the generic description of 1D charge density wave systems with important electronic correlations.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 71.30.+h Metal insulator transitions and other electronic transitions – 71.45.Lr Charge-density-wave systems

1 Motivation

Non-Fermi liquid behavior in correlated fermion systems is an exciting topic of current research. One-dimensional (1D) correlated electrons (more precisely: one-dimensional quantum systems with gapless excitations) are a paradigmatic example of non-Fermi liquids: their low-energy excitations are not quasi-particles but rather collective charge and spin density fluctuations which obey each to their proper dynamics [1]. The key features of these "Luttinger liquids" [2] are (i) anomalous dimensions of operators producing correlation functions with non-universal power-laws, parametrized by one renormalized coupling constant K_ν per degree of freedom $\nu = \rho$ (charge), σ (spin) which have the status of the Landau parameters familiar from Fermi liquid theory; (ii) charge-spin separation, leading to a fractionization of an electron into charged, spinless, and neutral, spin-carrying collective excitations, with different dynamics determined by velocities $v_\rho \neq v_\sigma$. Each of these features leads to (iii) absence of fermionic quasi-particles. Responsible are the electron-electron interaction which is marginal in one dimension and therefore transfers nonvanishing momentum in scattering processes at all energy scales, and the nesting properties of the 1D Fermi surface. They produce divergent $2k_F$ charge and spin density fluctuations which then interfere with Cooper-type superconducting fluctuations.

All three features clearly show up in the single-particle spectral function [3–5]

$$\rho(q,\omega) = -\pi^{-1}\mathrm{Im}\, G(k_F + q, \mu + \omega) \qquad (1.1)$$

which can be measured (within the "sudden approximation") by angle-resolved photoemission (ARPES) (with bad angular resolution, one essentially measures $N(\omega) = \sum_q \rho(q,\omega)$ and is able to probe only features (i) and (iii)). The spectral function is purely incoherent [3–5], at best with peaks at the dispersion energies of the elementary charge and spin excitations, indicating that the electron behaves as a composite particle built on more elementary excitations. In equation (1.1), G is the Fourier transform of the retarded electronic Green's function

$$G(xt) = -i\Theta(t)\langle\{\Psi(xt), \Psi^\dagger(00)\}\rangle \ , \qquad (1.2)$$

k_F the Fermi wave number, and μ (= 0) is the chemical potential.

Much experimental effort has been devoted to studying and attempting to "prove" Luttinger liquid correlations in various quasi-1D systems. Examples are organic conductors of the family based on the molecule TMTSF (Bechgaard salts) where both NMR [6] and (partially)

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photoemission [7] have provided evidence in favor of a Luttinger liquid picture, quantum wires fabricated into semiconductor nanostructures [8], or edge states in the fractional quantum Hall effect [9]. In all cases however, there appear to be problems with the precise values of the parameter K_ρ derived, or with some other aspects of the interpretation in terms of a Luttinger liquid. It is not clear to date to what extent these discrepancies are due to the neglect of some experimentally important factor in the theory (such as, *e.g.* three-dimensionality or electron-phonon coupling in the chain systems, or deviations from the special filling factors in the quantum Hall edge states), or indicative of more fundamental problems either with theory or experiment.

1D (organic and inorganic) charge density wave (CDW) systems apparently could provide an alternative field of search for these typically one-dimensional correlations. Photoemission indeed has produced results [10] similar to the Bechgaard salts when performed with low angular resolution. With high angular resolution, a broad dispersing feature has been identified in $(TaSe_4)_2I$ [11] while *two* such signals have been measured in the blue bronze $K_{0.3}MoO_3$ [12]. Even though the actual situation in $K_{0.3}MoO_3$ may be slightly more complictated because there are two almost degenerate bands cutting the Fermi energy, it is clearly of importance to first understand the photoemission spectrum expected from the metallic phase of a single-band CDW material. Finally, while this paper was prepared, new experiments on the organic two-chain conductor TTF–TCNQ became available which clearly show dispersing signals both on the TTF and TCNQ chains with very unusual lineshapes [13]. Specifically, the TCNQ signals are somewhat similar to $K_{0.3}MoO_3$, and we know from independent experiments that there are strong $2k_F$-CDW fluctuations on this chain in the metallic state [14]. (The TTF-chain exhibits strong $4k_F$-CDW fluctuations at very high temperature and is expected to be a Luttinger liquid.)

The association of the two dispersing signals of $K_{0.3}MoO_3$ with the charge and spin excitations of a Luttinger liquid is suggestive. As I will explain in the next section in more detail, it is incompatible, however, with the CDW transitions observed in these materials. This incompatibility motivates the consideration of the Luther-Emery model and is at the origin of the work reported here. Section 2 will discuss this model, its generic role as a low-energy fixed-point of 1D quantum systems which have both gapped and gapless degrees of freedom, and the picture we had of its correlations prior to this work.

Recently, photoemission experiments also have been performed on the 1D Mott insulator $SrCuO_2$ [15]. In Mott insulators, the charge fluctuations are gapped while the spins remain gapless. Their low-energy physics, therefore, can again be described by a Luther-Emery model, and our theory can be adapted to study the spectral functions of 1D Mott insulators. Earlier, angle-integrated photoemission on $BaVS_3$ has been interpreted as evidence for a Luttinger liquid [16]. The behavior of the conductivity, however, is more insulator-like, and the present theory might be of interest there, too.

Section 3 presents the construction of the single-particle spectral function (1.1). In Section 4 I present results for the spectral functions of the spin-gapped Luther-Emery model, *i.e.* 1D Peierls systems and superconductors. In Section 5, the spectral functions of 1D Mott insulators are presented. Section 6 shows how the construction procedure of Section 3 can be generalized to arbitrary correlation functions of local operators. I compare my results with information from other studies in Section 7 and use them for an interpretation of published experiments in Section 8. I conclude with a short summary and a brief perspective. Partial results have been presented earlier [17,18].

2 The Luther-Emery model

The Luther-Emery model extends the Luttinger model by including the backscattering of electrons across the Fermi surface. Its Hamiltonian is [19]

$$H = H_0 + H_1 + H_2 + H_4, \tag{2.1}$$

$$H_0 = \sum_{r,k,s} v_F(rk - k_F) : c^\dagger_{rks} c_{rks} :, \tag{2.2}$$

$$H_1 = \sum_{s,s'} \left[g_{1\parallel} \delta_{s,s'} + g_{1\perp} \delta_{s,-s'} \right] \times \int_0^L dx : \Psi^\dagger_{+,s}(x) \Psi_{-,s}(x) \Psi^\dagger_{-,s'}(x) \Psi_{+,s'}(x) : \tag{2.3}$$

$$H_2 = \frac{1}{L} \sum_{p,s,s'} \left[g_{2\parallel} \delta_{s,s'} + g_{2\perp} \delta_{s,-s'} \right] \times \rho_{+,s}(p) \rho_{-,s'}(-p), \tag{2.4}$$

$$H_4 = \frac{1}{2L} \sum_{r,p,s,s'} \left[g_{4\parallel} \delta_{s,s'} + g_{4\perp} \delta_{s,-s'} \right] : \rho_{r,s}(p) \rho_{r,s'}(-p) : . \tag{2.5}$$

c_{rks} describes fermions with momentum k and spin s on the two branches ($r = \pm$) of the dispersion varying linearly $[\varepsilon_r(k) = v_F(rk - k_F)]$ about the two Fermi points $\pm\, k_F$, $\Psi_{r,s}(x)$ is its Fourier transform, and

$$\rho_{r,s}(p) = \sum_k : c^\dagger_{r,k+p,s} c_{r,k,s} : = \sum_k \left(c^\dagger_{r,k+p,s} c_{r,k,s} - \delta_{q,0} \langle c^\dagger_{r,k,s} c_{r,k,s} \rangle_0 \right) \tag{2.6}$$

is the density fluctuation operator which obeys a bosonic algebra

$$[\rho_{r,s}(p), \rho_{r',s'}(-p')] = -\delta_{r,r'} \delta_{s,s'} \delta_{p,p'} \frac{rpL}{2\pi} \cdot \tag{2.7}$$

The Luttinger model is obtained for $g_1 = 0$ and includes only forward scattering.

In one dimension, fermions can be transformed into bosons, and for the Luttinger model, there is an exact

operator identity relating a fermion operator $\Psi_{rs}(x)$ to the bosonic density fluctuations (2.6) [1,2]. For our purposes, the approximate expression

$$\Psi_{rs}(x) \sim \lim_{\alpha\to 0} \frac{e^{irk_F x}}{\sqrt{2\pi\alpha}} \times \exp\left(\frac{-i}{\sqrt{2}}\left[r\Phi_\rho(x) - \Theta_\rho(x) + s\left\{r\Phi_\sigma(x) - \Theta_\sigma(x)\right\}\right]\right) \tag{2.8}$$

with the two phase fields

$$\Phi_\nu(x) = -\frac{i\pi}{L}\sum_{p\neq 0}\frac{e^{-\alpha|p|/2-ipx}}{p}\left[\nu_+(p)+\nu_-(p)\right], \tag{2.9}$$

and

$$\Theta_\nu(x) = \frac{i\pi}{L}\sum_{p\neq 0}\frac{e^{-\alpha|p|/2-ipx}}{p}\left[\nu_+(p)-\nu_-(p)\right], \tag{2.10}$$

found earlier by Luther and Peschel [20], is sufficient.

This formula allows for a boson representation of the Hamiltonian and of all correlation functions. Before, it is important, however, to recall the physics of the phase fields $\Phi_\nu(x)$ and $\Theta_\nu(x)$ in (2.8) [1,21,22]. The charge density *fluctuation* operator is related to $\Phi_\rho(x)$ by $\sum_r \rho_r(x) = -\pi^{-1}\partial\Phi_\rho(x)/\partial x$, and likewise for spin σ. When an additional particle is inserted into the system, a kink of amplitude π is formed in $\Phi_\nu(x)$. These fields therefore describe the scattering phase shifts of the particles present in the system, generated by the particles added. The operators inserting the particles are exponentials of the dual fields $\Theta_\nu(x) = \int \Pi_\nu(x)dx$, where Π_ν is the momentum conjugate to Φ_ν: $[\Pi_\nu(x), \Phi_\nu(x')] = -i\delta(x-x')$. In a general fluctuation operator whose correlation function we wish to evaluate, the prefactor of $i\Theta_\nu/\sqrt{2}$ measures the number of ν-particles it inserts into the system while the prefactor of $i\Phi_\nu/\sqrt{2}$ measures the number of ν-particles it rearranges at constant total ν-particle number to generate the desired fluctuation. By ν-particle, we label, in the first place,

$$\Psi_{r\nu}(x) = (2\pi\alpha)^{-1/4}\exp\{-i[r\Phi_\nu(x) - \Theta_\nu(x)]/\sqrt{2}\}, \tag{2.11}$$

the slowly-varying charge or spin part of the fermion operators $\Psi_{rx}(x)$ but, with phase factors reflecting the appropriate Fermi seas, these particles will describe the holons and the spinons of the 1D Bethe-Ansatz soluble models.

The boson form of the Luther-Emery Hamiltonian becomes

$$H_0 + H_4 = \frac{1}{L}\sum_{\nu r p\neq 0}(\pi v_F + g_{4\nu}) : \nu_r(p)\nu_r(-p) : \tag{2.12}$$

$$H_{1,\parallel} + H_2 = \frac{1}{L}\sum_{\nu p}(2g_{2\nu} - g_{1\parallel})\nu_+(p)\nu_-(-p), \tag{2.13}$$

$$H_{1\perp} = \frac{2g_{1\perp}}{(2\pi\alpha)^2}\int dx \cos\left[\sqrt{8}\Phi_\sigma(x)\right]. \tag{2.14}$$

$\nu_r(p)$ are the operators for the charge and spin densities

$$\rho_r(p) = \frac{1}{\sqrt{2}}\left[\rho_{r,\uparrow}(p) + \rho_{r,\downarrow}(p)\right],$$
$$\sigma_r(p) = \frac{1}{\sqrt{2}}\left[\rho_{r,\uparrow}(p) - \rho_{r,\downarrow}(p)\right], \tag{2.15}$$

and the interactions have been transformed as

$$g_{i\rho} = \frac{1}{2}\left(g_{i\parallel} + g_{i\perp}\right), \quad g_{i\sigma} = \frac{1}{2}\left(g_{i\parallel} - g_{i\perp}\right). \tag{2.16}$$

Diagonalizing the Luttinger part (*i.e.* H excluding $H_{1\perp}$) generates the renormalized velocities of the collective charge and spin excitations and their stiffness constants

$$v_\nu = \sqrt{\left[v_F + \frac{g_{4\nu}}{\pi}\right]^2 - \left[\frac{g_{2\nu} - g_{1\parallel}/2}{\pi}\right]^2},$$
$$K_\nu = \sqrt{\frac{\pi v_F + g_{4\nu} - g_{2\nu} + g_{1\parallel}/2}{\pi v_F + g_{4\nu} + g_{2\nu} - g_{1\parallel}/2}}. \tag{2.17}$$

The phase fields transform as $\Phi_\nu(x) \to \Phi_\nu(x)\sqrt{K_\nu}$ and $\Theta_\nu(x) \to \Theta_\nu(x)/\sqrt{K_\nu}$. The main effect of the g_4-interaction is a renormalization of v_ν. We therefore drop H_4 from explicit consideration in the following, and always assume correctly renormalized velocities v_ν.

For $K_\sigma - 1$ sufficiently large with respect to $|g_{1\perp}|$, backscattering is irrelevant, and the Luther-Emery model reduces to a Luttinger liquid. Its renormalized value of K_σ can be calculated, *e.g.* by perturbative renormalization group [23] which is well-controlled in this case or, if applicable, fixed to unity by the requirement of spin-rotation invariance. Charge and spin excitations are gapless, and depending on the value of K_ρ, the dominant correlations are spin density wave (SDW, $K_\rho < 1$, repulsive forward scattering) or triplet pairing (TS, $K_\rho > 1$, attractive forward scattering). Charge density wave (CDW) and singlet superconducting (SS) fluctuations, respectively, are subdominant.

The backscattering Hamiltonian $H_{1\perp}$ is, for $K_\sigma - 1$ small enough compared to $|g_{1\perp}|$, a relevant perturbation and opens a gap Δ_σ in the spin excitation spectrum

$$\varepsilon_\sigma(q) = \pm\sqrt{v_\sigma^2 q^2 + \Delta_\sigma^2}. \tag{2.18}$$

Luther and Emery have shown that for the special value $K_\sigma = 1/2$, the interaction Hamiltonian $H_{1\perp}$ (2.14) can be represented as a bilinear in spinless fermions, using the bosonization formula (2.8) for spinless fermions (multiply the argument of the exponential by $\sqrt{2}$ and drop the σ-fields), and diagonalized [19]. On this Luther-Emery line $K_\sigma = 1/2$, the gap is computed exactly to be $\Delta_\sigma = |g_{1\perp}|/2\pi\alpha$ (α is an infinitesimal in (2.8) but often associated with a cutoff of the order of a lattice constant). Renormalization group then allows to derive the gap for arbitrary K_σ. The charges remain gapless.

The Mott insulator is the consequence of an instability in the charge channel, caused by Umklapp scattering off the lattice for commensurate band-fillings. The Umklapp

Hamiltonian appropriate for a half-filled band is obtained by simply replacing spin by charge in equation (2.14), and its coupling constant often is denoted by $g_{3\perp}$. Here the spins are gapless while relevant Umklapp scattering opens a gap Δ_ρ in the charge channel. This generic picture applies (with little modification only) to all even commensurabilities ($k_F a = [r/s]\pi/2$, s even). The situation is different for s odd, where the Umklapp operator necessarily couples charges and spins [1], and we exclude these cases from our study. The Mott insulator is dominated by $4k_F$-CDW and/or SDW correlations.

While the Luther-Emery solution is essentially [24] exact, it is useless for computing correlation functions since there is no practical relation between the physical fermions and the spinless pseudofermions. Still, we have some qualitative information on the correlation functions. Several methods [25] support the idea that, in the gapped phase, correlations of the Φ_σ-field tend towards a non-zero constant as $|x|$ or $|t| \to \infty$ while those involving exponentials of its dual field $\Theta_\sigma(x)$ decay exponentially in space (or oscillate in time). The spin gap quenches low-energy spin fluctuations, therefore SDW and TS correlations should be exponentially suppressed. With a constant asymptotic value of Φ_σ, CDW and SS are enhanced with respect to a Luttinger liquid, and now dominate over SDW and TS. The opening of a spin gap is a necessary condition for the emergence of dominant SS or CDW correlations in a 1D metal. As a corollary, a Luther-Emery phase must exist in the normal state of CDW systems (or superconductors) between a Luttinger liquid and the 3D ordered low-temperatures phases. One therefore should be careful in interpreting the properties of the metallic "normal state" of a CDW system (or of a 1D superconductor) in terms of a Luttinger liquid.

For the one- and two-particle spectral functions, there is a general belief that the opening of a gap affects the system for frequencies smaller than this gap while the behavior of the ungapped system is essentially recovered at larger frequency scales. The exponential decay (resp. oscillations) of correlation functions involving operators $\exp[i(\dots)\Theta_\sigma]$ would cut off (shift) the divergences as functions of $q(\omega)$ they had possessed in the Luttinger model. Possibly important power-law prefactors to exponentials have not been discussed. There has been almost no calculation or systematic construction of such functions – in particular dynamical ones [26] – and, to my knowledge, no critical check of these hypotheses by numerical simulation prior to this work [17,18].

A wide variety of models fall into the Luther-Emery universality class and my results should be applicable there in a low-energy sector: Luttinger liquids coupled to phonons and related models so long as they are incommensurate, have wide regions of parameter space with gapped spin fluctuations and gapless charges [27]; the negative-U Hubbard model at any band-filling has a spin gap [28], and the positive-U Hubbard model at half-filling has a charge gap [29,30]; with longer-range interactions, charge gaps can occur at different rational band-fillings, too. The $t-J$-model has a spin gap at low density [31]. Spin gaps occur frequently in models of two Luttinger or Hubbard chains coupled by single-particle tunneling [32,33]. Also when a $2k_F$-CDW is established in many coupled Luttinger chains as a consequence of interchain Coulomb interaction, the system passes through a region of attractive backscattering which opens a spin gap [34].

3 Construction of the spectral function

I now present a systematic construction of the single-particle spectral function, equations (1.1, 1.2), for the *spin-gapped* Luther-Emery model. The Green's function exhibits the full complexity of the problem, involving all four phase fields Φ_ν, Θ_ν, while many others are easier [1]. They will be discussed in Section 6. Here, we limit ourselves to the diagonal terms of the Green's function, both in the branch index r and in the spin index s, and further assume spin-rotation invariance, so that s is dropped alltogether. This assumption, which I will make throughout the paper unless exceptions for the sake of an argument are stated explicitly, further implies $K_\sigma = 1$. With the non-vanishing expectation values of operators $\exp[i(\dots)\Phi_\sigma]$ generated by the gap opening, finite off-diagonal terms are possible, in principle, both here and in multi-particle correlation functions. They can be calculated in complete analogy to the terms discussed here, and we ignore them in the following.

Using bosonization (2.8), the retarded Green's function for right-moving fermions ($r = +$) can be represented as a product

$$G(xt) = -i\Theta(t)e^{ik_F x}\left[g_\rho(xt)g_\sigma(xt) + (x \to -x, t \to -t)\right], \tag{3.1}$$

of charge and spin correlation functions

$$g_\nu(xt) = \left\langle \Psi_{+\nu}(xt)\Psi^\dagger_{+\nu}(00)\right\rangle. \tag{3.2}$$

The product structure is a consequence of the charge-spin separation of the Hamiltonian (2.1). The spectral function (1.1) then is a convolution

$$\rho(q,\omega) = \frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} dq'\, d\omega'\, \left[g_\rho(q',\omega')g_\sigma(q-q',\omega-\omega') + (q \to -q\ ,\ \omega \to -\omega)\right]. \tag{3.3}$$

The charge part is easy and can be calculated in the Luttinger model (I only display the leading ω- and q-dependence)

$$g_\rho(q,\omega) \sim \Theta(\omega - v_\rho q)\Theta(\omega + v_\rho q) \times (\omega - v_\rho q)^{\gamma_\rho - 1}(\omega + v_\rho q)^{\gamma_\rho - 1/2} \tag{3.4}$$

with

$$\gamma_\rho = (K_\rho + K_\rho^{-1} - 2)/8 \quad \text{for} \quad K_\rho \neq 1, \text{ and}$$
$$g_\rho(q,\,\omega) \sim \frac{\Theta(\omega + v_\rho q)}{\sqrt{\omega + v_\rho q}}\delta(\omega - v_\rho q) \qquad (K_\rho = 1)\,. \tag{3.5}$$

Using a similar expression for the spins, one can reproduce in detail the spectral functions of the Luttinger model calculated elsewhere directly [3–5]. Notice that the divergences are stronger than for a spinless Luttinger model ensuring that singularities remain after performing the convolution integrals. For both $K_\nu \neq 1$, the coalescence of three of the four singularities of $g_\rho(q,\omega)$ and $g_\sigma(q,\omega)$ is needed to generate a singularity in the spectral function of the Luttinger model; if one of them, *e.g.* K_σ, is unity, the coalescence of two singularities is sufficient.

The determination of the spin correlation function is more involved because it has no simple representation in terms of the Luther-Emery pseudofermions, *excluding any exact calculation.* I now show that the leading behavior of this function can, however, be *uniquely constructed from symmetries, equivalences, and known limits* if the Ansatz is made that $g_\sigma(xt)$ is a product of power laws and exponentials in x and t. There is a variety of arguments requiring this form, and we will give them in the following, together with the construction procedure.

The important steps are: (i) representing the Hamiltonian in terms of right- and left-moving fermions requires g_σ to be a function of $x \pm v_\sigma t$ only. In general, g_σ will contain both power laws ($f_\pm$) and exponentials (f_{exp}) of these variables

$$g_\sigma(xt) \sim f_+(x - v_\sigma t) f_-(x + v_\sigma t) f_{exp}(x^2 - v_\sigma^2 t^2). \quad (3.6)$$

Interactions other than g_4 can only mix left- and right-moving excitations, producing products of $x \pm v_\sigma t$, or functions thereof, but cannot introduce new dependences on x and/or t. This is consistent both with the boson solution of the massless Luttinger phase and with the Luther-Emery solution of the gapped phase. (The Lorentz invariance of the Luther-Emery model requires all correlation functions of Luther-Emery *pseudofermions* to depend on $x^2 - v_\sigma^2 t^2$ only – and by implication all those of the physical fermions whose operators can be represented in terms on Luther-Emery fermions alone.) The exponential part f_{exp} necessarily is a function of $x^2 - v_\sigma^2 t^2$ only. All dependences on x and t other than through functions of $x^2 - v_\sigma^2 t^2$ must therefore be present also in the Luttinger model ($g_{1\perp} = 0$), and necessarily are of power-law form.

(ii) The limit of a vanishing gap $\Delta_\sigma \to 0$ can also be used to constrain the function $g_\sigma(xt)$, but is rather subtle. To make the argument clear, we momentarily relax the assumption of spin rotation invariance so that the spin channel of the model is described by $g_{1\perp}$ and general K_σ. (Alternatively, we can look at a Mott problem with Umklapp scattering $g_{3\perp}$ and $K_\rho \neq 1$ is more natural.) In the limit $\Delta_\sigma \to 0$, the function $f_{exp}(x^2 - v_\sigma^2 t^2) \to 1$ here, because the exponential dependences are introduced by the finite gap. Straightforwardly, one would now identify the product $f_+(x - v_\sigma t) f_-(x + v_\sigma t) = \langle \Psi_\sigma(xt) \Psi_\sigma^\dagger(00) \rangle_{g_{1\perp}=0}$ with the spin part of the spectral function of the remaining Luttinger model, *i.e.* equation (3.7) below with *anomalous* exponents $\delta_- = (K_\sigma + K_\sigma^{-1} - 2)/8$ and $\delta_+ = \delta_- + 1/2$. This physically appealing procedure was used in an earlier paper [17], and possibly could describe the physics of a small-gap Luther-Emery model.

Taking the limit $\Delta_\sigma \to 0$ to constrain eventual power-laws in $g_\sigma(xt)$ involves different physics, however, and the above argument must be modified. For vanishing gap, g_σ must reduce to the correlation function of the *free* Luttinger model ($K_\sigma = 1$), no matter what value of K_σ *would* describe the hypothetical Luttinger model obtained from the Luther-Emery model (2.1) for $g_{1\perp} = 0$, *i.e.* independently of any assumption on spin-rotation invariance. Physically, this is so because the anomalous operator dimensions $K_\sigma \neq 1$ of the Luttinger model are a consequence of singular low-energy virtual particle-hole excitations. When there is a gap at the Fermi surface, these processes are quenched, and one is left with the exponent $K_\sigma = 1$ of the free model [35]. Notice that this argument implies that we consider a rather large gap.

Accidentally, the spectral functions given earlier [17] remain correct. This, however, is due to the limitation to spin-rotation invariant interactions there. They impose $K_\sigma = 1$ for the power-law functions $f_\pm(x \mp v_\sigma t)$ in any case.

With $f_{exp}(x^2 - v_\sigma^2 t^2; \Delta_\sigma = 0) \sim 1$ one can determine all possible power-laws $f_\pm$ up to corrections varying more slowly than a power law, to be

$$f_\pm(x \mp v_\sigma t) = [\alpha - i(x \mp v_\sigma t)]^{-\delta_\pm} \quad (3.7)$$

with exponents

$$\delta_+ = 1/2 \ , \quad \delta_- = 0. \quad (3.8)$$

These are the exponents of a free Luttinger correlation function for the spin part of a right-moving fermion. I re-emphasize that they arise because of the quenching of low-energy particle-hole excitations by the spin gap and hold independent of any assumption on spin-rotation invariance. (As we will see below, the corresponding result for the charge channel implies that there cannot be any anomalous dimensions in a 1D Mott insulator with spin-rotation invariance respected).

(iii) From the equivalence of the Luther-Emery model to a classical 2D Coulomb gas [23] (using the Matsubara formalism of imaginary times $\tau = it$, putting $y = v_\sigma \tau$) and Debye screening of the charges above the Kosterlitz-Thouless temperature, one deduces an exponential factor

$$f_{exp}(x \pm v_\sigma t) \sim \exp(-c \Delta_\sigma \sqrt{x^2/v_\sigma^2 - t^2}) \quad (3.9)$$

with an undetermined constant c, in f_{exp}. This equivalence quite generally excludes any decay faster than (3.9).

In this picture, the perturbation Hamiltonian (2.14) generates a Coulomb gas of charges $q_e = \pm 1$, and the Φ_σ-fields of the Green's function appear as two test charges $q_e' = \pm 1/2$ whose bare (logarithmic) interaction is modified by screening from the Coulomb gas. The gapped Luther-Emery phase corresponds to the high-temperature plasma phase of unbound charges in the Coulomb gas, and the screening can then be treated in the Debye-Hückel approximation [36]. Here, the effective potential between the charges is $V(r) \sim \exp(-\kappa_D |\mathbf{r}|)/\sqrt{\kappa_D |\mathbf{r}|}$ with the Debye wavevector $\kappa_D = 2\Delta_\sigma / v_\sigma$ [23]. The Θ_σ-fields can then be

viewed as magnetic monopoles with strengths $q_m = \pm 1/2$. Their interaction is again logarithmic, and they couple to the electric charges with $V_{em}(\mathbf{r}) \sim -\arctan(y/x)$ [37]. Clearly, the high-temperature plasma of electric charges $q_e = \pm 1$ modifies the effective monopole-monopole interaction which becomes

$$V_{m-m}(\mathbf{q}) = -\frac{2\pi}{q^2} + \frac{2\pi}{q^2}\left(\frac{q_y}{q_x}\right)^2 \frac{1}{q^2+\kappa_D^2}, \tag{3.10}$$

where I have used the Debye-Hückel polarization propagator

$$\Pi(\mathbf{q}) = \frac{q^2}{2\pi}\frac{\kappa_D^2}{q^2+\kappa_D^2}\,. \tag{3.11}$$

Fourier-transforming back to real space, one obtains

$$V_{m-m}(\mathbf{r}) \sim \ln|\mathbf{r}| + c'|\mathbf{r}|\kappa_D \tag{3.12}$$

with an open constant $c' \propto c$. One observes an antiscreening effect here: in the presence of the electric charges, the magnetic monopoles are confined more strongly than without charges! Going back to real times, (3.12) produces the exponential dependence in (3.9) and, most importantly, gives additional (in fact, for those multi-particle correlation functions which only depend on $x^2 - v_\sigma^2 t^2$ the only firm) justification for the presence of power-law prefactors in addition to exponential terms in (3.6).

(iv) The open constant c in (3.9) can be determined from a spectral representation of f_{exp}, and our interpretation of the bosonization formula (2.8). Fourier transforming $f_{exp}(x,t)$, one obtains

$$f_{exp}(q,\omega) = 2\pi v_\sigma c \Delta_\sigma \frac{\Theta(\omega^2 - v_\sigma^2 q^2 - c^2\Delta_\sigma^2)}{(\omega^2 - v_\sigma^2 q^2 - c^2\Delta_\sigma^2)^{3/2}} \tag{3.13}$$

which has a gap of magnitude $c\Delta_\sigma$ in its spectrum. This gap must correspond to the excitation of $|n|$ spinons where n is the prefactor of $i\Theta_\sigma(x)/\sqrt{2}$ in the operator whose correlation function we wish to calculate. This constrains the prefactor in the exponential to $c = |n|$ quite generally. For the single-particle Green's function $n = 1$, and we obtain $c = 1$ here.

(v) The present construction of $g_\sigma(xt)$ is not an exact calculation. It is therefore important to look for exactly known cases which can be used as tests, to confirm the validity of this construction. Gulácsi has calculated explicitly the $t = 0$-Green's function of a 1D Mott insulator [38]: He finds $G(x) \sim \exp(-\Delta_\rho|x|)/|x|$ which is in complete agreement with the present theory when the $1/\sqrt{|x|}$-contribution from the ungapped channel is multiplied to equation (3.14) below. That there may be a power-law prefactor in the charge part of the spectral function has also been realized but well hidden in publications, by others [39].

In Section 6, I will discuss further tests of these rules based on two-particle correlation functions.

From the rules (i) – (v), I find

$$g_\sigma(x,t) \sim \exp\left(-\Delta_\sigma\sqrt{x^2 - v_\sigma^2 t^2}/v_\sigma\right)/\sqrt{\alpha + i(v_\sigma t - x)}. \tag{3.14}$$

Fourier transformation then gives

$$g_\sigma(q,\omega) \sim \left(1 + \frac{v_\sigma q}{\sqrt{v_\sigma^2 q^2 + \Delta_\sigma^2}}\right)\frac{\Theta(\omega + v_\sigma q)}{\sqrt{\omega + v_\sigma q}} \times\delta(\omega - \sqrt{v_\sigma^2 q^2 + \Delta_\sigma^2}). \tag{3.15}$$

The comparison of (3.15) with (3.5) (after $\rho \to \sigma$ there) is interesting. The δ-function translates the absence of anomalous dimensions in the gapped channel, a consequence of rule (ii), rather than spin-rotation invariance as in the σ-version of (3.5). The change in dispersion due to the spin gap enters through this δ-function. The frequency-dependent prefactor is the same as in the gapless system. However, due to the different argument in the δ-function, it no longer becomes singular in the limit $q, \omega \to 0$ but has an upper limit of $\Delta_\sigma^{-1/2}$ now. A similar effect occurs in the Green's function of 1D quantum antiferromagnets, where the opening of the spin gap cuts off a singularity of the prefactor of the delta function [40]. The factor in parentheses is a coherence factor translating the enhanced spin-pairing tendency at the origin of the spin gap, and one readliy recognizes the same structure as for the coherence factors $u_q,\ v_q$ familiar from the theory of superconductivity.

4 Spectral function for the spin-gapped Luther-Emery model

We now must convolute $g_\sigma(q,\omega)$, equation (3.15), with the charge part, equations (3.4) or (3.5). The results depend on the relative magnitudes of the charge and spin velocities. We therefore treat separately the cases of (A) repulsive interactions (in the sense that the effective forward scattering matrix element $g_{2\rho} - g_{1\|}/2 > 0$), *i.e.* $K_\rho < 1$, and $v_\rho > v_\sigma$, where Peierls-type $2k_F$-CDW fluctuations dominate, and (B) attractive forward scattering, *i.e.* $K_\rho > 1$ and $v_\rho < v_\sigma$, when singlet superconducting fluctuations are most important. (The inequalities on the velocities and K_ρ usually go with each other as listed when standard lattice models are treated. Of course, when one takes all $g_{i\nu}$ as free parameters, other combinations are possible. Relevant for the subsequent classification then are the velocities.)

What could we expect from our knowledge of the Luttinger liquid [3]? There the singularities at $\omega = v_{\rho(\sigma)}q$ arise from processes where the charge (spin) contributes all of the electron's momentum q and the spin (charge) none. The same argument applied to the Luther-Emery model predicts signals at the renormalized spin dispersion $\varepsilon_\sigma(q)$, equation (2.18), and at a shifted charge dispersion

$$\varepsilon_\rho(q) = v_\rho q + \Delta_\sigma. \tag{4.1}$$

Figure 1 shows the location of the signals expected from this argument. The Δ_σ-shift in the charge dispersion comes from the fact that the zero-momentum spin fluctuation can only be excited at a cost of Δ_σ. As will be

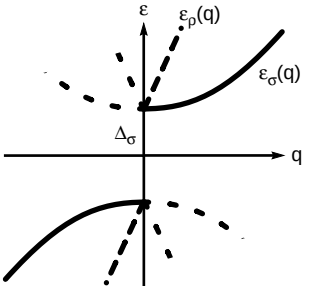

Fig. 1. Dispersion of peaks in the spectral function $\rho(q,\omega)$ of a spin-gapped Luther-Emery model with $v_\rho > v_\sigma$. The dispersion laws $\varepsilon_\rho(q)$ and $\varepsilon_\sigma(q)$ are given in the text. The heavy solid and dashed lines give the signals in the main band [sign(ω) = sign(q)] while the light dashed lines label the shadow bands [sign(ω) = – sign(q)].

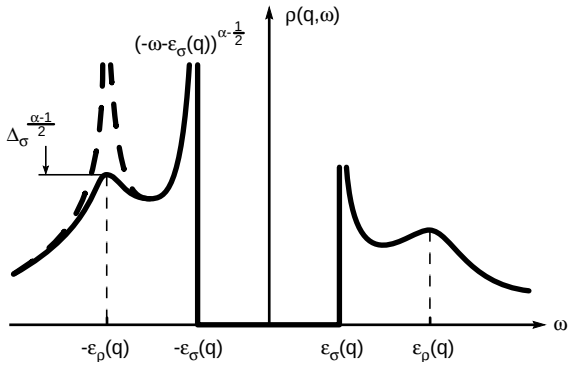

Fig. 2. Spectral function of the spin-gapped Luther-Emery model for $q < 0$. $v_\rho > v_\sigma$ has been assumed, as applies to a 1D Peierls insulator. The dashed line at $-\varepsilon_\rho(k)$ indicates the Luttinger liquid divergence which is suppressed here to a finite maximum.

seen below, however, the spectral functions of the Luther-Emery model never show two singularities with these dispersions. The intuitive predictions on the spectral function of the Luther-Emery model basically transcribe the standard argument that the behavior of correlation functions is modified on energy scales below the gap (correlations are suppressed there) but recovered almost unchanged on higher energy scales. Our results will show that for dynamical, *q and* ω-dependent correlations, this argument is not trustworthy.

4.1 One-dimensional Peierls "insulators"

We assume $v_\rho > v_\sigma$ and $K_\rho < 1$, implying dominant CDW correlations. Calling these systems "insulators" is a misnomer, however, because the charges are gapless and the systems are metallic. More precisely, we think about the Luther-Emery model here as describing the "normal" metallic state above a CDW transition.

The convolution of g_σ and g_ρ, equation (3.3), is rather straightforward now. After executing the ω'-integral, singularities are obtained from the coalescence of the two singularities carried by $g_\rho(q,\omega)$. The result of the calculation is shown schematically in Figure 2 for $q < 0$ (unlike previous papers, we present the spectral functions as those of the *occupied* states, *i.e.* as they would be measured by a photoemission experiment). There are indeed features at the special frequencies shown in Figure 1. On the spin dispersion $\varepsilon_\sigma(q)$, there is a true singularity

$$\rho[q,\omega \approx -\varepsilon_\sigma(q)] \sim \Theta[-\omega-\varepsilon_\sigma(q)][-\omega-\varepsilon_\sigma(q)]^{\alpha-1/2} \tag{4.2}$$

as in the Luttinger model. Here, α is *defined* as $\alpha = (K_\rho + K_\rho^{-1} - 2)/4 = 2\gamma_\rho$ since the notion of a K_σ does not make sense in a spin-gapped system. Folklore would then predict another singularity $|\omega + \varepsilon_\rho(q)|^{(\alpha-1)/2}$ (short dashed lines in Fig. 2) which is *not* observed here. It is cut off instead to a finite maximum of order

$$\rho[q,\omega \approx -\varepsilon_\rho(q)] \sim \Delta_\sigma^{(\alpha-1)/2}. \tag{4.3}$$

The reason for cutting of the Luttinger divergence on the charge dispersion is related to the non-singular prefactor (for $q \to 0$) in $g_\sigma(q,\omega)$, *cf.* equation (3.15) and the subsequent discussion, and the convolution makes this effect apparent on the charge dispersion $\varepsilon_\rho(q)$. *The spin gap therefore supresses the divergence associated with the charge dispersion while on the renormalized spin dispersion, the spectral response remains singular.*

At positive frequencies, the Luther-Emery model has pronounced shadow bands. Here, the Luttinger liquid only has very small weight. The weight in the Luther-Emery model is much stronger, and the spectral function has the same overall shape as at negative frequencies. For $q < 0$, the negative frequency part is enhanced by a coherence factor $1 - v_\sigma q/\varepsilon_\sigma(q)$ while a factor $1 + v_\sigma q/\varepsilon_\sigma(q)$ decreases its shadow. These factors translate the increased coherence due to the spin pairing and the finite spin gap, and are a consequence of the corresponding coherence factors in equation (3.15). Of course, as suggested by Figure 1, one can also view the shadow bands as bending back from the Fermi (or more precisely: the gap) energy as k is increased beyond k_F. This view perhaps is closer to a real photoemission experiment.

4.2 One-dimensional superconductors

We now take $v_\rho < v_\sigma$, *i.e.* attractive forward scattering. This implies $K_\rho > 1$, and such a system has dominant singlet pairing fluctuations. Interestingly, two true singularities occur here whose location is shown in Figure 3. There is one singularity on the renormalized spin dispersion

$$\begin{aligned}\rho[q,\omega \approx -\varepsilon_\sigma(q)] &\sim \Theta(q-q_c)\\ &\times \Theta[-\omega-\varepsilon_\sigma(q)][-\omega-\varepsilon_\sigma(q)]^{\alpha-1/2}\\ &+ \Theta(q_c-q)|-\omega-\varepsilon_\sigma(q)|^{\alpha-1/2},\end{aligned} \tag{4.4}$$

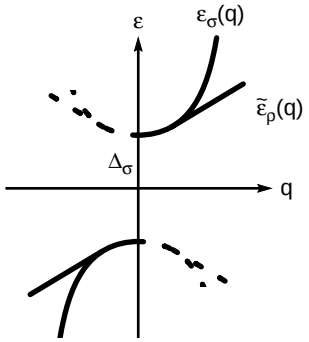

Fig. 3. Dispersion of singularities in the spectral function $\rho(q,\omega)$ of a spin-gapped Luther-Emery model with $v_\rho < v_\sigma$. The solid lines give the signals in the main band while the dashed lines label the shadow bands.

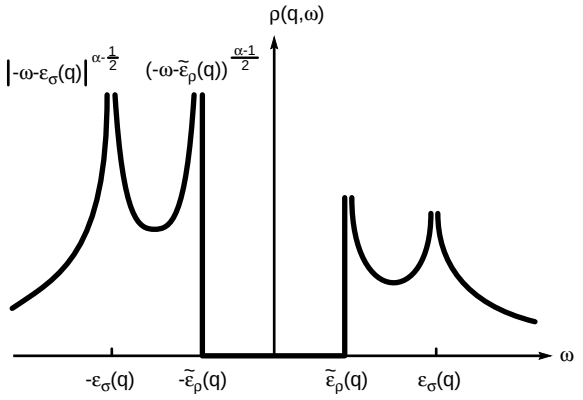

Fig. 4. Spectral function $\rho(q,\omega)$ of the spin-gapped Luther-Emery model with $v_\rho < v_\sigma$ (applying to 1D superconductors) for $q < 0$.

which is one-sided for $q > q_c$ and two-sided for $q < q_c$.

$$q_c = \mathrm{sign}(q)\frac{v_\rho}{v_\sigma}\frac{\Delta_\sigma}{\sqrt{v_\sigma^2 - v_\rho^2}} \tag{4.5}$$

is a critical wave vector which arises in the convolution procedure from searching the minimum of $\varepsilon_\sigma(q') + v_\rho(q - q')$ as a function of q'. At this wavevector, the dispersion

$$\tilde{\varepsilon}_\rho(q) = \varepsilon_\sigma(q_c) + v_\rho(q - q_c) \tag{4.6}$$

is tangential to $\varepsilon_\sigma(q)$. For $q < q_c$, a divergence

$$\rho[q, \omega \approx -\tilde{\varepsilon}_\rho(q)] \sim \Theta(-\omega - \tilde{\varepsilon}_\rho(q))[-\omega - \tilde{\varepsilon}_\rho(q)]^{\frac{\alpha-1}{2}} \tag{4.7}$$

on this shifted charge dispersion splits off the spin divergence. Again, there are strong shadow bands with the same functional forms as the main bands, specifically with two singularities, and with intensities controlled by coherence factors. The dispersions of the signals are displayed in Figure 3, and the shape of the spectral function is sketched in Figure 4.

Notice that, quite generally, that the behavior of $\rho(q, \omega \approx \pm\, \Delta_\sigma)$ is determined by that of the spin part close to Δ_σ and that of the charge part at $\omega \approx 0$. Unlike earlier conjectures [25], it is therefore *not* necessary to know details of the charge dynamics on a scale $\omega \approx \Delta_\sigma$ where the Luttinger description may have acquired significant corrrections.

The k-integrated density of states then is $N(\omega) \sim \Theta(\omega - |\Delta_\sigma|)(\omega - |\Delta_\sigma|)^\alpha$, independent of the magnitudes of the velocities. There is no weight below the gap, and the typical gap singularity in the density of states of the spin fluctuations is wiped out by convoluting with the gapless charges.

It is quite clear now that certain properties of 1D fermions – the dynamical ones involving (1+1)D Fourier transforms – are affected by the gap opening on *all* energy scales, contrary to common expectation, while those depending on one variable alone are modified only on scales below the gap energy. Despite the opening of a gap in the spin channel, singular spectral response remains possible in q- and ω-dependent correlation functions.

5 Spectral function of one-dimensional Mott insulators

The spectral function of a 1D Mott insulator can be computed as a special case of the generic solution presented above. One simply has to change $\sigma \leftrightarrow \rho$ *everywhere* and put $K_\sigma = 1$ in the gapless spin channel for spin-rotation invariance (which we assume to hold, again). Importantly, the exchange of ρ and σ also applies to the inequalities on the velocities v_ν, where again two cases must be distinguished.

Both factors g_ν in the convolution now involve δ-functions. In the case of repulsive forward scattering $v_\rho > v_\sigma$, one now finds a spectral function with two singularities, similar to the case of a 1D superconductor. Since $K_\sigma = 1$, the anomalous single-particle exponent $\alpha = 0$, *i.e.* one obtains two inverse square-root singularities. In the main band ($\omega < 0$ for $q < 0$), the spectral function becomes

$$\rho(q,\omega) \sim \frac{\Theta(q - q_c)\Theta[-\omega - \varepsilon_\rho(q)]}{\sqrt{-\omega - \varepsilon_\rho(q)}} + \frac{\Theta(q_c - q)\Theta[-\omega - \tilde{\varepsilon}_\sigma(q)]}{\sqrt{[-\omega - \tilde{\varepsilon}_\sigma(q)]| - \omega - \varepsilon_\rho(q)|}} \tag{5.1}$$

with $\tilde{\varepsilon}_\sigma(q) = \varepsilon_\rho(q_c) + v_\sigma(q - q_c)$. An important difference to the case of a superconductor occurs in the shadow band: since the spectral function of the gapless spin channel has no shadow band of its own, the singularity on $\tilde{\varepsilon}_\sigma(q)$ in the shadow band is missing. The shadow band therefore has a single singularity on the charge dispersion $\varepsilon_\rho(q)$ with a weight depressed by a coherence factor with respect to the weight of the main band signals. The effect is completely analogous to the appearence of a single nonanalyticity in the (very weak) shadow bands of a Luttinger liquid with spin-rotation invariant interactions [3–5]. The shape of this spectral function is sketched in Figure 5. The location of the singularities follows Figure 3 with the

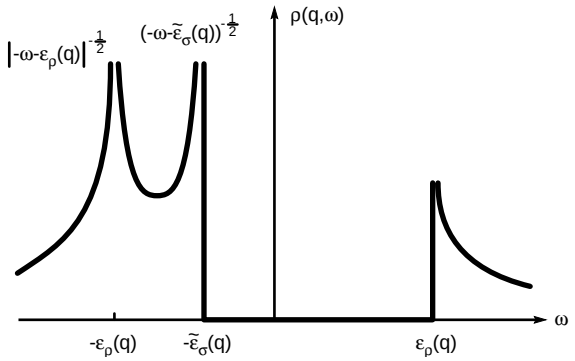

Fig. 5. Spectral function $\rho(q,\omega)$ of the charge-gapped Luther-Emery model, describing 1D Mott insulators, with $v_\rho > v_\sigma$ for $q < 0$. The dispersions of the signals follow Figure 3 with $\rho \leftrightarrow \sigma$ everywhere, and the straight dashed lines in the shadow bands must be ignored.

replacement $\rho \leftrightarrow \sigma$ except for the shadow bands where the straight lines should be ignored.

The case $v_\sigma > v_\rho$ again is different. Compared to the case of the 1D Peierls "insulator", the anomalous dimension α on the charge dispersion drops out due to spin-rotation invariance, giving an inverse square-root singularity on $\varepsilon_\rho(q)$. Also the finite maximum on the shifted spin-dispersion $\varepsilon_\sigma(q)$ does not occur. This is because the δ-function has zero weight in the energy domain where the square-root prefactor in equation (3.15) takes its maximum. The shadow band, of course, has a single inverse-square-root singularity with the usual coherence factors. Thus, the spectral function for this case becomes

$$\rho(q,\omega) \sim \frac{\Theta[|\omega| - \varepsilon_\rho(q)]}{\sqrt{|\omega| - \varepsilon_\rho(q)}}, \tag{5.2}$$

up to coherence factors, and the density of states

$$N(\omega) \sim \Theta(|\omega| - \Delta_\rho) \times \text{regular function}. \tag{5.3}$$

The spectral properties of a doped Mott insulator, of course, depend on the detailed scenario emerging from a more complete theory. Work on the Hubbard model shows, however, that the upper Hubbard band qualitatively survives a finite dopant concentration [30,38]. Continuity then suggests that as the insulating state is left by varying the band-filling, spectral weight is gradually taken out of both the main and shadow bands of a spectral function such as those discussed before, and transferred into the charge and spin divergences of a Luttinger liquid signal. Although the spins are left unaffected in the transition and only a charge gap opens, both the charge and the spin signals are predicted to be shifted and strongly modified by doping. This is a direct consequence of the convolution property (3.3) of the single-particle spectral function. When superposing (to a first approximation) the two signals, care must be taken, in addition, to account for the dependence of the chemical potential on doping level.

6 Generalization to other correlation functions

We now discuss the construction of other correlation functions for the Luther-Emery model. Clearly, due to charge-spin separation, they can again be written as convolutions of charge and spin correlation functions. Consider a general local operator

$$O_\nu^{(m,n)}(x) = \Psi_{r\nu}^m(x)\Psi_{r\nu}^n(x), \tag{6.1}$$

where $\Psi_{r\nu}(x)$ had been introduced in equation (2.11), and a positive (negative) exponent is understood as a creation (annihilation) operator. Bosonizing O_ν, the Φ_ν-field acquires a prefactor $(m-n)$, and Θ_ν is multiplied by $(m+n)$ with respect to the single-particle operator $\Psi_{r\nu}$. If gapless channel is assumed to be the charge $\nu = \rho$ (as we have done throughout this paper except in the preceding section), the correlation function of O_ρ behaves as

$$\begin{aligned} R_\rho^{(m,n)}(xt) &= \left\langle O_\rho^{(m,n)}(xt)\left[O_\rho^{(m,n)}(00)\right]^\dagger\right\rangle_{Luttinger} \\ &\sim (\alpha + iv_\rho t - ix)^{-m^2/2}(\alpha + iv_\rho t + ix)^{-n^2/2} \\ &\times \left(\frac{\alpha^2}{(\alpha+iv_\rho t)^2 + x^2}\right)^{\frac{(m-n)^2}{8}(K_\rho - 1) + \frac{(m+n)^2}{8}(K_\rho^{-1} - 1)}. \end{aligned} \tag{6.2}$$

Its Fourier transform is

$$\begin{aligned} R_\rho^{(m,n)}(q,\omega) &\sim \Theta(\omega - v_\rho q)\Theta(\omega + v_\rho q) \\ &\times (\omega - v_\rho q)^{\gamma_-^{(m,n)} - 1}(\omega + v_\rho q)^{\gamma_+^{(m,n)} - 1}, \end{aligned} \tag{6.3}$$

$$\begin{aligned} \gamma_+^{(m,n)} &= \frac{m^2}{2} + \frac{(m-n)^2}{8}(K_\rho - 1) \\ &+ \frac{(m+n)^2}{8}\left(\frac{1}{K_\nu} - 1\right), \\ \gamma_-^{(m,n)} &= \frac{n^2}{2} + \frac{(m-n)^2}{8}(K_\rho - 1) \\ &+ \frac{(m+n)^2}{8}\left(\frac{1}{K_\nu} - 1\right). \end{aligned}$$

We now turn to such an operator for spin, O_σ, in the presence of a spin gap. When the spin gap opens due to the Hamiltonian (2.14), the Φ_σ-field develops long-range order. Its dual field, Θ_σ, then is disordered, and its correlations will contain exponential terms similar to f_{exp}, equation (3.9). We now have to distinguish two cases. (i) If we have $m = -n$, the operator $O_\sigma^{(m,-m)}$ can be represented in terms of the Φ_σ-field alone. Since this is the ordering field, we simply can put it to a constant value, implying $R_\sigma^{(m,-m)}(xt) \sim 1$, and the space-time dependence of the total correlation function is then determined by the charge part $R_\rho^{(s,t)}(q,\omega)$ (which may carry different powers s,t of $\Psi_{r,\rho}$, depending on the spin directions) alone, and given by equation (6.3). One can, in principle, go one

step further and account for the long-wavelength fluctuations out of the ground state-value of Φ_σ. A convenient method for this again is the mapping onto a classical 2D Coulomb gas. Since the Φ_σ-field of the correlation functions introduces electric test charges, we know that in the massive Luther-Emery phase their interaction is exponentially screened (*cf.* Sect. 3). We then find the fluctuation contribution

$$\langle[\Phi_\sigma(xt) - \Phi_\sigma(00)]^2\rangle \sim \frac{\exp\left(-2\Delta_\sigma\sqrt{x^2/v_\sigma^2 - t^2}\right)}{(x^2/v_\sigma^2 - t^2)^{1/4}}\,. \tag{6.4}$$

I will discuss an interesting application in a moment.

However, if (ii) $m \neq -n$, the spin correlations contain the disorder field Θ_σ dual to the Φ_σ, and the gap opening will lead to exponential factors as in equation (3.9). This is the case for the Green's function, *cf.* equation (3.2). We apply the same rules (i) – (v) as in Section 3. Specifically, the prefactor of the gap in the exponential is $c = |m+n|$, by comparing the energy for the insertion of $|m+n|$ σ-particles into the system with the gap obtained in the spectral representation of the exponential. The power-law prefactor is that of the free Luttinger model because there cannot be any anomalous dimensions in a gapped fermion system. In (xt)-space, the correlation function then is

$$\begin{aligned} R_\sigma^{(m,n)}(xt) &= \left\langle O_\sigma^{(m,n)}(xt)\left[O_\sigma^{(m,n)}(00)\right]^\dagger\right\rangle \\ &\sim (\alpha + iv_\sigma t - ix)^{-m^2/2}\,(\alpha + iv_\sigma t + ix)^{-n^2/2} \\ &\quad\times \exp\left(-|m+n|\Delta_\sigma\sqrt{x^2/v_\sigma^2 - t^2}\right). \end{aligned} \tag{6.5}$$

This expression can be Fourier transformed and convoluted with an appropriate charge part.

What the present construction cannot do, however, is to give information on the magnitude, or a possible vanishing, of the prefactor of the correlation function. One example is the $2k_F$-CDW correlation function in the half-filled replusive Hubbard model, where a naive use of the construction above would predict (in real space at $t = 0$) a dependence $\sim x^{-1}$ which, on physical grounds, is not expected to be important in that model [19]. Qualitative information can be obtained in that situation from renormalization group studies, where one can monitor how the amplitude of a correlation function changes as one moves *away* from a Luttinger liquid fixed point [41]. A complete solution of this problem presumably would require an exact boson representation of the *physical* fermions in a Luther-Emery model, including fermion raising operators.

To conclude this section, I discuss two more test cases for my construction procedure. Consider the transverse $2k_F$-spin-correlation functions [1,25]

$$\begin{aligned} R_{SDW\perp}(xt) &= \langle O_{SDW\perp}(xt) O_{SDW\perp}^\dagger(00)\rangle \\ &= \langle \Psi_{-\downarrow}^\dagger(xt)\Psi_{+\uparrow}(xt)\Psi_{+,\uparrow}^\dagger(00)\Psi_{-\downarrow}(00)\rangle \end{aligned} \tag{6.6}$$

in the Luther-Emery spin-gap regime. The spin density wave operator can also be represented as

$$\begin{aligned} O_{SDW\perp}(xt) &= \frac{e^{2ik_Fx}}{2\pi\alpha}\exp\left\{-i\sqrt{2}\,[\Phi_\rho(x) + \Theta_\sigma(x)]\right\} \\ &= e^{2ik_Fx}O_\rho^{(-1,1)}(xt)O_\sigma^{(-1,-1)}(xt). \end{aligned} \tag{6.7}$$

We now limit ourselves to the spin component of the correlation function and obtain, using equation (6.5),

$$R_\sigma^{(-1,-1)}(xt) \sim \frac{\exp\left(-2\Delta_\sigma\sqrt{x^2/v_\sigma^2 - t^2}\right)}{\sqrt{x^2 - v_\sigma^2 t^2}}\,. \tag{6.8}$$

Fourier transformation gives

$$R_\sigma^{(-1,-1)}(q,\omega) \sim \frac{\Theta(\omega^2 - v_\sigma^2q^2 - 4\Delta_\sigma^2)}{\sqrt{\omega^2 - v_\sigma^2q^2 - 4\Delta_\sigma^2}}\,. \tag{6.9}$$

One the other hand, *on the Luther-Emery line* $K_\sigma = 1/2$, one can refermionize the operator

$$O_\sigma^{(-1,-1)}(x) = \sqrt{2\pi\alpha}\Psi_-^\dagger(x)\Psi_+^\dagger(x) \tag{6.10}$$

in terms of spinless fermions $\Psi_r(x)$, by inverting the spinless variant [1] of the bosonization formula (2.8). The limitation of this procedure to the Luther-Emery line is inessential because different coupling constants will only affect the magnitude of the spin gap but not the form of the excitation spectrum, so long as $\Delta_\sigma > 0$. Now, one can calculate $R_\sigma^{(-1,-1)}(q,\omega)$ as the pairing correlation function of spinless fermions *in a fermion representation.* Such a calculation has been outlined by Lee [25], and the result derived from his expressions agrees with equation (6.9) both concerning the regions of nonvanishing spectral weight, and the critical exponents of the singularities. Incidentally, my own expressions are more complicated than Lee's by additional terms and additional occupation functions $n(k)$ and $1 - n(k)$. They conspire with the coherence factors $[1 \pm v_\sigma q/\varepsilon_\sigma(q)]$ to produce a prefactor $v_\sigma^2q^2/(v_\sigma^2q^2 + 4\Delta_\sigma^2)$ to the leading inverse-square-root singularity which vanishes as $q \to 0$. At $q = 0$, a subleading term $\propto \Theta(|\omega| - 2\Delta_\sigma)$ times a regular function remains. Apart these subtle prefactors, the exact fermionic calculation reproduces the result of the construction procedure advocated here for the correlation functions of the Luther-Emery model.

A final test is provided by the charge correlations of a 1D Mott insulator. In general, the charge density operator $\hat{n}(x)$ has contributions at wavevectors $q \approx 0,\ 2k_F,\ 4k_F$, *etc.*

$$\begin{aligned} \hat{n}(x) \sim\ & -\frac{\sqrt{2}}{\pi}\frac{\partial\Phi_\rho(x)}{\partial x} \\ &+ \frac{1}{\pi\alpha}\exp\left\{-2ik_Fx + \sqrt{2}i\Phi_\rho(x)\right\}\cos[\sqrt{2}\Phi_\sigma(x)] \\ &+ \frac{2}{(2\pi\alpha)^2}\exp\left\{-4ik_Fx + \sqrt{8}i\Phi_\rho(x)\right\}. \end{aligned} \tag{6.11}$$

In a half-filled band, $4k_F = 2\pi/a$, a reciprocal lattice vector so that the $4k_F$-term effectively does not oscillate when

measured on the lattice sites. When the Mott gap Δ_ρ opens, the field Φ_ρ orders at a finite constant value. The third term in (6.11) then translates the long-range charge order, the first term measures the long-wavelength fluctuations out of this ordered ground state, and the second term measures $2k_F$ charge fluctuations. Using the arguments at the beginning of this section (after $\sigma \leftrightarrow \rho$), we obtain from the first two terms a spectral function

$$R_n(q,\omega) \sim \delta(q)\delta(\omega) + q^2 \frac{\Theta(\omega^2 - v_\rho^2 - 4\Delta_\rho^2)}{\omega^2 - v_\rho^2 - 4\Delta_\rho^2} \cdot \qquad (6.12)$$

The zero-frequency δ-function comes from the "$4k_F$"-part, and the high-frequency signal from the $\partial\Phi_\rho/\partial x$-term. In principle, one could also calculate the $2k_F$-part. However, experience with the Hubbard model suggests that prefactors not specified here suppress the $2k_F$-CDW fluctuations on the lattice sites [1], and we do not consider them here (similar, and nonvanishing contributions, however appear in $2k_F$-SDW correlation functions, and in a "bond order wave" which is best described as a $2k_F$-CDW centered midway between two sites).

The spectral function $R_n(q,\omega)$ has been calculated recently by Mori and Fukuyama [26]. They do not give an explicit expression which would allow to check the critical exponents, but the region of nonvanishing spectral weight, and the overall shape of the high-frequency signal are consistent with equation (6.12), whereas the δ-function in equation (6.12) seems to be missing. It is present, however, in a numerical diagonalization of an extended Hubbard model [42], and provides another, though more superficial test of our construction.

7 Relation to other work

In the preceding sections, we have discussed some tests for the dynamical correlation functions of the Luther-Emery model constructed here [25,38]. Independent verification comes from work on many models which fall into the Luther-Emery universality class.

In particular, numerical studies have attempted to look into the spectral properties of correlated fermion models. Quantum Monte-Carlo simulations of the 1D Hubbard model at half-filling, a prototypical Mott insulator with $v_\rho > v_\sigma$ provides evidence for pronounced shadow bands, much stronger than those of the doped systems which form Luttinger liquids [30]. At present, the resolution is not good enough to directly visualize the two dispersing inverse-square-root singularities found here. However, recent improvements on doped Hubbard models [43] lend hope that Quantum Monte-Carlo will be able, in the near future, to confirm the predicitons made here.

The 1D $t-J$-model at half-filling also forms a Mott insulator with $v_\rho > v_\sigma$, and exact diagonalization of lattices up to 22 sites has allowed a calculation of the spectral function of this model [15]. While the location of regions of finite spectral weight, and of the singularities agrees with the present study, numerical diagonalization on such small systems does not allow to determine the critical exponents of the divergences of the 1D Mott insulator.

Spin gaps also arise in many lattice models. *E.g.* for two coupled Luttinger, Hubbard, or $t-J$-chains, there are wide regions of parameter space where the spin fluctuations are massive, and the single-particle spectral function has been calculated occasionally [33]. Again, exact diagonalization finds important shadow bands [33] but the resolution is not good enough to separate the two dispersing divergences found in Section 4 for a superconductor, not to speak of the much weaker signal on the shifted charge dispersion $\varepsilon_\rho(q)$ predicted above for a CDW system.

Evidence for such a weak signal, and for a divergent signal on the gapped spin dispersion $\varepsilon_\sigma(q)$ comes, however, from exact diagonalization of a $t-J-J'$-model where a spin gap opens for certain values of J' [44]. These authors observe a very strong spinon signal, and the holon peak is anomalously weak, as predicted here.

A Bethe Ansatz calculation of spectral functions for a 1D Mott insulator has recently been performed by Sorella and Parola (SP) based on the 1D supersymmetric $t-J$ model [45], and also confirms essential aspects of the present work. In their model, $v_\rho < v_\sigma$ so that we predict a single inverse-square-root singularity on $\varepsilon_\rho(q)$. Such a singularity is also found from the Bethe Ansatz solution used by SP. When a finite magnetization is included, SP find critical exponents which explicitly depend on the momentum of the hole created. One would expect from universality and the possibility to transform a positive-U Hubbard model into one with negative U by a particle-hole transformation on one spin species alone, that such spectral functions should also describe spin-gapped systems with $v_\rho > v_\sigma$. We do not find such momentum-dependences in the work presented here. SP's method, however, requires the calculation of the ground state and low-energy properties of the spin Hamiltonian at finite total momentum of the spin system. These explicitly depend on the momentum, and produce the momentum-dependent exponents. In the Luther-Emery model, one calculates a spinon excitation with some momentum with respect to a zero momentum ground state. The momentum-dependent correlation exponents found by SP certainly are beyond scope and possibilities of the present model. On the other hand, their method does not allow to look into more subtle features than critical exponents, such as the finite maximum which we found in this case.

8 Applications to experiments

Importantly, our results could prove useful in the description of the photoemission properties of certain quasi-1D materials.

There have been angle-resolved photoemission experiments on the 1D Mott insulator $SrCuO_2$ with a gap $2\Delta_\rho \sim 1.8$ eV [15]. The lineshapes observed were anomalously broad and showed unsual dispersion. As a consequence, the authors proposed a description in terms of a system with charge-spin separation, where the broad feature would, in fact, be composed of the unresolved spin

and charge signals. In addition, a strong shadow band bends back from the gap edge for $k > k_F$. Its dispersion is consistent with the one of the charge signal for $k < k_F$. Clearly, these observations are fully consistent with the theory presented here, which predicts two inverse-square-root singularities beyond some critical wave vector (*cf.* Fig. 5), and a single one below, as are the accompanying diagonalization results on a 1D $t-J$-model [15].

More interesting in the present context are a number of unexplained ARPES results on organic and inorganic materials which undergo Peierls transitions at low temperatures. Specifically, ARPES experiments on the blue bronze $K_{0.3}MoO_3$ by several groups show *two* dispersing peaks [12]. Also in the organic conductor TTF–TCNQ, anomalous lineshapes are observed [13]. Of interest here is the TCNQ-band which shows $2k_F$-CDW fluctuations in the metallic state [14] and triggers a series of transitions into a low-temperature CDW phase. While some materials such as the Bechgaard salts [7], or the TTF-band of TTF–TCNQ (which has strong $4k_F$-CDW fluctuations [14]) may well fall into the Luttinger liquid universality class, it is particularly surprising that CDW systems such as $K_{0.3}MoO_3$, or the TCNQ-band in TTF–TCNQ, should behave as Luttinger liquids. In fact, the photoemission properties are in striking contrast to the established picture of a fluctuating Peierls insulator which has been applied quite universally to describe the normal state of CDW systems [46]. It predicts a strongly temperature dependent, narrow [$|\omega| \leq \Delta_{CDW}(T=0)$] pseudogap and $\rho(q<0,\omega)$ is governed by a broadened quasi-particle peak at $\omega < 0$ and a weak shadow at $\omega > 0$ [18,47].

A Luttinger liquid interpretation for the CDW photoemission is highly suggestive but encounters problems which are all resolved in a Luther-Emery framework. (i) As has been explained before, Luttinger liquids have no dominant $2k_F$-CDW correlations: for repulsive interactions ($K_\rho < 1$), spin density waves are logarithmically stronger than CDWs [1], and the behavior of lattice models is consistent with this picture [48]. For attractive interactions, the system is dominated by superconductivity [1]. A spin gap is a necessary condition for promoting CDW correlations in correlated 1D electron systems and is realized in the Luther-Emery model! (ii) $2k_F$-CDWs often are due to electron-phonon coupling, and renormalization group provides us with a detailed scenario [1,27]. The dependence of the spin gap on electron-phonon coupling λ, the phonon frequency ω_D, and K_ρ, can be calculated reliably [27]. A spin gap also opens if $2k_F$-CDWs are caused by Coulomb interaction between chains [34]. (iii) The spin susceptibility of CDW systems above the Peierls temperature decreases significantly with decreasing temperature indicative of activated spin fluctuations. This applies applies both to $K_{0.3}MoO_3$ at temperatures from T_P to beyond 700 K [49], and to the TCNQ-chain in TTF–TCNQ where the magnetic susceptibility contributions of both chains can be separated by NMR [50]. Notice in this context that at finite temperature, the density of states in the spin channel of the Luther-Emery model is essentially the same as for the Lee-Rice-Anderson theory of a fluctuating Peierls insulator [51], implying that both models will have similar $\chi(T)$. The temperature-dependent susceptibility alone therefore cannot discriminate between these two theories. Remarkably however, in $K_{0.3}MoO_3$ the conductivity is metallic in the same temperature range: early experiments over a restricted temperature range find the resistance $\rho(T) \sim T$ [52] while very recent data taken to much higher temperatures even suggest a sublinear temperature dependence [53] – not unlike the one found in Luttinger liquids with repulsive electron-electron interactions [54]. In TTF–TCNQ, $\rho(T) \sim T$ has been found [55], but it is not known how the individual chains contribute to this dependence. The experiments are incompatible with the temperature dependence of the conductivity expected in a fluctuating Peierls insulator [18] which indeed is observed in some organic materials and also $(TaSe_4)_2I$. (iv) For a Luttinger model, the stronger divergence in $\rho(q,\omega)$ is associated with the charge mode and disperses more quickly than the weaker signal. In the experiment on $K_{0.3}MoO_3$, the quickly dispersing signal is less peaked than the slow one. On the other hand, the important feature of the Luther-Emery spectral function, Figure 1, is that the spin gap supresses the divergence of the charge signal which disperses more quickly than the divergent spin contribution. (v) A CDW transition out of a Luther-Emery liquid by opening a charge gap at the Peierls temperature, is also consistent with subtle transfers of spectral weight in regions *away* from the Fermi energy, observed in spectra taken through the true CDW transition [56]. In these experiments, the spectral weight at the Fermi energy is essentially zero at any temperature. However, at some finite energy below E_F, the weight drops with a temperature dependence consistent with a BCS-like gap. In a naive charge-spin separating, Luther-Emery scenario, one would postulate the opening of a charge gap Δ_ρ at the Peierls temperature (as a consequence of the establishment of 3D coherence, allowing for the finite-T transition), in addition to the preexisting spin gap. Thus one expects a drop of spectral weight at the Peierls transition in an energy range between $E_F - \Delta_\sigma$ and $E_F - \Delta_\sigma - \Delta_\rho$ which, on a sufficiently coarse temperature scale, would amount to a shift of the leading edge by Δ_ρ. More likely, the establishment of 3D coherence will destroy to some extent the ideal spin-charge separation of the 1D Luther-Emery model, and produce a single CDW gap $\Delta_{CDW} > \Delta_\sigma$ below the transition, both for charges and spins.

On a quantitative level, there is one major problem for the description of the normal state of most CDW systems: the spin gap derived from an analysis of the magnetic susceptibilities is much smaller than the spin gaps derived from the peak maxima of the ARPES signals. At present it is not clear if this indicates a fundamental problem with a Luther-Emery model (the problem would however not be solved with any competing theory), if this is due to some ununderstood effect in the photoemission process, or if it is due to some extrinsic sample property. In another language, it is not clear what mechanism is responsible for

apparent gaps which systematically are a sizable fraction of the valence band widths.

This phenomenology is not consistent with many other theories proposed for 1D fermions. Theories based on a fluctuating Peierls insulator would have to explain the two dispersing bands seen in $K_{0.3}MoO_3$ as two separate bands. Two such bands indeed exist but the implication would be that band structure calculations get one of them too narrow by a factor of 5, but get the correct dispersion for the other one [57]. Moreover, they cannot reconcile the activated susceptibility with the essentially metallic conductivity above the Peierls temperature.

Standard Luttinger liquids [1,43], but also the anomalous ground states obtained from coupling Luttinger chains so long as their low-energy fixed point is a Fermi liquid [34], do neither produce the CDW correlations, nor the activated susceptibility. Notice, however, that both transversely coupled Luttinger liquids (Kopietz *et al.* [34]) and the 1D Hubbard model [43] can, under some circumstances, produce spectral functions where the peak on the spinon dispersion is stronger than that on the charge dispersion. They, however, would predict a Fermi surface crossing of the photoemission signal which is not observed experimentally, in addition to the problems listed above. In the experiments, instead, the dispersing spectral features bend back from the Fermi energy as k is increased beyond k_F, in a manner strongly reminiscent of the shadow bands discussed before.

Depsite (important) quantitative problems, the Luther-Emery spectral function is consistent with the photoemission experiments on $K_{0.3}MoO_3$ and TTF–TCNQ, and beyond that, the model is consistent with much of the other experimental phenomenology available. I emphasize that while the agreement of the Luther-Emery spectral function with the observed photoemission lineshapes certainly is an argument in favor of this model, it is the consistency of its predictions with most other experiments available which suggests that it might be a natural starting point for a description of the low-energy physics of these CDW materials.

Obviously, this suggestion is somewhat speculative and independent support is called for. Its virtue is that it comes to grips with the puzzle that the spin susceptibilities of $K_{0.3}MoO_3$ and TTF–TCNQ decrease with decreasing temperature while the conductivity are metallic, that it leaves space for the good description of optical properties as a fluctuating Peierls insulator (they only probe the charge fluctuations which will form CDW precursors at temperatures much below the spin gap opening, presumably as a consequence of emerging 3D coherence), and that it provides an (admittedly phenomenological) description of the photoemission properties of these materials with extremely 1D *electronic* properties [58]. As in the Bechgaard salts [7], a single-particle exponent $\alpha \sim 1/2 \ldots 1$ would be required implying strong long-range electron-electron interactions, and there is at best preliminary support from transport measurements [53], for such strong correlations in $K_{0.3}MoO_3$. Retarded electron-phonon coupling could increase α over its purely electronic value [27]. To what extent this mechanism contributes could be gauged from the measured α which must be larger than the one derived from the enhancement of v_ρ over the band velocity (hélas strongly depending on the accuracy of band structure calculations). In TTF–TCNQ, the analysis is made difficult by the presence of two chains. There is evidence for strong long-range electron-electron interactions on the TTF-chain from the observation of $4k_F$-CDW fluctuations, but the situation for TCNQ is less clear. If a sizable enhancement of the dispersion of the ARPES signals over the estimated bandwidths can be interpreted as evidence for long-range electronic correlations, they would indeed be present on both chains.

9 Summary

In this paper, I have presented a construction of the dynamical correlation functions of the 1D Luther-Emery model. This model has one gapped degree of freedom, and an ungapped one, and describes 1D superconductors and Peierls insulators (spin gap) and 1D Mott insulators (charge gap). It is a natural extension of Luttinger liquid theory to the peculiar phase intermediate between metal and band insulator, made possible in one dimension by the phenomenon of charge-spin separation. The dynamical correlation functions presented here show where and to what extent the two typically 1D features of a Luttinger liquid: charge-spin separation, and anomalous dimensions of operators, survive in the presence of a gap in one channel. Since an exact calculation of such correlation functions usually is not possible in a Luther-Emery model, our construction relied heavily on limiting cases, symmetries, and equivalences to other models. However, it successfully passed several tests in situations where exact results were available from other methods.

The main emphasis of the paper was on the single-particle spectral function which is measured in photoemission. We showed that, generically, charge-spin separation and anomalous dimensions are also visible in the spectral functions of the Luther-Emery model. Specifically, for a spin gapped system with repulsive interactions, describing a 1D charge density wave system, the spectral function has a true singularity on the gapped spin dispersion with an anomalous exponent $\alpha - 1/2$ while on the charge dispersion, the Luttinger liquid divergence is cut off to a finite maximum by the spin gap – a results which finds a straightforward explanation in terms of convolution of charge and spin correlation functions. For attractive interactions, *i.e.* a 1D superconductor, two divergences with anomalous dimensions are found. For 1D Mott insulators, *i.e.* a charge gap, one finds one or two inverse-square-root singularities, *i.e.* no anomalous dimension (due to spin-rotation invariance), depending on the order of the velocities of the charge or spin fluctuations. It was also shown how these procedures can be generalized to two- and multi-particle correlation functions.

Besides predicting spectral functions for the many 1D models falling into the Luther-Emery universality class, there are a few experimental situations where these results

can be usefully applied. They successfully describe the photoemission spectrum of the 1D Mott insulator $SrCuO_2$ [15], to an extent leaving few questions open, the most notable one being experimental resolution. Less clearcut but perhaps more interesting are CDW materials such as $K_{0.3}MoO_3$ and TTF–TCNQ which show very unusual photoemission spectra. These are qualitatively consistent with a Luther-Emery model, and we have proposed that these materials might, most naturally, be described in this framework. A Luther-Emery phase is necessary as an intermediate between a Luttinger liquid and a long-range ordered CDW, and $K_{0.3}MoO_3$ and TTF–TCNQ are natural candidates for searching for such a strange metal. This scenario requires strong electron-electron interactions at least at high energies, and not all CDW materials need fall into this scheme. If the electron-phonon interaction is so strong as to produce CDW precursor fluctuations at very high temperature, and the electronic correlations are weak enough, the establishment of a Luttinger liquid, and the crossover to a Luther-Emery liquid at lower temperature, may be quenched, and a fluctuating Peierls insulator [46] or a bipolaron liquid [59] may be a more appropriate picture. Some CDW materials such as $(TaSe_4)_2I$ [11], $(perylene)_2PF_6$ [18], $(fluoranthene)_2PF_6$ [60] apparently are consistent with this picture. However, $K_{0.3}MoO_3$ and TTF–TCNQ are not consistent, and the consistency of the spectral functions constructed in this paper with the published experiments, and the analysis of further experiments indicate that, besides electron-phonon coupling, electronic correlations must be important in these CDW systems.

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