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LETTER TO THE EDITOR

Spectral properties of Luther–Emery systems

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Abstract. We construct the spectral function of the Luther–Emery model which describes one-dimensional fermions with gapless charge and gapped spin degrees of freedom. We find a true singularity with interaction dependent exponents on the gapped spin dispersion and a finite maximum depending on the magnitude of the spin gap on a shifted charge dispersion. We apply these results to photoemission experiments on charge density wave systems and discuss the spectral properties of a one-dimensional Mott insulator.

Non-Fermi liquid behaviour in correlated fermion systems is an exciting topic of current research. One-dimensional (1D) metals 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 each obey their proper dynamics [1]. The key features of these 'Luttinger liquids' [2] clearly show up in the single-particle spectral function

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

which can be measured in photoemission: (i) absence of fermionic quasi-particles, (ii) anomalous dimensions of operators producing correlation functions with non-universal power laws, (iii) charge–spin separation [3]. (In equation (1), G is the electronic Green function, k_F the Fermi wave number, and μ the chemical potential.) Responsible for this 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 $2k_F$ charge and spin density fluctuations which then interfere with Cooper-type superconducting fluctuations.

In a Luttinger liquid, both the charge and the spin excitations are gapless. One-dimensional Peierls or Mott insulators or superconductors are, however, characterized by one gapless and one gapped degree of freedom. The model describing this situation,

$$H = H_0^{(\rho)} + H_0^{(\sigma)} + H_{1\perp} \tag{2}$$

$$H_0^{(\nu)} = \frac{1}{2\pi}\sum_{\nu=\rho,\sigma}\int \mathrm{d}x\,\left\{ v_\nu K_\nu\,\pi^2\Pi_\nu^2(x) + \frac{v_\nu}{K_\nu}\left(\frac{\partial\Phi_\nu(x)}{\partial x}\right)^2\right\} \tag{3}$$

$$H_{1\perp} = \frac{2g_{1\perp}}{(2\pi\alpha)^2}\int \mathrm{d}x\,\cos\left[\sqrt{8}\Phi_\sigma(x)\right] \tag{4}$$

has been solved by Luther and Emery [4]. Here, H_0 describes harmonic charge ($\nu=\rho$) and spin ($\nu=\sigma$) density fluctuations through the bosonic phase fields $\Phi_\nu(x)$ and their canonically conjugate momenta $\Pi_\nu(x)$. Their dispersions are gapless $\omega_\nu(q) = v_\nu|q|$ with velocities v_ν, and H_0 contains, in addition, stiffness constants K_ν. The backscattering

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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 (else, (2) reduces to a Luttinger liquid). The *umklapp* Hamiltonian for a half-filled band is obtained by simply replacing spin by charge in equation (4). Luther and Emery have shown that for the special value $K_\sigma = 1/2$, the interaction Hamiltonian (4) can be represented as a bilinear in spinless fermions, and diagonalized. The resulting spectrum $\varepsilon_\sigma(q) = \pm\sqrt{v_\sigma^2 q^2 + \Delta_\sigma^2}$ shows a gap Δ_σ at the Fermi level. Systems in these classes would be dominated by singlet superconducting (SS) [5] or charge density wave (CDW) correlations [6, 7] or be 1D Mott insulators [8, 9]—problems of high experimental and theoretical interest. We concentrate on the spin-gap problem because it is more generic: here all values of K_ρ are physically sensible (giving SS for $K_\rho > 1$ and CDW for $K_\rho < 1$) while spin-rotation invariance enforces $K_\sigma = 1$ for the Mott problem.

There is a fairly complete picture of the properties of Luttinger liquids [1], but much less is known for systems with both gapless and gapped degrees of freedom. There is a general belief that the opening of a gap affects the system for frequencies smaller than this gap while the behaviour of the ungapped system is essentially recovered at larger frequency scales. Moreover, several methods [10] support the idea that 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 $\int \mathrm{d}x\, \Pi_\sigma(x)$ decay exponentially in space (or oscillate in time) which would cut off (shift) the divergences as functions of q (ω) 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—due to the absence of any practical relation between the physical fermions and the spinless pseudofermions emerging from the Luther–Emery solution [11] and, to my knowledge, no critical check of these hypotheses by numerical work. It is the purpose of this letter to discuss the spectral function of a model with gapless and gapped degrees of freedom and to comment on recent photoemission experiments on quasi-1D CDW systems where this model could be relevant.

Here, I construct the single-particle spectral function $\rho(q, \omega)$, equation (1), for the Luther–Emery model. Other correlation functions may be obtained along the same lines. The charge–spin separation manifest in the Hamiltonian (2) allows us to represent $G(xt)$ as a product of certain charge and spin correlation functions $g_\nu(x, t) = \langle \Psi_{rx}^{(\nu)}(xt) \Psi_{rs}^{(\nu)\dagger}(00) \rangle$ where the notation $\Psi^{(\nu)}$ indicates that only the ν-part of the boson representation of Ψ is to be taken, and $\rho(q, \omega)$ as a convolution of their Fourier transforms. The charge part is simply calculated in the Luttinger model [3].

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 behaviour of this function can, however, be *uniquely constructed from symmetries, equivalences, and known limits*. The important steps are the following. (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

$$g_\sigma(xt) \sim f_+(x - v_\sigma t) f_-(x + v_\sigma t) f_{\exp}(x \pm v_\sigma t). \tag{5}$$

(ii) For vanishing gap, g_σ must reduce to the correct Luttinger form. This requires $f_{\exp}(x \pm v_\sigma t; \Delta_\sigma = 0) \equiv 1$ and determines all possible power laws up to corrections $\mathrm{O}(\Delta_\sigma)$ in the exponents, or terms varying more slowly than a power law. (iii) From the equivalence of the Luther–Emery model to a classical 2D Coulomb gas, and Debye screening of the charges above the Kosterlitz–Thouless temperature $\propto \exp(-\Delta_\sigma |\boldsymbol{r}|)$ [12], one deduces an exponential factor $\exp(-c\Delta_\sigma \sqrt{x^2/v_\sigma^2 - t^2})$, with an undetermined constant

c, in $f_{\rm exp}$. (iv) Exponential terms with the same (or slower) decay but different dependences on $x \pm v_\sigma t$ can be excluded by imposing $g_\sigma(x,t) = g_\sigma^\star(-x,-t)$ derived from translational invariance. (v) Gulácsi has calculated explicitly the $t = 0$ Green function of a 1D Mott insulator [13]: his calculation excludes the possible corrections to the power laws of $O(\Delta_\sigma)$ mentioned in (ii) and therefore fixes the power-law contributions $f_\pm$ to be just of the usual Luttinger form. Moreover, exponential decay faster than determined in (iii) is excluded, too, and the open constant $c = 1$ is determined. I thus find

$$g_\sigma(x,t) \sim \exp\left(-\Delta_\sigma \sqrt{x^2 - v_\sigma^2 t^2}/v_\sigma\right) \Big/ \sqrt{\alpha + \mathrm{i}(v_\sigma t - x)}. \tag{6}$$

Fourier transformation then gives

$$g_\sigma(q,\omega) \sim \left(1 + \frac{v_\sigma q}{\sqrt{v_\sigma^2 q^2 + \Delta_\sigma^2}}\right) \frac{\Theta(\omega + v_\sigma q)}{\sqrt{\omega + v_\sigma q}} \delta\left(\omega - \sqrt{v_\sigma^2 q^2 + \Delta_\sigma^2}\right). \tag{7}$$

This result can then be convoluted with the charge part.

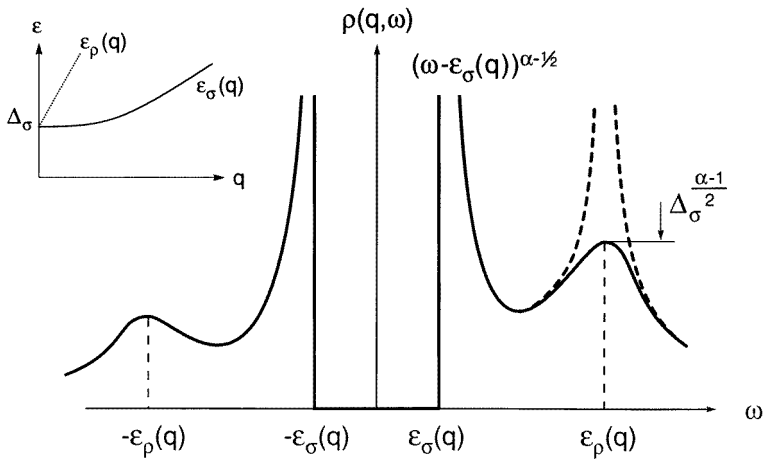

Figure 1. Spectral function of the Luther–Emery model for $q > 0$. The thick dashed line at $\varepsilon_\rho(q)$ gives the Luttinger liquid divergence which is supressed here. The inset shows the dispersion of the two $\omega > 0$ features.

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 $\varepsilon_\sigma(q)$ and at a shifted charge dispersion $\varepsilon_\rho(q) = v_\rho q + \Delta_\sigma$ (inset in figure 1). The result of the calculation is shown schematically in figure 1 for $q > 0$ and the (realistic) case $v_\rho > v_\sigma$. There are indeed features at these frequencies. At $\varepsilon_\sigma(q)$, there is a true singularity $[\omega - \varepsilon_\sigma(q)]^{\alpha-1/2}$ as in the Luttinger model (however, here α is *defined* as $\alpha = (K_\rho + K_\rho^{-1} - 2)/4$ since the notion of a K_σ does not make sense). Folklore would then predict another singularity $|\omega - \varepsilon_\rho(q)|^{(\alpha-1)/2}$ (dashed lines in figure 1) which is *not* observed here. It is cut off instead to a finite maximum of order $\Delta_\sigma^{(\alpha-1)/2}$: as in the 1D quantum antiferromagnet, the opening of the spin gap cuts off the singularity of the prefactor of the delta function in (7) as $q \to 0$, 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 negative 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 positive frequencies. For $q > 0$, the positive 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.

Can we expect structured spectral functions for α larger than 1/2 or 1? The present construction, which amounts to determining the leading behaviour and does not fulfill sum rules, does not allow a definite answer. Experience with the Luttinger model shows, however, that, once all sum rules are enforced, when the exponents increase so as to change a divergence into a cusp singularity the prefactor changes sign so as to turn upward the cusps [14]. Such a crossover, keeping peaky structures also for large α, is natural and is expected to occur in the present problem, too.

Notice finally that the behaviour of $\rho(q, \omega \approx \pm\Delta_\sigma)$ is determined by that of the spin part close to Δ_σ and the charge part at $\omega \approx 0$. Unlike earlier conjectures [10], 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 $N(\omega) \sim \Theta(\omega - |\Delta_\sigma|)(\omega - |\Delta_\sigma|)^\alpha$. 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 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 this, singular spectral response remains possible in q- and ω-dependent correlation functions.

The spectral function of a 1D Mott insulator can be computed as a special case of the generic solution presented above ($\sigma \leftrightarrow \rho$ everywhere and $K_\sigma = 1$ for spin-rotation invariance). Then

$$\rho(q, \omega) \propto \Theta\Big(\omega - \sqrt{v_\rho^2 q^2 + \Delta_\rho^2}\Big) \Big/ \sqrt{\omega - \sqrt{v_\rho^2 q^2 + \Delta_\rho^2}}$$

and $N(\omega) \sim \Theta(\omega - \varepsilon_\rho)$ times a regular function here. 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 [9, 13]. Continuity then suggests that as the Mott transition is approached by varying the band-filling spectral weight is gradually taken out of both the charge and spin divergences of the Luttinger liquid parts of the spectral function to reappear in the Luther–Emery function possessing only a charge divergence, although the transition leaves the spins unaffected and opens only a charge gap. When superposing (to a first approximation) the two signals, care must be taken, however, to account for the dependence of the chemical potential on doping level.

A wide variety of models fall into the Luther–Emery universality class and the present 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 [5]; the negative-U Hubbard model at any band-filling has a spin gap [15], the positive-U Hubbard model at half-filling has a charge gap [8, 9], spin gaps occur frequently in models of two coupled Luttinger or Hubbard chains

[16, 17] etc. Some numerical studies have attempted to calculate spectral properties [9, 17]. While consistent with the present work on the existence of shadow bands, their resolution is not good enough to probe the finer structures computed here.

A more microscopic calculation of spectral functions for the 1D Mott insulator has recently been performed by Sorella and Parola (SP) based on the 1D t–J model [18], and confirms the essential aspects of the present work. Specifically, it supports the present work in (i) the suppression of the signal living on the shifted charge (spin) dispersion when a spin (charge) gap opens, but the possibility of a finite maximum remaining is not discussed (as pointed out above, neither do we find such a maximum for $K_{\rho(\sigma)} = 1$ in the gapless channel, the case studied by SP); (ii) a true singularity associated with a branch cut in $G(k, \omega)$ is found on the spin (charge) dispersion. The momentum-dependent correlation exponents found by SP are, however, beyond the scope and possibilities of the present model. On the other hand, it is not clear how their results reduce to a Luttinger spectrum when $\Delta \to 0$ where *momentum-independent* exponents are expected [18].

Importantly, our results could prove useful in the description of the photoemission properties of certain quasi-1D materials. There is now a considerable number of such experiments on quasi-1D conductors in their 'normal' metallic state (above low-temperature phase transitions) [6, 7, 19]. Usually, they measure the density of states $N(\omega)$, which universally shows an absence of spectral weight at the Fermi edge, and a gradual increase with energy only over a considerable fraction of the conduction band width, these two features being essentially temperature independent. This behaviour is formally consistent with the Luttinger liquid picture, predicting $N(\omega) \propto |\omega|^{\alpha}$ with some interaction-dependent exponent $\alpha > 0$. More strikingly even, an angle-resolved photoemission experiment on $K_{0.3}MoO_3$ shows *two* dispersing peaks [19]. While some materials, such as the Bechgaard salts, may well fall into this universality class [20], it is particularly surprising that CDW systems such as the blue bronze $K_{0.3}MoO_3$ or $(TaSe_4)_2I$ should behave similarly. In fact, the photoemission properties are in striking contrast to the established picture of a fluctuating Peierls insulator [21]. It predicts a strongly temperature-dependent, narrow ($|\omega| \leqslant \Delta_{CDW}(T = 0)$) pseudogap and $\rho(q > 0, \omega)$ is governed by a broadened quasi-particle peak at $\omega > 0$ and a weak shadow at $\omega < 0$.

A Luttinger liquid interpretation for the CDW photoemission is highly suggestive but encounters problems which are all resolved in a Luther–Emery framework. (i) Luttinger liquids have no dominant $2k_F$-CDW correlations: for repulsive interactions ($K_\rho < 1$) spin density waves are logarithmically stronger than CDWs, and for attractive interactions the system is dominated by superconductivity [1]. A spin gap is a necessary condition for dominant CDW correlations in 1D and 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, 5]. The dependence of the spin gap on electron–phonon coupling λ, the phonon frequency ω_D and K_ρ can be calculated reliably [5]. A spin gap also opens if CDWs are caused by Coulomb interaction between chains [22]. (iii) The spin susceptibility of CDW systems above the Peierls temperature decreases with decreasing temperature indicative of activated spin fluctuations. Remarkably, in $K_{0.3}MoO_3$ the conductivity is metallic in the same temperature range. (iv) For a Luttinger model, the stronger divergence in $\rho(q, \omega)$ is associated with the charge mode. For repulsive interactions $v_\rho > v_\sigma$, while 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 [23]. The Luther–Emery spectral function is consistent with the experiments and this model therefore might be a natural starting point for a description of the low-energy physics of CDW materials such as $K_{0.3}MoO_3$.

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 susceptibility of $K_{0.3}MoO_3$ decreases with decreasing temperature while the conductivity is 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 this material with extremely 1D *electronic* properties [24]. As in the Bechgaard salts [20], a single-particle exponent $\alpha \sim 1$ would be required, implying strong long-range electron–electron interactions, and there is at best preliminary support from transport measurements for such strong correlations in $K_{0.3}MoO_3$. Retarded electron–phonon coupling could increase α over its purely electronic value [5]. To what extent this mechanism contributes can be gauged from the measured α which must be larger than the one derived from the enhancement of v_ρ over the band velocity (alas strongly depending on the accuracy of band structure calculations). In the perspective of the present work, high-resolution photoemission studies on the organic conductor TTF-TCNQ are desirable because there is independent evidence both for strong electronic correlations and electron–phonon coupling, and a crossover between regimes dominated by one or the other seems to take place as the temperature is varied.

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