Local density of states of 1D Mott insulators and CDW states with a boundary

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We determine the local density of states (LDOS) of one-dimensional incommensurate charge density wave (CDW) states in the presence of a strong impurity potential, which is modeled by a boundary. We find that the CDW gets pinned at the impurity, which results in a singularity in the Fourier transform of the LDOS at momentum $2k_F$. At energies above the spin gap we observe dispersing features associated with the spin and charge degrees of freedom respectively. In the presence of an impurity magnetic field we observe the formation of a bound state localized at the impurity. All of our results carry over to the case of 1D Mott insulators by exchanging the roles of spin and charge degrees of freedom. We discuss the implications of our result for scanning tunneling microscopy experiments on spin-gap systems such as two-leg ladder cuprates.

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In recent years scanning tunneling microscopy (STM) and spectroscopy (STS) techniques have proved to be very useful tools for studying strongly correlated electron systems such as high temperature superconductors (HTSC) [3], carbon nanotubes [2], and rare-earth compounds [4]. The usage of magnetic tips has also enabled the investigation of magnetic properties [4]. These experiments have motivated an intense research effort on the theory of STS [3,4], the main focus being on quasiparticle properties in HTSC. STM measures the local differential conductance $dI/dV(x)$, which is directly related to the LDOS. Impurities break translational invariance and lead to a modification of the LDOS in their vicinity, from which one can infer characteristic properties of the bulk state of matter as well as the nature of its electronic excitations. Interestingly this holds even in strongly correlated systems without quasiparticle excitations as was demonstrated for a non-magnetic impurity placed in a gapless Luttinger liquid [5,6], which can be regarded as a quantum critical CDW state. In this case, at low energies the impurity behaves effectively as a physical boundary [3] where the phase of the CDW order parameter gets pinned, giving rise to induced CDW order.

Here we consider STS in a 1D strongly correlated system with a spin gap in the presence of an impurity. This problem is of interest to the study of (quasi) 1D CDW systems, two-leg ladder materials with strong superconducting correlations, and the stripe phases of HTSC [3]. We focus on the regime in which the scattering at the impurity is strong and hence at sufficiently low energies it acts as a physical boundary [11]. The inherently non-perturbative nature of STS in gapped (quasi)-1D systems requires an entirely different treatment compared to previously studied cases. Following Ref. [3] we consider the spatial Fourier transform of the LDOS throughout, as this allows physical properties to be more easily identified and is commonly used in experiments [3,8].

The starting point of our analysis is the continuum description of a CDW state. The latter arises in two rather different kinds of 1D correlated electron systems: (1) A partially filled band of spinful electrons coupled to optical phonons of frequency $\omega_{ph}$. At energies small compared to $\omega_{ph}$ the electron-phonon coupling results in an attractive interaction between electrons that can overcome the Coulomb repulsion [11] (2) Strongly correlated two- and three-leg ladder systems [4,12]. Here, in spite of strongly repulsive electron interactions, a Mott state with a finite spin gap occurs for a range of dopings around half filling [13]. In both cases there is a broad range of parameters such that at low energies the system gives rise to a CDW state characterized by a gapped spin sector and a gapless charge sector. Regardless of the microscopic origin of the spin gap, by taking the continuum limit and bosonizing one arrives at a spin-charge separated theory describing collective charge and spin degrees of freedom.

We now imagine a potential impurity to be present which at low energies and temperatures effectively cuts the system into two disconnected parts [14]. We then can model the impurity by a boundary condition on the continuum electron field $\Psi_{c}(x=0) = 0$, resulting in a spin-charge separated Hamiltonian of the form $H = H_c + H_s$:

$$H_c = \frac{v_c}{16\pi} \int_{-\infty}^{0} dx \left[ \frac{1}{K^2_c} (\partial_x \Phi_c)^2 + K^2_c (\partial_x \Theta_c)^2 \right],$$

$$H_s = \frac{v_s}{16\pi} \int_{-\infty}^{0} dx \left[ \frac{1}{K^2_s} (\partial_x \Phi_s)^2 + K^2_s (\partial_x \Theta_s)^2 \right] - \frac{g_s}{(2\pi)^2} \int_{-\infty}^{0} dx \cos \Phi_s.$$

Here $\Phi_{c,s}$ are canonical Bose fields which satisfy the boundary conditions $\Phi_{c,s}(x=0) = 0$, and $\Theta_{c,s}$ are their dual fields. The charge and spin velocities $v_{c,s}$, the Luttinger parameters $K_{c,s}$ and coupling constant $g_s$ are functions of the parameters defining the underlying microscopic model. In the case of single chain electron-phonon systems we have $v_s > v_c$ and $K_c > 1$ as we deal-
ing with attractive electron-electron interactions. On the other hand, in the case of two-leg ladders there is a spin gap with \( v_s < v_c \) and \( K_c < 1 \). We will consider both situations in what follows. The charge sector describes gapless collective charge excitations propagating with velocity \( v_c \), whereas the spin excitations are described by a sine-Gordon model with a boundary \( [12] \). In the regime considered here the bulk spectrum of the latter consists of gapped (anti)soliton excitations. At the Luther-Emery point \( K_s = 1/\sqrt{2} \) the spin sector is equivalent to a free massive Dirac fermion \([13] \). As is well known, \([1] - [6] \) reduces to the low-energy theory of a half-filled one-band Mott insulator, provided we interchange charge and spin sector and then set \( K_s = 1 \) and \( k_F = \pi/2 \). By virtue of this connection all our results for CDW states carry over to 1D Mott insulators.

The central object of our study is the time-ordered Green’s function in Euclidean space,

\[
G_{\sigma \sigma'}(\tau, x_1, x_2) = -\langle 0 | T_\tau \Psi_{\sigma}(\tau, x_1) \Psi_{\sigma'}^+(0, x_2) | 0 \rangle. \tag{3}
\]

Here \( | 0 \rangle \) is the ground state and \( \tau = i t \) denotes imaginary time. At low energies the electron annihilation operator can be decomposed into right- and left-moving components as \( \Psi_{\sigma}(x) = e^{i k_F x} R_\sigma(x) + e^{-i k_F x} L_\sigma(x) \), which reduces \([3] \) to

\[
G_{\sigma \sigma'} = e^{i k_F x_1-x_2} G_{LR}^{RR} + e^{-i k_F x_1-x_2} G_{LR}^{LL} + e^{i k_F x_1+x_2} G_{RL}^{RR} + e^{-i k_F x_1+x_2} G_{RL}^{LL}, \tag{4}
\]

where e.g. \( G_{LR}^{RR} = -\langle 0 | T_\tau R_{\sigma}(\tau, x_1) L_{\sigma'}^+(0, x_2) | 0 \rangle \). As we are interested in the LDOS, we ultimately want to set \( x_1 = x_2 \). As was noted in Ref. \([6] \) it is useful to consider the Fourier transform of the LDOS as physical properties can be more easily identified. In momentum space the \( RL \) and \( LR \) contributions occur in a different region \( Q \approx \pm 2 k_F \) compared to the \( RR \) and \( LL \) parts \( Q \approx 0 \).

In absence of a boundary we have \( G_{RL}^{RR} = G_{RL}^{LL} = 0 \) as the charge parts of these Green’s functions vanish. In presence of a boundary left and right sectors are coupled and the Fourier transform of the Green’s function \([4] \) concomitantly acquires a nonzero component at \( Q \approx \pm 2 k_F \), which gives a particularly clean way of investigating impurity effects. For this reason we focus on the \( 2 k_F \)-part of the Green’s function in what follows but note that the small momentum regime can be analyzed analogously.

The Green’s function \( G_{RL}^{RL} \) factorizes into a product of correlation functions in the spin and charge sectors. The charge part can be determined by a standard mode expansion \([16] \). The sine-Gordon model on the half-line \([12] \) is known to be integrable for quite general boundary conditions \([17] \). This enables us to calculate the correlation functions in the spin sector using the boundary state formalism introduced by Ghoshal and Zamolodchikov \([17] \) together with a form-factor expansion \([16] \). Taking into account only the leading terms we arrive at (\( \tau > 0 \)) \( g_{\tau}(\tau, x) \).

\[
g_{\tau}(\tau, x) = \frac{\delta_{\sigma\sigma'}}{2\pi} \frac{1}{(v_c \tau - 2i x)^a} \frac{1}{(v_c \tau + 2i x)^b} \left[ \frac{4 x^2}{v_c^2 \tau^2} \right]^c, \tag{5}
\]

where \( g_{\tau}(\tau, x) \) are the contributions of the charge and spin sectors respectively. Here \( K_0 \) is a modified Bessel function, the normalization constant \( Z_1 \) was obtained in Ref. \([18] \) and explicit expressions for the boundary reflection amplitude \( K(\theta) \) are given in Ref. \([17] \) (at the Luther-Emery point we have \([19] K(\theta) = \tan h \frac{\theta}{2} \)). The exponent in the charge sector is related to the Luttinger parameters by \( a = (K_c + 1/K_c)^2/8, b = (K_c - 1/K_c)^2/8 \), and \( c = (1/K_c^2 - K_c^2)/8 \). The subleading terms in \([13] \) involve three or more particles in the intermediate state or higher orders in the boundary \( K \)-matrix \([20] \). The Fourier transform of the LDOS for \( E > 0 \) is

\[
N_\sigma(E, Q) = -\int_0^\infty dx \int_{-\infty}^\infty \frac{dt}{2\pi} e^{i(Et-Qx)} G_{\sigma\sigma'}(t, x), \tag{7}
\]

where the Green’s function has been analytically continued to real time. For \( Q \approx 2 k_F \) only \( G_{RL}^{RL} \) contributes and using \([4] \) we arrive at our main result

\[
N_\sigma(E, 2 k_F + q) \propto -\Theta(E - \Delta) \sum_{i=1}^2 N_i(E, q), \tag{8}
\]

\[
N_i(E, q) = \int_A^{\infty} d\theta \left[ \frac{h_1(\theta) u_1^{2a+1} e^{2 i q \Delta \cos \theta} - u_2^{2 a-b} e^{2 i q \Delta \sin \theta} + i \sgn(v_c q/\Delta - 2 \sin \theta) \delta_{\sigma \sigma'}}{E - \Delta \cos \theta} \right] F_2(2c + 1, a, b, a + b + 2c; u_1^*, -u_2), \tag{8}
\]

Here \( | q | \ll 2 k_F, A = \arccosh(\frac{Q}{2 k_F}), F_1 \) denotes Appell’s hypergeometric function, \( h_1(\theta) = 1, h_2(\theta) = K(\theta + i \frac{\pi}{4}) e^{\theta/2} \), \( u_1 = 2(E - \Delta \cos \theta) / v_c q + i \sgn(v_c q/\Delta - \sin \theta) \), and \( u_2 = 2 v_c(E - \Delta \cos \theta) / v_c q - i \sgn(v_c q/\Delta - 2 \sin \theta) \), where \( \delta \rightarrow 0^+ \). Below we plot \([5] \) for two different parameter regimes. We smoothen the singularities in the LDOS by taking \( \delta \) small but finite. In experiments the singularities are broadened by instrumental resolution and temperature. The results presented below apply to the regime \( T < E, \Delta, v_c q/\Delta_0 \) (\( \Delta_0 \) is the lattice spacing), where temperature effects are negligible.

**Repulsive Case:** We first consider the case of repulsive electron interactions \( v_s < v_c, K_c < 1 \). In Fig. \([4] \) we plot \( N_\sigma(E, 2 k_F + q) \) for the case of unbroken spin rotational symmetry \( (K_s = 1) \). The LDOS is dominated by the strong peak at momentum \( 2 k_F \), which has its origin in \( N_1(E, Q) \) and is indicative of the CDW order being pinned at the boundary. This is analogous to the Luttinger liquid case \([6] \). At low energies above the spin gap \( \Delta \) we further observe two dispersing features associated with the collective spin and charge degrees.
energy peak appears at $E$ whereas the spin peak has its origin in low freedom respectively: (1) a “charge peak” that follows $E_c = v_c|q|/2 + \Delta$ and (2) a “spin peak” at position $E_s = \sqrt{\Delta^2 + (v_s q/2)^2}$. The charge peak arises from the contribution $N_1(E, Q)$ to the Fourier transform of the LDOS, whereas the spin peak has its origin in $N_2(E, Q)$, which encodes the effects of the boundary on the spin degree of freedom. We note that like in the Luttinger liquid case the phase of $N_\sigma$ exhibits characteristic jumps at the peak positions.

**Attractive Case:** In Fig. 2 we show $N_\sigma(E, 2k_F + q)$ for the case of attractive electron interactions ($v_s > v_c$, $K_s > 1$) and unbroken spin rotational symmetry. The peak at $2k_F$ is much less pronounced than in the repulsive case. We again observe charge and spin peaks that follow $E_c$ and $E_s$ respectively. For momenta $q$ above a critical value $q_0 = 2\Delta v_c/v_s \sqrt{v_s^2 - v_c^2}$ a third dispersing low-energy peak appears at $E = v_s|q|/2 + \Delta \sqrt{1 - (v_c/v_s)^2}$. This feature can be thought of as arising from a spin excitation with momentum $q_0$ and a charge excitation with momentum $q - q_0$. This is reminiscent of what is found for the single-particle spectral function in the bulk.

So far we have considered the simplest possible boundary conditions corresponding to a spin-independent phase shift $\pi$. In reality one may expect an impurity to give rise to a local potential or local magnetic field, which result in more general phase shifts upon reflection of particles at the boundary. In particular, these more general boundary conditions can give rise to boundary bound states, see e.g. [22]. In order to exhibit the signature of boundary bound states in LDOS measurements we now consider boundary conditions of the form $\Phi_{\sigma}(\tau, 0) = 0$, $\Phi_{\sigma}(\tau, 0) = \Phi_0^\sigma$ with $0 \leq \Phi_0^\sigma \leq \pi$. In terms of the right- and left-moving fields this corresponds to $R_{\sigma}(\tau, 0) = -e^{-i f_1 \Phi_0^\sigma/2} L_{\sigma}(\tau, 0)$, where $f_1 = 1 = -f_1$. We note that these boundary conditions break spin rotational symmetry. If we go over to the case of the 1D Mott insulator by exchanging spin and charge degrees of freedom the spin rotational symmetry remains intact and the boundary conditions correspond to a local potential.

A discussion of the general case with nontrivial boundary phase shifts in both spin and charge sectors is left for a longer publication.

The leading terms in the form-factor expansion for the chiral Green’s function $G^R_{\sigma \sigma'}$ are still given by [20], but now the boundary reflection amplitude depends on $\sigma$. For example, at the Luther-Emery point we have $K^\sigma(\theta) = \sin(\theta/2 - f_\sigma \Phi_0^\sigma/2)/\cos(\theta/2 + f_\sigma \Phi_0^\sigma/2)$. We note that nevertheless the Green’s function is still diagonal in spin indices $G^R_{\sigma \sigma'} \propto \delta_{\sigma \sigma'}$. If $\pi/2 \leq \Phi_0^\sigma$, $K^\sigma(\theta)$ has a pole in the physical strip $0 < \pi/2 < \pi/2$, which gives rise to an additional term linear in the boundary reflection matrix in the form-factor expansion. The resulting contribution to $N_\sigma(E, Q)$ has a non-dispersing singularity at the lower threshold $\Delta \sin \Phi_0^\sigma$, see Fig. 3. The emergence of a non-dispersing feature within the gap signals the presence of a boundary bound state. We note that the boundary bound state appears only in the down-spin channel $N_\downarrow(E, Q)$. On the other hand, if we were to consider $N_\uparrow(E < 0, Q)$, the additional feature would appear in the up-spin channel only.

Finally we wish to discuss the implications of our results for STM experiments on quasi-1D materials. Our results apply for energies above the 1D-3D cross-over scale, which is set by the strength of the 3D couplings. Perhaps the most interesting materials to which our findings may be applied are two-leg ladders like Sr$_{14}$Cu$_{24}$O$_{41}$. The model we have studied captures the essential features of the low-energy description of (weakly doped) two-leg ladders, namely a gapless charge sector and a gapped spin sector. The tunneling current measured in STM experiments is directly related to the local density of states $N_\sigma(E, Q)$. From the $2k_F$ component of the current one can hence extract informa-
tions about the CDW correlations in the presence of an impurity. In particular, we expect the various peaks in $N_s(E, Q)$ corresponding to the pinned CDW order and the dispersing spin and charge degrees of freedom to appear in the Fourier transform of the local differential conductance. A possible asymmetry $N_{↓}(E, Q) - N_{↑}(E, Q)$ may be detected using a magnetic STM tip [4].

In summary, we have determined the low energy LDOS in strongly correlated gapped 1D systems such as Mott insulators and CDW states in the presence of a strong impurity potential. We have shown that the spatial Fourier transform of the LDOS can be used to infer characteristic properties of the bulk state of matter. The LDOS is dominated by a singularity at $2k_F$, which is indicative of the pinning of the CDW order at the position of the impurity. The LDOS further exhibits clear signatures of propagating collective spin and charge modes, which reflect the nature of the underlying electron-electron interactions. We have investigated the modification of the LDOS in the presence of impurity bound states and discussed the relevance of our results to STM measurements on two-leg ladder materials like Sr$_2$CuO$_2$Cl$_2$.

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![FIG. 3: |$N_{↑}(E, 2k_F + q)$| (full line) and |$N_{↓}(E, 2k_F + q)$| (dashed line) for $v_s q/\Delta = 6$, $K_c = 1$, $K_r = 1/\sqrt{2}$, $v_s = 2v_c$, and $4\phi^s_0 = 0.9\pi$. The singularity of $N_{↓}(E, 2k_F + q)$ at $E = \Delta \sin \phi^s_0$ is due to the boundary bound state. The broad maximum of $N_{↓}$ at $E \approx 1.8$ is due to the excitation of the boundary bound state and additional charge excitations.](image)

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