Local density of states of 1D charge density wave states in the presence of an impurity

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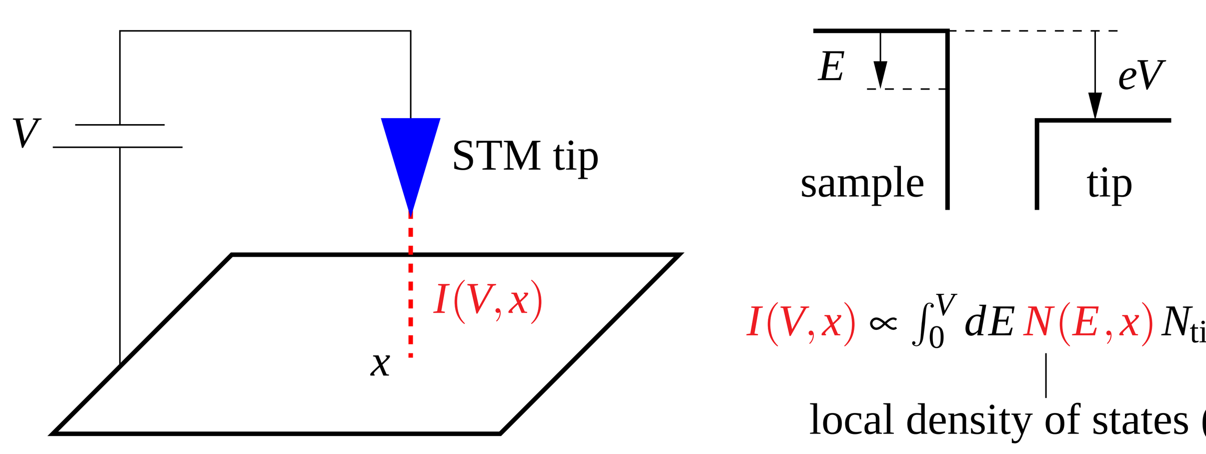
Motivation

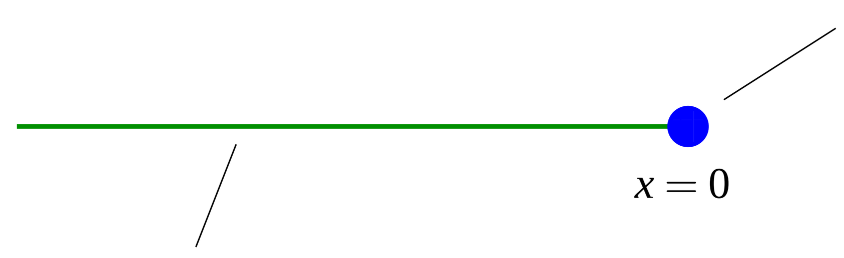
In recent years scanning tunneling microscopy (STM) techniques have proved to be very useful tools for studying strongly correlated electron systems such as high-temperature superconductors (HTSC), carbon nanotubes, and rare-earth compounds. STM measures the local density of states:



$I(V,x) \propto \int_0^V dE\, N(E,x)\, N_{\rm tip}(E-eV)$

local density of states (LDOS)

In one-dimensional systems an impurity effectively acts as a boundary. In particular, the low-energy properties of strongly correlated systems are typically described by boundary field theories. We consider STM in a one-dimensional strongly correlated system with a spin gap in the presence of a non-magnetic impurity:



impurity
equivalent to boundary
BC: $\Psi_\sigma(x=0)=0$

charge density wave (CDW) state
gapless charge excitations, gapped spin excitations
examples: 2-leg ladders ($SrCu_2O_3$), stripes in HTSC, carbon nanotubes
analog: Mott insulators (Bechgaard salts, NaV_2O_5)

Model

We consider the effective low-energy Hamiltonian

$$H = H_c + H_s,$$
$$H_c = \frac{v_c}{16\pi}\int_{-\infty}^{0} dx \left[\frac{1}{K_c^2}\left(\partial_x\Phi_c\right)^2 + K_c^2\left(\partial_x\Theta_c\right)^2\right],$$
$$H_s = \frac{v_s}{16\pi}\int_{-\infty}^{0} dx \left[\frac{1}{K_s^2}\left(\partial_x\Phi_s\right)^2 + K_s^2\left(\partial_x\Theta_s\right)^2\right] - \frac{g_s}{4\pi^2}\int_{-\infty}^{0} dx \cos\Phi_s,$$

where $\Phi_{c,s}$ are canonical Bose fields which satisfy the boundary conditions $\Phi_{c,s}(x=0)=0$, and $\Theta_{c,s}$ are their dual fields. The Mott insulator is given by replacing $H_c \leftrightarrow H_s$. The LDOS is obtained from the time-ordered Green's function

$$-\langle T_\tau \Psi_\sigma(\tau,x_1)\,\Psi^\dagger_{\sigma'}(0,x_2)\rangle = e^{ik_F r}G^{RR}_{\sigma\sigma'} + e^{-ik_F r}G^{LL}_{\sigma\sigma'} + e^{2ik_F R}G^{RL}_{\sigma\sigma'} + e^{-2ik_F R}G^{LR}_{\sigma\sigma'},$$

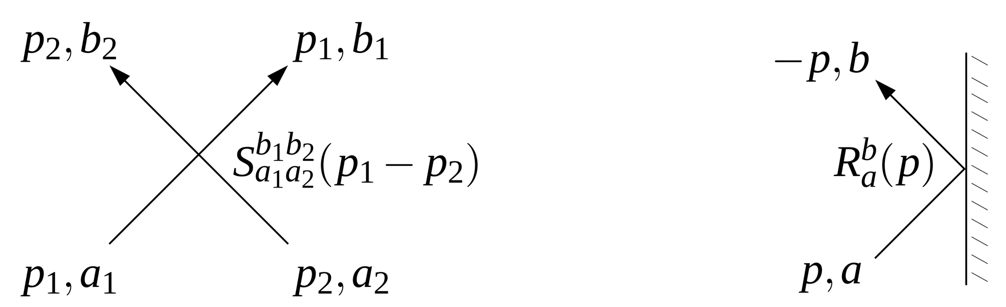
where $\tau = it$, $R=(x_1+x_2)/2$, $r = x_1 - x_2$. In the bulk one finds $G^{RL}_{\sigma\sigma'}=0$. In the presence of the boundary one has $G^{RL}_{\sigma\sigma'}\neq 0$, which results in a $2k_F$-component of the LDOS.

Technique

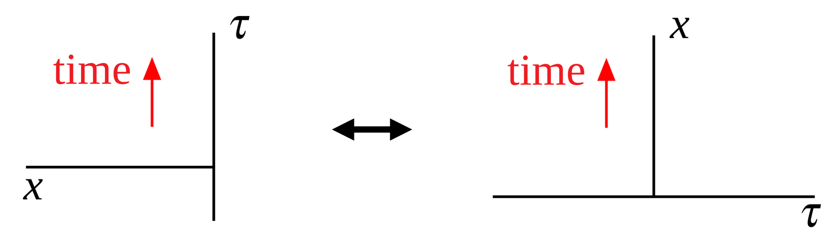
Bosonization yields

$$G^{RL}_{\sigma\sigma'} \propto \left\langle e^{-\frac{i}{2}\phi_c}\, e^{-\frac{i}{2}\bar{\phi}_c}\right\rangle_c \left\langle e^{-\frac{i}{2}f_\sigma\phi_s}\, e^{-\frac{i}{2}f_{\sigma'}\bar{\phi}_s}\right\rangle_s .$$

The correlations in the charge part can be calculated by standard mode expansion. The spin sector is a sine-Gordon model with a boundary, which is integrable. The Hilbert space is spanned by solitons and antisolitons which fulfill the scattering rules



As was shown by Ghoshal and Zamolodchikov [Int. J. Mod. Phys. **9**, 3841 (1994)] the correlation functions in the presence of the boundary can be calculated via a rotation in Euclidean space-time



$$\langle 0_B|\, T_\tau O_1(\tau,x_1)\, O_2(0,x_2)\,|0_B\rangle \quad = \quad \langle 0|\, T_x O_1(\tau,x_1)\, O_2(0,x_2)\,|B\rangle .$$

The boundary condition translates into an initial condition for the system on the infinite line; the boundary conditions are encoded in the boundary state $|B\rangle$. The correlation functions can now be calculated by a form-factor expansion using the known matrix elements $\langle 0|\,e^{\pm\frac{i}{2}\phi_s}\,|p_1,\ldots,p_n\rangle_{a_1,\ldots,a_n}$ in the bulk [S. Lukyanov and A. B. Zamolodchikov, Nucl. Phys. B **607**, 437 (2001)].

Results

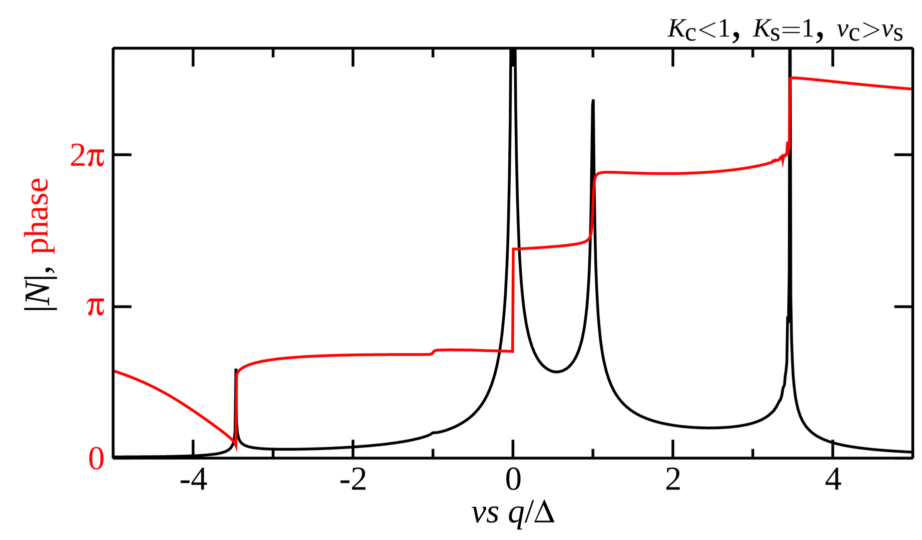
The form-factor expansion in the spin sector yields a series expansion for $N_\sigma(E,2k_F+q)$, the Fourier transform of the LDOS ($|q|\ll 2k_F$):

$$N_\sigma(E>0,2k_F+q) \propto \Theta(E-\Delta)\left[N_1^{RL}(E,q)+N_2^{RL}(E,q)+\ldots\right],$$

$$N_i^{RL}(E,q) = \int_{-\mathrm{Arcosh}\frac{E}{\Delta}}^{\mathrm{Arcosh}\frac{E}{\Delta}} \frac{d\theta\, h_i(\theta)\, u_i^{2c+1}}{(E-\Delta\cosh\theta)^{2-a-b}}\, F_1(2c+1,a,b,a+b+2c;u_i+i\delta,-u_i-i\delta),$$

where $h_1=1$, $h_2=R_+^+(-\theta)\,e^{\theta/2}$, $u_i=u_i(E,q,\theta)$, F_1 is Appell's hypergeometric function, and a,b,c are functions of K_c. We have determined the subleading terms N_i^{RL}, $i\geq 3$, and found them to be negligible. Below we plot $N_\sigma(E>0,2k_F+q)$.

Pinned CDW order



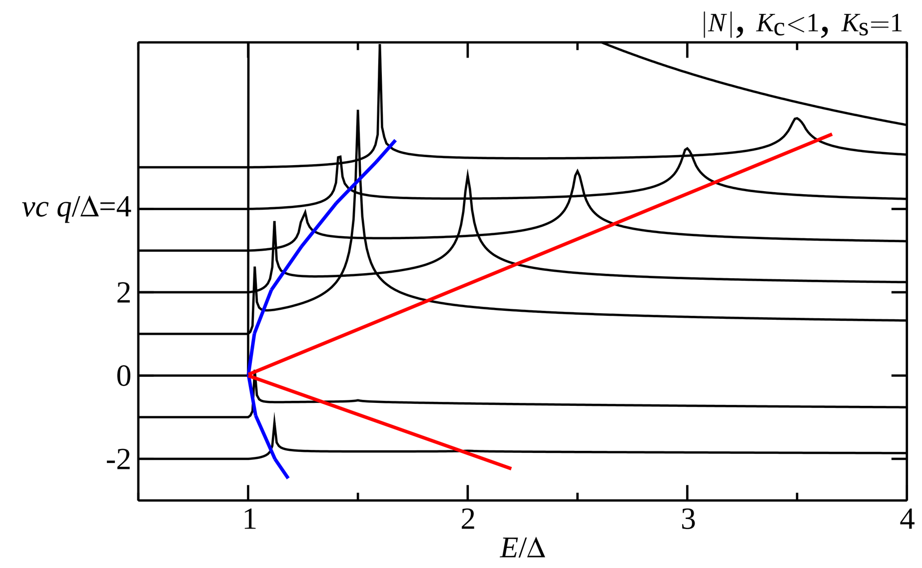
singularity for $q\to 0$:

$$N(2k_F+q)\sim\left(\frac{1}{v_c q}\right)^{1-\frac{K_c^2}{2}}$$

$\rightarrow$ density modulation with wave length $1/2k_F$

other peaks are due to propagating charge and spin excitations

Quasiparticle dispersions: $v_c > v_s$



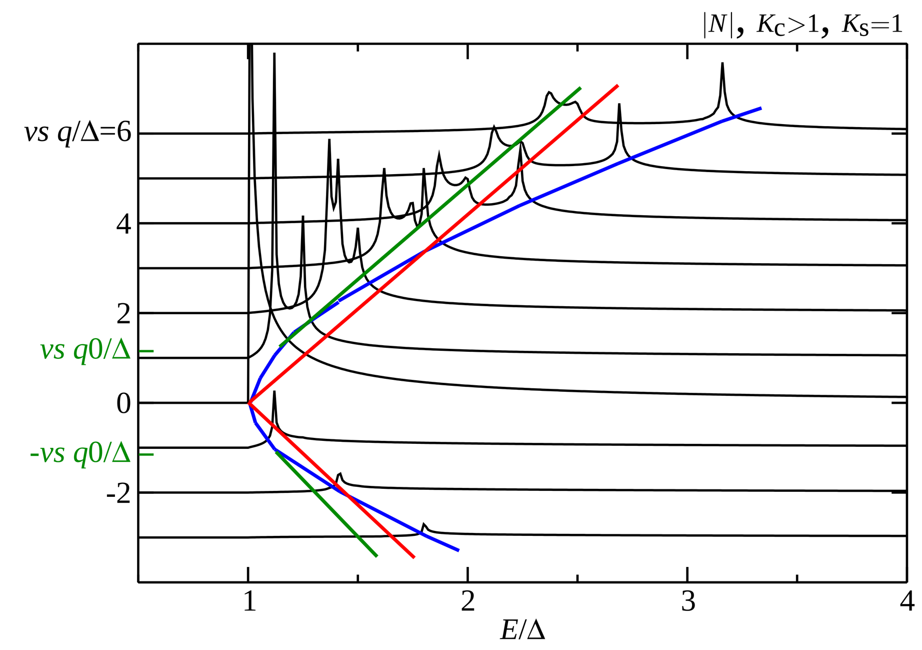
propagating charge excitations (holons):

$$E=\Delta+\frac{v_c}{2}|q|$$

propagating spin excitations (spinons):

$$E=\sqrt{\Delta^2+\left(\frac{v_s q}{2}\right)^2}$$

Quasiparticle dispersions: $v_c < v_s$

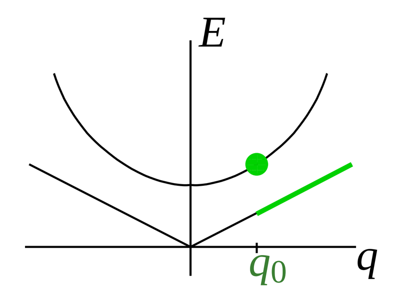


above critical momentum

$$q_0=\frac{2\Delta v_c}{v_s\sqrt{v_s^2-v_c^2}}$$

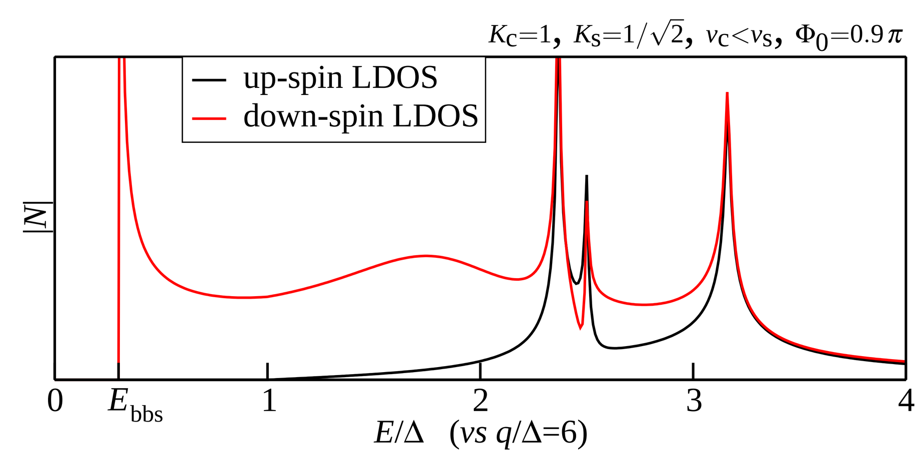
third dispersing peak

$$E=\Delta\sqrt{1-(v_c/v_s)^2}+\frac{v_c}{2}|q|$$



Boundary bound states

A static magnetic field at the impurity results in the boundary conditions $\Phi_c(0)=0$, $\Phi_s(0)=\Phi_0$. If $\Phi_0>\pi K_s^2$ there exists a stable boundary bound state with energy $E_{\rm bbs}<\Delta$. This results in a non-dispersing singularity within the spin gap.



The boundary bound state appears in the down-spin channel only.

$$N_\sigma\propto\delta_{\sigma\downarrow}(E-E_{\rm bbs})^{-\alpha},$$

$$\alpha=1-\frac{1}{2K_c^2}.$$

Conclusion

We have developed a method for determining 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. Our results are relevant to STM measurements on two-leg ladder materials like $Sr_{14}Cu_{24}O_{41}$.

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