Local Density of States in 1D Mott Insulators with a Boundary

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D. Schuricht and F.H.L. Essler, JSTAT P11004 (2007)

D. Schuricht, F.H.L. Essler, A. Jaefari and E. Fradkin, PRL 101, 086403 (2008).

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Outline

- Statement of the problem.
- Introduction and experimental motivation.
- 1D Mott insulators.
- Low-energy limit and bosonization.
- Correlators is presence of a boundary.
- Fermion autocorrelator.
- Boundary state form factor approach to correlation functions.
- Some results.
- Summary.

Statement of the Problem

Take the U(1) Thirring model on the half-line

$$\mathcal{H} = \int_{-\infty}^{0} dx \left[i v_F \sum_{a=1}^{2} \bar{\Psi}_a(t,x)\ \gamma_1 \partial_x \Psi_a(t,x) - \sum_{\alpha} g_\alpha J_\mu^\alpha(t,x)\ J^{\alpha\mu}(t,x) \right],\ g_x = g_y.$$

$$J_\mu^\alpha = \frac{1}{2} \bar{\Psi}_a(t,x)\ \gamma_\mu\ \sigma_{ab}^\alpha\ \Psi_b(t,x)\ , \quad \Psi_1 = \begin{pmatrix} R_\uparrow(t,x) \\ L_\uparrow(t,x) \end{pmatrix}\ ,\ \Psi_2 = \begin{pmatrix} R_\downarrow^\dagger(t,x) \\ L_\downarrow^\dagger(t,x) \end{pmatrix}\ .$$

Boundary Conditions: e.g.

$$R_\sigma(0) = -L_\sigma(0).$$

Calculate the retarded fermion autocorrelation function

$$\int_0^\infty dt e^{i\omega t} \int_{-\infty}^{0} dx e^{-iqx} \langle 0| \{ R(t,x), L^\dagger(0,x) \} |0\rangle$$

by combining form factor bootstrap and boundary state approaches.

Introduction

Reduced Dimensionality $\rightarrow$ large $\hbar$ $\Big\}$ Unusual Collective Many-Body
Strong Interactions $\qquad$ Physics at $T = 0$

- **Numerous experimental realizations and measurements.**
- **Integrable models allow calculation of measurable quantities:**

  (effects of integrability breaking perturbations smaller than experimental error)

  – Neutron scattering $\longrightarrow$ 2-point function of spin operators

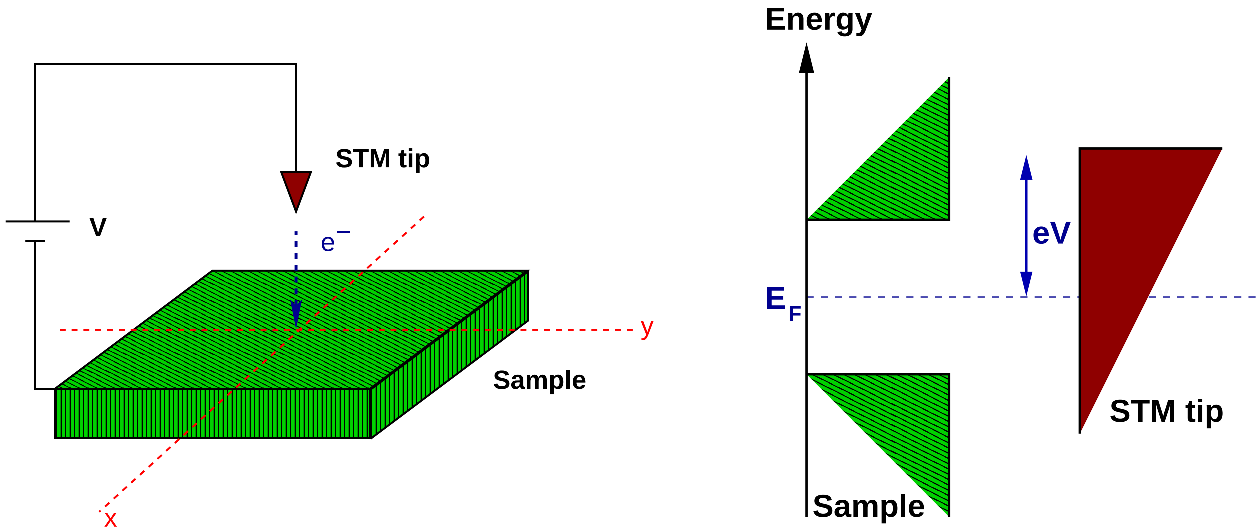
$$
\begin{aligned}
I(\omega, \boldsymbol{Q}) &\propto \sum_{\alpha,\gamma} \left[\delta_{\alpha\gamma} - \frac{Q_\alpha Q_\gamma}{\boldsymbol{Q}\cdot\boldsymbol{Q}} \right] S^{\alpha\gamma}(\omega, \boldsymbol{Q}) \ , \\
S^{\alpha\gamma}(\omega, \boldsymbol{Q}) &= \int_{-\infty}^{\infty} \frac{dt}{2\pi}\ e^{i\omega t}\ \frac{1}{N} \sum_{l,l'} e^{-i\boldsymbol{Q}\cdot(\boldsymbol{R}_l - \boldsymbol{R}_{l'})} \langle 0 | S_l^\alpha(t)\ S_{l'}^\gamma | 0 \rangle
\end{aligned}
$$

  – Photoemission $\longrightarrow$ 2-point function of electron operators

  – **Scanning Tunneling Spectroscopy ?**

Scanning Tunneling Spectroscopy (STS)

Precise measurement of local single-particle density of states (LDOS)



Current : $$I(V,\mathbf{x}) \propto \int_0^{eV} dE\ N_{\text{sample}}(E_F+E,\mathbf{x})\ N_{\text{tip}}(E_F+E-eV)$$

$$N_{\text{tip}} \approx \text{const} \Rightarrow \boxed{\frac{dI(V,\mathbf{x})}{dV} \propto N_{\text{sample}}(eV,\mathbf{x})}$$

LDOS related to **local** single-particle Green's function:

$$\begin{aligned} N_{\text{sample}}(E,\mathbf{x}) &= -\frac{1}{\pi}\text{Im}\int_0^\infty dt\ e^{iEt}\ G_{\text{ret}}(t,\mathbf{x})\ , \\ G_{\text{ret}}(t,\mathbf{x}) &= -i\theta(t)\langle 0|Tc(t,\mathbf{x})\ c^\dagger(0,\mathbf{x})|0\rangle. \end{aligned}$$

Translational invariance: no $\mathbf{x}$-dependence.

Idea of STS: impurities break translational invce $\longrightarrow$ $\mathbf{x}$-dependence emerges.

Measure $N_{\text{sample}}(E,\mathbf{x})$ for many $\mathbf{x}$, use it to extract **bulk** dynamical properties

" Use impurities as measurement device".

In practice: determine

$$N(E,\mathbf{k}) = \sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}} N(E,\mathbf{x}).$$

Can this technique see spin-charge separation 1D Mott insulators?

Field Theory of 1D Mott Insulators

"Standard Model" of Mott insulator: (extended) Hubbard model (Lieb/Wu '68)

$$H = -t \sum_{j,\sigma=\uparrow,\downarrow} c^\dagger_{j,\sigma} c_{j+1,\sigma} + h.c. + U \sum_j (n_{j,\uparrow} - \frac{1}{2})(n_{j,\downarrow} - \frac{1}{2})$$
$$+V \sum_j (n_j - 1)(n_{j+1} - 1), \quad n_j = n_{j,\uparrow} + n_{j,\downarrow}, \; n_{j,\sigma} = c^\dagger_{j,\sigma} c_{j,\sigma}.$$

- $U = V = 0$: metal. Gapless fermionic excitations.
- $U > V > 0$: "Mott insulator" (dynamical mass generation). Single-electron excitations have gap, but gapless spin excitation.

Low-energy continuum limit for $U, V \ll t$: linearize dispersion around $\pm k_F = \pm\frac{\pi}{2a_0}$

$$c_{j,\sigma} \rightarrow \sqrt{a_0}\left[R_\sigma(x) e^{ik_F x} + L_\sigma(x) e^{-ik_F x}\right] \ , \quad x = ja_0.$$

$H \longrightarrow$ 2 Dirac fermions with 4-fermion interactions

Bosonization

$$L^{\dagger}_{\sigma}(\tau,x) \;=\; \frac{\eta_\sigma}{\sqrt{2\pi}} e^{if_\sigma \pi/4} \exp\left(-\frac{i}{2}\bar{\varphi}_c(\tau,x)\right) \exp\left(-\frac{if_\sigma}{2}\bar{\varphi}_s(\tau,x)\right),$$

$$R^{\dagger}_{\sigma}(\tau,x) \;=\; \frac{\eta_\sigma}{\sqrt{2\pi}} e^{if_\sigma \pi/4} \exp\left(\frac{i}{2}\varphi_c(\tau,x)\right) \exp\left(\frac{if_\sigma}{2}\varphi_s(\tau,x)\right).$$

$\varphi_{c,s}$ chiral Bose fields, $f_\uparrow = 1 = -f_\downarrow$, η_a Klein factors.

$$\mathcal{H} \;=\; \int dx\, [\mathcal{H}_c(x) + \mathcal{H}_s(x)]\,,$$

$$\mathcal{H}_c \;=\; \frac{v_c}{16\pi}\left[(\partial_x \Phi_c)^2 + (\partial_x \Theta_c)^2\right] - \frac{g}{(2\pi)^2}\cos(\beta\Phi_c) + \text{irrelevant}\;,$$

$$\mathcal{H}_s \;=\; \frac{v_s}{16\pi}\left[(\partial_x \Phi_s)^2 + (\partial_x \Theta_s)^2\right] + \text{irrelevant}.$$

$$\Phi_s = \varphi_s + \bar{\varphi}_s,\ \Theta_s = \varphi_s - \bar{\varphi}_s, \qquad \beta\Phi_c = \varphi_c + \bar{\varphi}_c,\ \frac{1}{\beta}\Theta_c = \varphi_c - \bar{\varphi}_c$$

Free spin boson and sine-Gordon model in charge sector $\longrightarrow$ integrable.

Single Impurity

Place strong potential impurity at $x = 0 \longrightarrow$ cuts line into two.

Hard-wall boundary conditions: $\boxed{R_\sigma(0) = -L_\sigma(0)}$ (have also considered additional phase shift)

$$\begin{aligned} \mathcal{H} &= \int_{-\infty}^{0} dx \left[\mathcal{H}_c^B(x) + \mathcal{H}_s^B(x)\right], \\ \mathcal{H}_c^B &= \frac{v_c}{16\pi}\left[(\partial_x\Phi_c)^2 + (\partial_x\Theta_c)^2\right] - \frac{g}{(2\pi)^2}\cos(\beta\Phi_c) , \\ \mathcal{H}_s^B &= \frac{v_s}{16\pi}\left[(\partial_x\Phi_s)^2 + (\partial_x\Theta_s)^2\right]. \end{aligned}$$

Boundary Conditions: $\boxed{\Phi_{c,s}(0) = 0.}$ Compatible with spin-charge separation.

Ground state in presence of boundary

$$|0_B\rangle = |0_{B,c}\rangle \otimes |0_{B,s}\rangle.$$

Imaginary-time Fermion Autocorrelator

$$\begin{aligned}
G(\tau,x,x) &= -\langle 0_B|T_\tau c_{j,\sigma}(\tau)c^\dagger_{j,\sigma}|0_B\rangle \\
\longrightarrow \quad &- a_0\left[\langle 0_B|T_\tau R_\sigma(\tau,x)R^\dagger_\sigma(0,x)|0_B\rangle + \langle 0_B|T_\tau L_\sigma(\tau,x)L^\dagger_\sigma(0,x)|0_B\rangle\right] \\
&- a_0 e^{2ik_F x}\langle 0_B|T_\tau R_\sigma(\tau,x)L^\dagger_\sigma(0,x)|0_B\rangle \\
&- a_0 e^{-2ik_F x}\langle 0_B|T_\tau L_\sigma(\tau,x)R^\dagger_\sigma(0,x)|0_B\rangle
\end{aligned}$$

Fourier transform

$$G(\tau,q) = \int_{-\infty}^{0} dx\ e^{-iqx} G(\tau,x,x)$$

Dominant contribution at $q \approx 2k_F$

$$G(\tau,2k_F+k) \approx a_0 \int_{-\infty}^{0} dx\ e^{-ikx}\ \underbrace{\langle 0_B|T_\tau R_\sigma(\tau,x)L^\dagger_\sigma(0,x)|0_B\rangle}_{G_{RL}(\tau,x)}.$$

Focus on this from now on (other pieces work the same).

Bosonize:

$$G_{RL}(\tau,x) = \langle 0_{B,s}|T_\tau e^{-\frac{i}{2}\varphi_s(\tau,x)} e^{-\frac{i}{2}\bar{\varphi}_s(0,x)}|0_{B,s}\rangle \langle 0_{B,c}|T_\tau \mathcal{O}^1_{-\frac{\beta}{4}}(\tau,x)\mathcal{O}^{-1}_{-\frac{\beta}{4}}(0,x)|0_{B,c}\rangle$$

$$\mathcal{O}^n_{-\frac{\beta}{4}} = e^{-i\frac{\beta}{4}\Phi_c - \frac{in}{4\beta}\Theta} \ , \quad \text{spin: } \frac{n}{4} \ , \quad \text{topological charge: } n$$

Spin Sector

Free boson on the halfline. Calculate the correlator by mode expansion

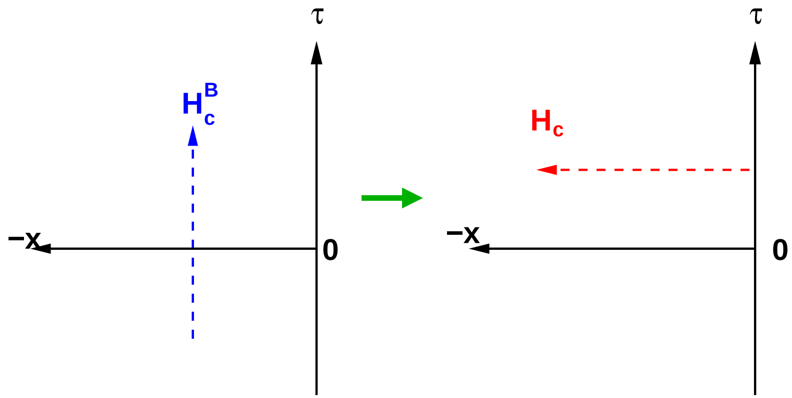
$$\langle 0_{B,s}|T_\tau e^{-\frac{i}{2}\varphi_s(\tau,x)} e^{-\frac{i}{2}\bar{\varphi}_s(0,x)}|0_{B,s}\rangle = \frac{1}{2\pi\sqrt{v_s\tau - 2ix}}.$$

Charge Sector: sine-Gordon on the halfline

Want to calculate

$$G_c(\tau, x) = \langle 0_{B,c}| T_\tau \mathcal{O}^1_{-\frac{\beta}{4}}(\tau, x) \mathcal{O}^{-1}_{-\frac{\beta}{4}}(0, x) |0_{B,c}\rangle \ , \qquad \mathcal{O}(\tau, x) = e^{\mathcal{H}_c^B \tau} \mathcal{O}(0, x) e^{-\mathcal{H}_c^B \tau}$$

Now change "transfer direction" Ghoshal/Zamolodchikov '94



$$G_c(\tau, x) = \frac{\langle 0| T_x \mathcal{O}^1_{-\frac{\beta}{4}}(\tau, x) \mathcal{O}^{-1}_{-\frac{\beta}{4}}(0, x) |B\rangle}{\langle 0|B\rangle} \ , \quad \mathcal{O}(\tau, x) = e^{-\mathcal{H}_c x} e^{-iP\tau} \mathcal{O}(0, 0) e^{iP\tau} e^{\mathcal{H}_c x}$$

$\longrightarrow$ particular matrix element in **bulk** SGM!

Boundary State

Ghoshal/Zamolodchikov '94: $|B\rangle$ can be constructed from bulk sine-Gordon scattering states.

$$|\theta_1, \ldots, \theta_n\rangle_{a_1,\ldots,a_n} = A^\dagger_{a_1}(\theta_1)\ldots A^\dagger_{a_n}(\theta_n)\,|0\rangle$$

Faddeev-Zamolodchikov algebra:

$$\begin{aligned}
A_{a_1}(\theta_1)A_{a_2}(\theta_2) &= S^{b_1b_2}_{a_1a_2}(\theta_1-\theta_2)A_{b_2}(\theta_2)A_{b_1}(\theta_1),\\
A^\dagger_{a_1}(\theta_1)A^\dagger_{a_2}(\theta_2) &= S^{b_1b_2}_{a_1a_2}(\theta_1-\theta_2)A^\dagger_{b_2}(\theta_2)A^\dagger_{b_1}(\theta_1),\\
A_{a_1}(\theta_1)A^\dagger_{a_2}(\theta_2) &= 2\pi\delta(\theta_1-\theta_2)\delta_{a_1a_2} + S^{b_2a_1}_{a_2b_1}(\theta_1-\theta_2)A^\dagger_{b_2}(\theta_2)A_{b_1}(\theta_1).
\end{aligned}$$

$$|\mathrm{B}\rangle = \exp\left(\frac{1}{2}\int_{-\infty}^{\infty}\frac{d\xi}{2\pi}K^{ab}(\xi)A^\dagger_a(-\xi)A^\dagger_b(\xi)\right)|0\rangle\,,$$

$K^{ab}(\xi)$ obtained from solution of **reflection equations** $K^{ab}(\xi) = R_{\bar{a}}^{b}(i\pi/2 - \xi)$

$R_{a_2}^{c_2}(\theta_2) S_{a_1 c_2}^{c_1 d_2}(\theta_1 + \theta_2) R_{c_1}^{d_1}(\theta_1) S_{d_2 d_1}^{b_2 b_1}(\theta_1 - \theta_2) = S_{a_1 a_2}^{c_1 c_2}(\theta_1 - \theta_2) R_{c_1}^{d_1}(\theta_1) S_{c_2 d_1}^{d_2 b_1}(\theta_1 + \theta_2) R_{d_2}^{b_2}(\theta_2)$

"Boundary cross-unitarity"

$$K^{ab}(\xi) = S_{cd}^{ab}(2\xi) K^{dc}(-\xi).$$

Boundary unitarity

$$R_a^c(\theta) R_c^b(-\theta) = \delta_a^b.$$

Form of $K^{ab}(\xi)$ generally quite complicated; for $\beta = 1/\sqrt{2}$ and $\Phi_c(\tau, 0) = \Phi_0$

$$R_-^+(\theta) = R_+^-(\theta) = -\frac{\cosh\left(i\frac{\pi}{4} \pm i\frac{\Phi_0}{2} + \frac{\theta}{2}\right)}{\cosh\left(i\frac{\pi}{4} \pm i\frac{\Phi_0}{2} - \frac{\theta}{2}\right)}, \quad R_\pm^\mp(\theta) = 0.$$

Ameduri/Konik/LeClair '95

For all cases we study: $K^{aa}(\xi) = 0$, $K^{+-}(\xi) = K^{-+}(\xi) \equiv K(\xi)$

Spectral Representation

$$\langle 0|\mathcal{O}^1_{-\frac{\beta}{4}}(\tau,x)\mathcal{O}^{-1}_{-\frac{\beta}{4}}(0,x)|B\rangle = \sum_{n=0}^{\infty}\sum_{a_j}\int \frac{d\theta_1\dots d\theta_n}{(2\pi)^n n!}\langle 0|\mathcal{O}^1_{-\frac{\beta}{4}}(\tau,x)|\theta_1,\dots,\theta_n\rangle_{a_1\dots a_n}$$
$$\times\ {}_{a_n\dots a_1}\langle\theta_n,\dots,\theta_1|\mathcal{O}^{-1}_{-\frac{\beta}{4}}(0,x)|B\rangle$$

Idea:

- Expand boundary state
  $|B\rangle = |0\rangle + \frac{1}{2}\int \frac{d\xi}{2\pi} K^{ab}(\xi) A^\dagger_a(-\xi)A^\dagger_b(\xi)|0\rangle + \dots$
- Evaluate terms in spectral rep with lowest numbers of particles using **Form Factor Bootstrap Approach**
- Observe that terms quadratic/cubic in K^{ab} and/or large n are (very) small except at $x \approx 0$. To get $x \ll \xi = v_c\Delta$ must sum full series.
- But $x \approx$ has small contribution to Fourier transform in x.
- Rapidly "converging" expansion for Fourier transform.

Form Factor Bootstrap Approach

Karowski/Weisz '78, **Smirnov** '93, Lukyanov '95, Delfino/Mussardo '95...

Basis of scattering states:

$$|\theta_1, \ldots, \theta_n\rangle_{a_1 \ldots a_n} \;, \qquad E_n = \sum_{k=1}^{n} \Delta \cosh \theta_n \;, \; P_n = \sum_{k=1}^{n} \frac{\Delta}{v} \sinh \theta_n .$$

Matrix Elements ("Form Factors"):

$$\langle 0|\mathcal{O}(0,0)|\theta_1, \ldots, \theta_n\rangle_{a_1 \ldots a_n}$$

Idea: analytic properties of S-matrix $\longrightarrow$ analytic properties of form factors $\longrightarrow$ form factors.

Form Factor Axioms

$\langle 0|\mathcal{O}(0,0)|\theta_n,\ldots,\theta_1\rangle_{a_n\ldots a_1}$ are **meromorphic** in the strip $0\leq \mathrm{Im}(\theta_n)<2\pi$ and fulfil

1. **Scattering Axiom**

$$\begin{aligned}\langle 0|\mathcal{O}(0,0)|\theta_n,\cdots,\theta_i,\theta_{i+1},\cdots,\theta_1\rangle_{a_n,\cdots,a_i,a_{i+1},\cdots,a_1} \quad &= \\ S_{a_i a_{i+1}}^{a'_i,a'_{i+1}}(\theta_i-\theta_{i+1})\langle 0|\mathcal{O}(0,0)|\theta_n,\cdots,\theta_{i+1},\theta_i,\cdots,\theta_1\rangle_{a_n,\cdots,a'_i,a'_{i+1},\cdots,a_1}\ .\end{aligned}$$

2. **Periodicity Axiom:**
$\langle 0|\mathcal{O}(0,0)|\theta_n,\ldots,\theta_1\rangle_{a_n\ldots a_1} = l_{\mathcal{O}\Psi_{a_n}}\langle 0|\mathcal{O}(0,0)|\theta_{n-1},\ldots,\theta_1,\theta_n-2\pi i\rangle_{a_{n-1}\ldots a_1 a_n}$

3. **Annihilation Pole Axiom** pole at $\theta_n=\theta_{n-1}+\pi i$ with residue

$$i\ \mathrm{res}\langle 0|\mathcal{O}(0,0)|\theta_n,\ldots,\theta_1\rangle_{a_n\ldots a_1} \quad = \quad \langle 0|\mathcal{O}(0,0)|\theta_{n-2},\ldots,\theta_1\rangle_{a'_{n-2}\cdots a'_1}\delta_{a_n a'_{n-1}}$$

$$\times\left[\delta_{a_1}^{a'_1}\cdots\delta_{a_{n-1}}^{a'_{n-1}} - l_{\mathcal{O}\Psi_{a_n}} S_{\tau_1 a_1}^{a'_{n-1}a'_1}(\theta_n-\theta_1)S_{\tau_2 a_2}^{\tau_1 a'_2}(\theta_n-\theta_2)\cdots S_{a_{n-1}a_{n-2}}^{\tau_{n-3}a'_{n-2}}(\theta_{n-1}-\theta_{n-2})\right].$$

4. **Lorentz Covariance:**
$\langle 0|\mathcal{O}(0,0)|\theta_n+\alpha,\ldots,\theta_1+\alpha\rangle_{a_n\ldots a_1} = e^{s\alpha}\langle 0|\mathcal{O}(0,0)|\theta_n,\ldots,\theta_1\rangle_{a_n\ldots a_1}$

We need more general matrix elements

$$ {}_{a_n \ldots a_1}\langle \theta_n, \ldots, \theta_1 | \mathcal{O} | \theta'_1, \ldots, \theta'_m \rangle_{b_1 \ldots b_m} $$

Use crossing: if $\theta_j \neq \theta'_k \ \forall j, k$

$$ {}_{a_n \ldots a_1}\langle \theta_n, \ldots, \theta_1 | \mathcal{O} | \theta'_1, \ldots, \theta'_m \rangle_{b_1 \ldots b_m} \langle 0 | \mathcal{O} | \theta'_1, \ldots, \theta'_m, \theta_n - i\pi, \ldots, \theta_1 - i\pi \rangle_{b_1 \ldots b_m, \bar{a}_n \ldots \bar{a}_1} $$

In general: extra "disconnected" pieces $\propto \delta(\theta_j - \theta'_k)$

Can be worked out following Smirnov

$$ \begin{aligned} \langle A | \, O \, | B \rangle &= \sum_{\substack{A = A_1 \cup A_2 \\ B = B_1 \cup B_2}} S_{AA_1} S_{B_1 B} \langle A_2 | \, B_2 \rangle \langle A_1 + \mathrm{i}0 | \, O \, | B_1 \rangle \\ | A \rangle &= S_{AA_1} | A_2 A_1 \rangle = S_{AA_2} | A_1 A_2 \rangle \end{aligned} $$

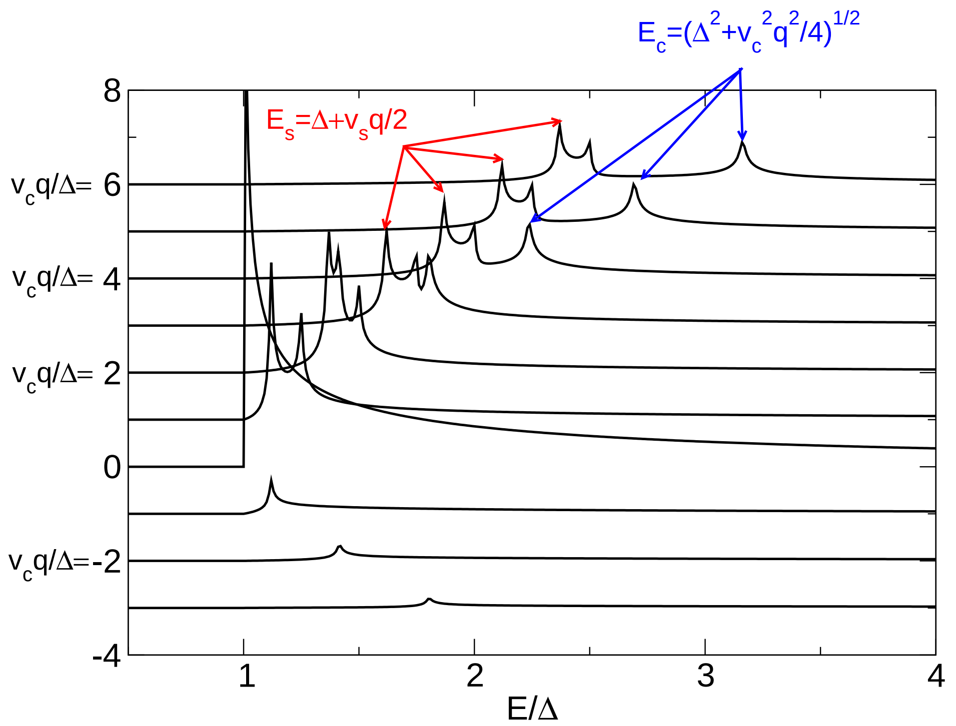
Results

$$G_c(\tau,x) = \frac{\langle 0|\mathcal{O}^1_{-\frac{\beta}{4}}(\tau,x)\mathcal{O}^{-1}_{-\frac{\beta}{4}}(0,x)|B\rangle}{\langle 0|B\rangle}$$
$$\approx Z\left[K_0(\Delta\tau) + \int_{-\infty}^{\infty}\frac{d\theta}{2}\,K(\theta+i\tfrac{\pi}{2})\,e^{\theta/2}\,e^{2i\frac{\Delta}{v_c}x\sinh\theta}\,e^{-\Delta\tau\cosh\theta}+\dots\right],$$

- Multiply by contribution of spin sector.
- Analytically continue to real times.
- Fourier transform to get quantity

$$N(E>0,2k_F+q) = \sum_{j=-\infty}^{0} e^{-i(2k_F+q)ja_0}\int dt e^{iEt}A(t,j)\ ,$$
$$A(t,j) = -\frac{1}{\pi}\mathrm{Im}\left[-i\theta(t)\langle 0_B|\{c_{j,\sigma}(t),c^\dagger_{j,\sigma}\}|0_B\rangle\right]$$

$N(E, 2k_F + q)$:



Direct evidence for spin-charge separation!

Third Peak: occurs for $q > q_0 = \frac{2\Delta v_s}{v_c\sqrt{v_c^2 - v_s^2}}$

$$E_c(q_0) + E_s(q - q_0) = \Delta\sqrt{1 - \frac{v_s^2}{v_c^2}} + \frac{v_s q}{2}$$

Further Results

- Small momenta $k \approx 0$.
- More general boundary conditions (phase shift)
  $\longrightarrow$ boundary bound state.
- Attractive electron-electron interactions (CDW state) $\longrightarrow$ spin gap.

Conclusions

- Developed method for calculating 2-point functions in massive integrable models with a boundary.
- Applied it to calculate LDOS in a 1D Mott insulator with a boundary/impurity.
- Boundary effects reveal information about **bulk** state of matter.
- Boundaries that mix spin and charge?
- More complicated models: SO(6) Gross-Neveu for doped 2-leg ladders.