Bounded Luttinger liquids as a universality class of quantum critical behavior

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(August 6, 2018)

Abstract

We show that one-dimensional quantum systems with gapless degrees of freedom and open boundary conditions form a new universality class of quantum critical behavior, which we propose to call “bounded Luttinger liquids”. They share the following properties with ordinary (periodic) Luttinger liquids: absence of fermionic quasi-particle excitations, charge-spin separation, anomalous power-law correlations with exponents whose scaling relations are parametrized by a single coupling constant per degree of freedom, $K_\nu$. The values of $K_\nu$ are independent of boundary conditions, but the representation of the critical exponents in terms of these $K_\nu$ depends on boundary conditions. We illustrate these scaling relations by exploring general rules for boundary critical exponents derived earlier using the Bethe Ansatz solution of the 1D Hubbard model together with boundary conformal field theory, and the theory of Luttinger liquids in finite-size systems. We apply this theory to the photoemission properties of the organic conductors (TMTSF)$_2$X, and discuss to what extent the assumption of finite strands with open boundaries at the sample surface can reconcile the experimental results with independent

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information on the Luttinger liquid state in these materials.

PACS numbers: 05.70.Jk, 68.35.Rh, 71.10.Pm, 79.60.-i
I. MOTIVATION

Phase transitions take place in a different way on surfaces and in the bulk of a sample. Order parameters, critical temperatures, critical exponents, and their scaling relations may be different, i.e. entirely new universality classes may be realized. Moreover, one may observe new phenomena due to anisotropy and the breaking of translational invariance caused by the boundary, like oscillations in correlation functions which, in the bulk, are monotonous, coordinate dependences, and in particular Friedel oscillations, in local quantities, etc.

Here, we discuss such boundary critical phenomena in one-dimensional (1D) strongly correlated electron systems which possess, in the bulk, a quantum critical point at zero temperature. Conformal invariance, a consequence of the combined Lorentz and scale invariance at a critical point, allows an exact determination of all critical exponents in 1+1D. The conformal field theory is parametrized by a unique constant – the conformal anomaly or the central charge $c$ of the corresponding Virasoro algebra. Strongly correlated electron systems of the kind we are interested in here, have $c = 1$, and their critical exponents continuously depend on the coupling of the fields. They can be calculated exactly from the low-energy excitations of the underlying Hamiltonians. The excitation spectra, in turn, can be obtained by a variety of methods, notably Bethe Ansatz for integrable models, and exact numerical diagonalization on small lattices quite generally.

Conformally invariant, 1D strongly correlated electron systems are metals, and are also described as Luttinger liquids. In that perspective, the main focus is on their non-Fermi liquid properties which are embodied in their critical exponents (anomalous dimensions) and different velocities for excitations in different conformally invariant sectors (for two sectors only, charge and spin, this leads to charge-spin separation). In Luttinger liquid theory, the scaling relations between the different critical exponents are parametrized by a single renormalized coupling constant per degree of freedom $K_\nu$ (here $\nu = \rho$, charge, and $\nu = \sigma$, spin), playing the role of the Landau parameters familiar from Fermi liquid theory. The “Luttinger liquid universality class” then corresponds to unique dependences of all critical exponents on the $K_\nu$. The connection between both methods is well established in bulk systems.

Recently, both approaches have been extended to boundary critical phenomena in 1D fermion systems with open boundary conditions. Boundary conformal field theory has been used to derive the boundary critical exponents of integrable 1D electron systems in terms of the dressed charge matrices of these models. (Following the early work of Gaudin, Bethe Ansatz solutions have been produced, and integrability proven, for certain 1D electron models with boundaries.) Also Luttinger liquid theory has been formulated for systems with open boundaries. While Wang et al. gave the rules for evaluating critical exponents, explicit expressions for the exponents of specific correlation functions, relevant values for specific models such as the 1D Hubbard model, and their relation to those derived within Luttinger liquid theory, are still missing. An exception are Friedel oscillations in the 1D Hubbard model which have been studied by Bedürftig et al. Here, and for spinless fermions, accurate DMRG calculations are in impressive agreement with predictions from conformal field theory. Related problems have also been studied in the context of quantum spin chains.

Here, we provide explicit expressions for the critical exponents of a variety of correlation...
functions, and explicitly connect the predictions of conformal field theory in terms of the dressed charge matrices of integrable models to standard Luttinger liquid notation. We discuss the consequences of such mappings for nonintegrable systems and for experiments. We discuss the consequences of broken translational invariance in open systems. To be specific, we discuss the 1D Hubbard model throughout this paper, except when stated otherwise. The results can be carried over to other integrable models without difficulty.

Quite generally, we are interested in how quantum critical 1D strongly correlated electron systems fit into the general framework of surface critical phenomena, and of different universality classes in the bulk and at surfaces. We find that the boundary critical exponents of gapless (conformally invariant) 1D electron systems define a new universality class which we propose to call bounded Luttinger liquids, and which affect almost all physical quantities.

We are motivated by several recent developments, both theoretical and experimental. Recent theoretical work on boundary effects in photoemission emphasizes the need for exact information on the spectral function of 1D Hubbard models with open boundaries. Approximate results would indicate an enhancement of spectral weight in a large energy range around the chemical potential $\mu$. On the other hand, unexplained photoemission experiments on the quasi-1D Bechgaard salts $22$, $23$ have been tentatively associated with the possible influence of boundary effects $16$, $24$. Finally, boundary critical exponents are relevant in mesoscopic quantum wires and quantum Hall edge states and carbon nanotubes $25$, $26$, and the Luttinger liquid language has been preferred in all these articles.

As we shall see, integrable models can be used to illustrate relations between bulk and boundary critical exponents which are valid beyond the realm of integrability, in nonintegrable Hamiltonians and even in experimental Luttinger liquids, provided they exist. Remarkably, they allow to propose boundary effects as a possible resolution of the qualitative discrepancy of the photoemission spectra of the 1D Bechgaard salts, and the information provided by almost all other experiments on these materials.

The reminder of this paper is organized as follows. In Section II we discuss the determination of critical exponents of 1D correlated electron systems with periodic and open boundary conditions. We show which quantities determining the critical exponents are independent of boundary conditions, and which do depend on them. We do this for the 1D Hubbard model where we discuss the results from the Bethe Ansatz solution and use boundary conformal field theory, and for Luttinger liquids. For Luttinger liquids, we rewrite all critical exponents in a form similar to conformal field theory, i.e. in terms of the coupling constants $K_\nu$, and the quantum numbers which an operator inserts into a system. The rules derived here are used in Section III to give explicit expressions for a variety of correlation functions of bounded Luttinger liquids, and to illustrate the new scaling relations found here. Section IV discusses the application of boundary critical phenomena to problems posed by photoemission experiments on a class on 1D organic conductors, and Section V summarizes the open questions remaining.

II. MODELS

While our results are valid generally for interacting 1D electron systems, we shall concentrate our discussion on the 1D Hubbard model as a prototypical example of an integrable (or
Bethe ansatz solvable, used synonymously) system, and on the 1D Luttinger model. Here, we briefly describe how their critical properties are calculated, and how the solutions with periodic and open boundary conditions are related.

A. The 1D Hubbard model

The 1D Hubbard model is defined by the Hamiltonian

\[ H = - \sum_{i=1}^{N-1} \sum_{\sigma = \pm} (C_{i\sigma}^\dagger C_{i+1\sigma} + H.c.) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i=1}^{N} \sum_{\sigma = \pm} n_{i\sigma} - \frac{\hbar}{2} \sum_{i=1}^{N} (n_{i\uparrow} - n_{i\downarrow}), \]

(2.1)

where \( C_{i\sigma} \) (\( C_{i\sigma}^\dagger \)) is the electron annihilation (creation) operator; \( \mu \) denotes the chemical potential and \( \hbar \) is the external magnetic field. We shall consider \( \hbar = 0 \) in much of, and non-half-filled bands throughout this paper. Eq. (2.1) represents the Hamiltonian on \( N \) sites with open boundary conditions (OBC). For periodic boundary conditions (PBC), extend the first sum to \( N \) and identify \( C_{N+1} = C_1 \).

This model is solved by Bethe Ansatz\(^2\) for periodic and by reflection Bethe Ansatz for open boundary conditions\(^1\), and the energies of the ground and excited states are given as the solution of certain integral equations. Here we do not repeat these equations from the literature but emphasize the main physical results on passing from periodic to open boundary conditions. The basic idea of the reflection Bethe Ansatz is to superpose, in order to obtain the solution for open boundaries, the Bethe solution of the periodic system with its reflection at the origin\(^1\). In a similar way, one can pass from a particle on a ring to a particle in a box in elementary quantum mechanics, from a Luttinger liquid with periodic boundary conditions to one with open boundaries\(^1\), and from conformal to boundary conformal field theory\(^9\). A many-particle eigenstate with \( N_c = N_\uparrow + N_\downarrow \) electrons out of which \( N_s = N_\downarrow \) have spin projection \(-1/2\), is parametrized by the set of rapidities \((k, \Lambda)\) for charge and down-spin, basically a generalization of the wavenumbers of free electron states to include the correct scattering phase shifts) of the occupied states\(^3\). While for PBC, rapidites \(+k\) and \(-k\) give linearly independent solutions, for open boundaries only one sign (say \(+\) for these rapidites is allowed (as in elementary quantum mechanics), but the spacing of solutions is half as big and their density twice as big as for PBC. The equations determining the energies are formally different for open and periodic boundary conditions. However, they can be transformed into each other (cf. below for the entries of the dressed charge matrix), and consequently, their solutions are equal. The energies thus are independent of the boundary conditions, as are the velocities of the low-lying collective charge and spin modes (holons and spinons).

The critical properties are determined by the low-energy excitations, more specifically by the quantum numbers associated with the operators whose correlations at criticality we wish to determine, and a “dressed charge matrix” \( Z^{(p,b)} \). This \( 2 \times 2 \)-matrix contains the effective renormalized coupling constants within and between the low-energy (charge and spin) sectors of the Hilbert space of the Hubbard model, and therefore directly determines the non-universal critical exponents. It is defined as

\[ Z^{(p,b)} = \begin{pmatrix} Z_{cc} & Z_{cs} \\ Z_{sc} & Z_{ss} \end{pmatrix}, \]

(2.2)
The superscripts $p, b$ label periodic and bounded systems. In the absence of a magnetic field, $Z^{(p,b)}$ is completely determined by its first element $Z^{(p,b)}_{cc}$ as

$$Z^{(p,b)} = \begin{pmatrix} \xi^{(p,b)}(k_0) & 0 \\ \frac{\xi^{(p,b)}(k_0)}{2} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

(2.3)

where $k_0$ is a cutoff determined by the particle density, again identical for periodic and open boundary conditions.

$\xi^{(p,b)}(k_0)$, for a periodic system, obeys the integral equation

$$\xi^{(p)}(k) = 1 + \frac{1}{2\pi} \int_{-k_0}^{k_0} dk' \cos(k') K^{(p)}(\sin k - \sin k') \xi^{(p)}(k')$$

(2.4)

with the kernel

$$K^{(p)}(z) = \int_{0}^{\infty} d\omega \frac{\exp(-\omega U/4)}{\cosh(\omega U/4)} \cos(\omega z) .$$

(2.5)

For open boundary conditions, on the other hand, the integral equation for $\xi^{(b)}(k_0)$ reads

$$\xi^{(b)}(k) = 1 + \frac{1}{2\pi} \int_{0}^{k_0} dk' \cos(k') K^{(b)}(\sin k, \sin k') \xi^{(b)}(k')$$

(2.6)

with the kernel

$$K^{(b)}(z, z') = K^{(p)}(z - z') + K^{(p)}(z + z') .$$

(2.7)

Using $K^{(b)}(-z, z') = K^{(b)}(z, z')$, a consequence of $K^{(p)}(-z) = K^{(p)}(z)$, Eq. (2.3), we find that $\xi^{(b)}(k)$ can be continued to negative $k$ with $\xi^{(b)}(-k) = \xi^{(b)}(k)$. We can then change variables $k \to -k$ in the contribution of the second term of $K^{(b)}$ to the integral in (2.6), and find

$$\xi^{(b)}(k) = \xi^{(p)}(k)$$

and thus $Z^{(b)} = Z^{(p)}$.

Despite the differences between Eqs. (2.4), (2.5), and (2.6), (2.7), the dressed charge matrices are identical for open and periodic boundary conditions. This translates the fact that they are a property of the Hamiltonian only and independent of boundary conditions. The boundary effects are contained completely in the representation of the boundary critical exponents in terms of the entries of the dressed charge matrices. This representation depends on the boundary conditions.

With a magnetic field, one has a set of four coupled equations for the four entries of $Z^{(p,b)}$, containing different kernels. However, all symmetries used, and all transformations carried out above continue to be applicable. Consequently, the dressed charge matrices of open and periodic systems are identical also in a finite magnetic field.

The rapidities $k, \Lambda$, describing a general quantum state of the 1D Hubbard model depend on two sets of quantum numbers $I_{c,j}$ and $I_{s,j}$ of integers or half-odd integers, parametrizing the solutions (the “occupied states”). There are certain parity rules for the $I_{c,j}, I_{s,j}$, depending on $N_c, N_s$ being even or odd. In the ground state, their distributions are filled up
to a cutoff, a pseudo-Fermi number. Acting with an operator $O$ on a state of the system will change the distribution of rapidities. Both for the charge and spin channels, in the periodic systems, there are three types of excitations: particle addition (often also termed “charge” excitations\cite{foot}), current excitations, and particle-hole excitations. The single-particle operator $C^+_n$, e.g., adds a particle, i.e. $\Delta N_c = 1$, and, depending on spin, $\Delta N_s = 0$ for $s = \uparrow$, or $\Delta N_s = 1$ for $s = \downarrow$. Changing $N_{c,s}$ by unity changes the $I_{c,j}$ and/or $I_{s,j}$ between integers and half-odd integers. This backflow is accounted for by current quantum numbers $D_c = (\Delta N_c + \Delta N_s)/2 \mod 1$, and $D_s = \Delta N_s/2 \mod 1$. The role of these excitations, and of the particle-hole excitations, can best be seen by considering, e.g. the density operator $\sum_s c^\dagger_{n,s} c_{n,s}$ or $\sum_k c^\dagger_{k,q,s} c_{k+q,s}$. This operator does not change the particle number, i.e. $\Delta N_c = \Delta N_s = 0$. For small $q$, this operator creates particle-hole excitations, i.e. changes the distribution of the positive (or negative) $I_{c,j}$ or $I_{s,j}$ by some $\Delta I_c$ or $\Delta I_s$. If $q$ is not small and rather a multiple of $2k_F$, particles are transferred across the Fermi surface which will generate a persistent current in the system. These large-$q$ excitations therefore change the symmetry of the distribution of the $I_{c,j}$ and $I_{s,j}$, and therefore have a finite $D_{c,s}$. Permissible values of the $D_{c,s}$ follow from the expressions above. The finite $D_{c,s}$ values then generate the $2k_F$, $4k_F$, etc. excitations.

This set of quantum numbers is characteristic for an operator $O(x)$. Conformal field theory then determines its correlation functions as\cite{foot}

$$
\langle O(x) O^\dagger(0) \rangle \sim \frac{a(D_c, D_s) \exp(-2iD_c k_F t x) \exp(-2i[D_c + D_s] k_F t x)}{(x - v_\sigma t)^2\Delta_c^2 (x + v_\sigma t)^2\Delta_c (x - v_\sigma t)^2\Delta_s (x + v_\sigma t)^2\Delta_s}. 
$$

The anomalous dimensions of the operator

$$
\Delta_c^\pm = \frac{1}{2} \left( \pm \frac{Z_{ss}\Delta N_c - Z_{cc}\Delta N_s}{2 \det Z} + Z_{cc} D_c + Z_{sc} D_s \right)^2 + \Delta I_c^\pm \tag{2.10}
$$

$$
\Delta_s^\pm = \frac{1}{2} \left( \pm \frac{Z_{sc}\Delta N_c - Z_{cc}\Delta N_s}{2 \det Z} + Z_{cs} D_c + Z_{ss} D_s \right)^2 + \Delta I_s^\pm \tag{2.11}
$$

are determined by the entries of the dressed charge matrix and the changes in the quantum numbers $\Delta N_{c,s}$ and $D_{c,s}$ which the action of the operator generates.

For bounded systems, only positive rapidities are relevant, cf. Eq. (2.9), there is only one pseudo-Fermi point for each channel, and there are no current excitations. Consequently, there are only charge excitations $\Delta N_c$, $\Delta N_s$, and particle-hole excitations $\Delta I_c$, $\Delta I_s$. The backflow terms, resp. asymmetries of the rapidity distributions, $D_c$, $D_s$ are absent.

The complete, explicit behavior of correlation functions is rather complicated close to an open boundary, cf. Eq. (8) of Wang et al.\cite{foot}, for an example for a single channel (charge or spin). Asymptotically, however, the correlation functions $G_O$ of an operator $O$ simplify considerably and behave, close to an open boundary at $x = 0$,

1. in time (for $x_1, x_2 \approx 0$, and $vt \gg x_1, x_2$) as

$$
G_O(x_1, x_2, t) \sim t^{-2x_O h}. \tag{2.12}
$$
2. in space (specifically: \( x_1, t \approx 0, x_2 \gg x_1, vt \)) as

\[
G_O(x_1, x_2, t) \sim x_2^{-(x_O,b+d_O)}.
\] (2.13)

(Only the conformally invariant, i.e. slowly varying part of the correlation function is given. This must be multiplied by a factor oscillating with an appropriate multiple of \( k_F x_2 \).)

3. in temperature \((x_1, x_2 \approx 0, \omega \ll T)\)

\[
G_O(x_1, x_2, \omega, T) \sim T^{2x_O,b-1},
\] (2.14)

where the Fourier-transformed (in time) correlation function is used. That the boundary critical exponent \( x_O,b \), describing temporal correlations, comes in for temperature is most easily rationalized from the perspective of the Matsubara formalism of imaginary times (frequencies) in many-body physics.

The exponents \( x_O,b \) and \( d_O \) are the boundary critical exponent and bulk scaling dimension, respectively. The different exponents for spatial and time decays, and the appearance of a new boundary critical exponent describing the time correlations, translate the combined influences of the interactions and of broken translational invariance, on the low-energy properties of interacting 1D electron systems close to boundaries. In terms of the dressed charge matrix \( Z \), and the quantum numbers \( \Delta N_c, \Delta N_s, \Delta I_c, \) and \( \Delta I_s \) associated with the operator \( O \), \( x_O,b \) is given by

\[
x_O,b = \frac{1}{2} (Z^{-1} \Delta N)^T \cdot (Z^{-1} \Delta N) + \Delta I_c + \Delta I_s
\] (2.15)

with \((\Delta N)^T = (\Delta N_c, \Delta N_s)\), and the superscript \(T\) denotes the transpose. The bulk critical exponent is

\[
d_O = \Delta_c^+ + \Delta_c^- + \Delta_s^+ + \Delta_s^-.
\] (2.16)

Finally notice that when the system has boundaries on both sides, i.e. is of finite length \( L \), the power laws of space and time are changed to power laws of \( \sin(\pi x/2L) \), resp. \( \sin(\pi vt/2L) \) with the same exponents.

B. Luttinger liquid theory

At low energies, models of correlated 1D electrons such as the 1D Hubbard model, reduce to Luttinger liquids. Haldane’s Luttinger liquid conjecture postulates that, in a low-energy subspace, gapless one-dimensional quantum systems are described by an effective Luttinger Hamiltonian

\[
H = \frac{1}{2\pi} \sum_{\nu=\sigma} \int dx \left\{ v_\nu K_\nu \pi^2 \Pi_\nu^2(x) + \frac{v_\nu}{K_\nu} \left( \frac{\partial \Phi_\nu(x)}{\partial x} \right)^2 \right\}.
\] (2.17)
\( \Phi_\nu \) and \( \Pi_\nu \) are phase fields and their conjugate momenta for charge \((\nu = \rho)\) and spin \((\nu = \sigma)\) fluctuations

\[
\Phi_\nu(x) = -\frac{i\pi}{L} \sum_{p \neq 0} \frac{e^{-\alpha|p|/2-ipx}}{p} [\nu_+(p) + \nu_-(p)] ,
\]
(2.18)

and

\[
\Pi_\nu(x) = \frac{1}{\pi} \frac{\partial \Theta_\nu(x)}{\partial x} \text{ with } \Theta_\nu(x) = \frac{i\pi}{L} \sum_{p \neq 0} \frac{e^{-\alpha|p|/2-ipx}}{p} [\nu_+(p) - \nu_-(p)] ,
\]
(2.19)

which obey bosonic commutator relations, as do the long-wavelength fluctuation operators \( \nu_\nu(p) \). The \( K_\nu \) are the renormalized coupling constants in the charge and spin sectors. Zero-modes \((p = 0)\) do not influence the dynamics, and have been neglected.

Correlation functions and their critical exponents can then be calculated by bosonization

\[
\Psi_{rs}(x) \sim \lim_{\alpha \to 0} \frac{e^{ik_F x}}{\sqrt{2\pi \alpha}} \exp \left( -\frac{i}{\sqrt{2}} [r\Phi_\rho(x) - \Theta_\rho(x) + s \{r\Phi_\sigma(x) - \Theta_\sigma(x)\}] \right) .
\]
(2.20)

The chirality label \( r = \pm \) here and in Eqs. (2.18) and (2.19), refers to right- and left-moving fermions, with \( k \approx rk_F \). Consider a general local operator

\[
O_{\{m\}}(x) \equiv O_{m_\uparrow m_\downarrow,m_\uparrow m_\downarrow}(x) = \Psi_{m_\uparrow m_\uparrow}(x)\Psi_{m_\downarrow m_\downarrow}(x)\Psi_{m_\downarrow m_\uparrow}(x)\Psi_{m_\uparrow m_\downarrow}(x) ,
\]
(2.21)

where positive (negative) exponents label powers of creation (annihilation) operators, and higher powers of the operators are understood to be point-split, e.g., \((m_\uparrow \uparrow > 1)\)

\[
\Psi_{m_\uparrow m_\uparrow}(x) = \prod_{i=1}^{m_\uparrow \uparrow} \Psi_{m_\uparrow m_\uparrow}^{(i)}(x + [i - 1]a) .
\]
(2.22)

The two-point correlation function of such an operator decays as

\[
\langle O_{\{m\}}(xt)O_{\{m\}}(00) \rangle \sim \frac{\exp(-ik_F x J_\rho)}{(x - v_\rho t)^{2d_\rho^+} (x + v_\rho t)^{2d_\rho^-} (x - v_\sigma t)^{2d_\sigma^+} (x + v_\sigma t)^{2d_\sigma^-}}
\]
(2.23)

where the scaling dimensions

\[
2d_\rho^+ = \frac{1}{8} \left[ (\Delta N_\rho + J_\rho)^2 + (K_\rho - 1)J_\rho + (K_\rho^{-1} - 1)\Delta N_\rho \right]
\]
\[
2d_\rho^- = \frac{1}{8} \left[ (\Delta N_\rho - J_\rho)^2 + (K_\rho - 1)J_\rho + (K_\rho^{-1} - 1)\Delta N_\rho \right]
\]
\[
2d_\sigma^+ = \frac{1}{8} \left[ (\Delta N_\sigma + J_\sigma)^2 + (K_\sigma - 1)J_\sigma + (K_\sigma^{-1} - 1)\Delta N_\sigma \right]
\]
\[
2d_\sigma^- = \frac{1}{8} \left[ (\Delta N_\sigma - J_\sigma)^2 + (K_\sigma - 1)J_\sigma + (K_\sigma^{-1} - 1)\Delta N_\sigma \right]
\]
(2.24)
are determined by the two Luttinger liquid parameters $K_\nu$ and the number of charge and current excitations in the charge and spin sectors, created by the operator $O_{\{m\}}(xt)$

$$\Delta N_\rho = \sum_{r,s} m_{r,s} \, , \quad J_\rho = \sum_{r,s} r m_{r,s} \, , \quad \Delta N_\sigma = \sum_{r,s} s m_{r,s} \, , \quad J_\sigma = \sum_{r,s} r s m_{r,s} \, . \quad (2.25)$$

In addition, there are particle-hole excitations with chirality $r$ in each sector, given by

$$\rho_r(x) = \sum_s \Psi_{rs}^\dagger(x) \Psi_{rs}(x) \, , \quad \sigma_r(x) = \sum_s s \Psi_{rs}^\dagger(x) \Psi_{rs}(x) \, . \quad (2.26)$$

If an operator $\tilde{O}$ differs from $O$ above by $\Delta I_{r,\nu}$ powers of $\nu_r(x)$-type particle-hole excitations, the exponent of its correlation function will be increased as

$$d'_\nu \rightarrow d'_\nu + \Delta I_{r,\nu} \, . \quad (2.27)$$

Up to now, these critical exponents have been derived case by case, by an explicit bosonization calculation. Our Eqs. (2.23) and (2.24) show that, in complete analogy with conformal field theory, it is possible to give a general construction rule for the correlation functions, only based on the knowledge of the $K_\nu$ and the quantum numbers associated with the operators.

This picture is well-established for periodic systems. For open systems, the same basic ideas as outlined above, for integrable models and boundary conformal field theory, continue to hold: as a consequence of the boundary conditions, right- and left-moving fermion fields are no longer independent,

$$\Psi_{+,s}(x) = -\Psi_{-,s}(-x) \, , \quad (2.28)$$

and the physical fermions are described as superpositions of a chiral fermion with its reflection at the origin. The basic bosonization formula (2.20) is then replaced by

$$\Psi_{+,s}(x) \sim \lim_{\alpha \rightarrow 0} \frac{e^{ikFx}}{\sqrt{2\pi \alpha}} \exp \left( \frac{-i}{\sqrt{2}} \left[ \Phi_{+,\rho}(x) + s \Phi_{+,\sigma}(x) \right] \right) \, , \quad (2.29)$$

where the fields $\Phi_{+,\nu}(x)$ are obtained from Eqs. (2.18) or (2.19) by dropping the $\nu_-(p)$-operators. Due to the open boundary conditions, the full correlation functions of these operators are quite involved. While the single-particle Green’s function has been calculated by others, general correlation functions have not been published to date. Here, we give simple rules how the exponents describing the asymptotic decay of the correlation functions of more complicated operators, close to an open boundary, can be constructed in complete analogy to the recipes of boundary conformal field theory.

In the presence of open boundaries, the general operator $O_{\{m\}}(x)$ is represented in terms of only one type of chiral fermion, say $r = +$. There is thus only a single Fermi point, and no current excitations can be defined. There are only charge and particle-hole excitations. We therefore have $O_{\{m\}}^{(p)} \rightarrow O_{\{m\}}^{(b)}$ where the superscripts refer to boundary conditions

$$O_{\{m\}}^{(b)}(x) = \Psi_{+\uparrow +\downarrow}^{m+1+m-1}(x) \Psi_{+\downarrow +\uparrow}^{m+1+m-1}(x) = \Psi_{+\uparrow}^{\Delta N_\uparrow}(x) \Psi_{+\downarrow}^{\Delta N_\downarrow}(x) \quad (2.30)$$

with the same conventions as for $O_{\{m\}}^{(p)}$, Eq. (2.21). The first equality directly translates the bulk operator, in terms of its bulk quantum numbers, into a boundary operator, while the
second equality only uses the quantum numbers defined for the boundary operator: $\Delta N_s$ is the number of spin-$s$ particles the operator $O$ adds to the system. One now can calculate the correlations functions of $O_{(m)}^{(b)}(x)$ by the methods developed by others\textsuperscript{13–17}.

Close to an open boundary in a semi-infinite system, the complicated expressions simplify considerably in the limits $t \gg x$ and $x \gg t$ where $x$ is close to the boundary. From these limits, a boundary critical exponent $x_{O,b}$ can be defined for each operator $O_{(m)}(xt)$, and the behavior of the correlation functions as functions of the variables $x$, $t$, and $T$ is formally identical to Eqs. (2.12)–(2.14). For a Luttinger liquid, the boundary critical exponent $x_{O,b}$ then is given by

$$2x_{O,b} = x_{O,b}^{(\rho)} + x_{O,b}^{(\nu)} , \quad x_{O,b}^{(\nu)} = \frac{(\Delta N_{\nu})^2}{4K_{\nu}} .$$

(2.31)

Formally, $\Delta N_{\nu}$ is calculated in the same way as above, Eqs. (2.23), when the operator is represented in terms of the bulk chiral fermions, resp. with the correct number of $m_{+,s}$ and $m_{-,s} \equiv 0$ when it is set up directly as a boundary operator. Physically, an operator which generated current excitations in a periodic system, will now generate particle-hole excitations. The spatial decay of the correlations of $O(x)$ close to a boundary involves the bulk scaling dimension $d_{O} = \sum_{r, \nu} d_{\nu}^{r}$ of the operator $O(x)$ as in (2.13), and the $d_{\nu}^{r}$ are taken from Eqs. (2.24). The temperature variation again is determined by the boundary critical exponent $x_{O,b}$ as in (2.14). Bosonization of a Luttinger liquid with open boundaries therefore precisely reproduces the structure of correlation functions, and the boundary critical exponents that boundary conformal field theory extracts for integrable systems.

Notice further that for Luttinger liquids with open boundaries, the value of $K_{\rho}$ again comes out identical to that for periodic systems, translating the fact that it is a property of the Hamiltonian, resp. thermodynamics of the system, and as such independent of boundary conditions. Besides determining the boundary critical exponents of 1D fermions with open boundaries, our work therefore provides rules, in terms of $K_{\rho}$, how to connect bulk and boundary critical exponents of different correlation functions. Below, we shall discuss an application of this procedure.

Both methods, boundary conformal field theory and the Luttinger liquid, must lead to identical critical exponents. The relation between the entries of the dressed charge matrix, and the Luttinger liquid $K_{\rho}$ in the absence of magnetic fields (then $K_{\rho} \equiv 1$ for spin-rotation invariance) is

$$\xi^2(k_0) = 2K_{\rho} ,$$

(2.32)

both for bounded and for periodic systems.

In a finite magnetic field, the situation is far more complicated. In the 1D Hubbard model, there are (at least) three important effects of a finite magnetic field \textsuperscript{11}:

1. All entries of the dressed charge matrix acquire $h$-dependent corrections. This implies that the Luttinger coupling constant $K_{\rho}$, to the extent that it still makes sense, would depend on $h$ and therefore that charge-spin separation is violated, even in a low-energy subspace. Explicit expressions have been given by Frahm and Korepin\textsuperscript{11}. Specifically, $Z_{cs} \neq 0$ now.
2. The correction to the matrix element $Z_{ss}$ is particular in that it is logarithmic in $h$

$$Z_{ss} = \frac{1}{\sqrt{2}} \left( 1 + \frac{1}{4 \ln(h_c/h)} \right),$$  \hspace{1cm} (2.33)

while all other corrections have weaker $h$-dependences. $h_c$ is the critical field for a completely spin-polarized state. For the 1D Hubbard model, it has been calculated by Frahm and Korepin\cite{31} and varies from a finite constant at $U = 0$ to a $1/U$ behavior as $U \rightarrow \infty$. For non-interacting 1D electrons, one has $h_c = \varepsilon(2k_F)$ where $k_F$ is the Fermi wavevector for $h = 0$ and $\varepsilon(k)$ is the single-particle dispersion taken from the bottom of the band, $\varepsilon(0) = 0$. Thus $h_c = 2t[1 - \cos(2k_Fa)]$ for 1D tight-binding electrons.

3. There are different Fermi wave vectors for up- and down-spin electrons, $k_{F\uparrow} \neq k_{F\downarrow}$.

Quite generally, the mapping to a Luttinger liquid is problematic and cannot be carried out any more. If one is interested in boundary critical properties of 1D integrable systems, the conformal field theory approach (2.12)–(2.15) must be preferred.

In the (apparently realistic) limit $h \ll h_c$, the situation simplifies, however, and a mapping to a Luttinger liquid can still be done to logarithmic accuracy. To this accuracy, the only effect of the magnetic field is the correction to $Z_{ss}$, Eq. (2.33). This translates in a $h$-dependent deviation from unity, of the Luttinger coupling constant

$$K_\rho = \left( 1 + \frac{1}{4 \ln(h_c/h)} \right)^2 \approx 1 + \frac{1}{2 \ln(h_c/h)}.$$  \hspace{1cm} (2.34)

We obtained this equation by evaluating the finite-size corrections to the ground state energy\cite{4},

$$E(\Delta N, D) - E_0 = \frac{2\pi}{N} \left[ v_\rho(\Delta^c_\uparrow + \Delta^\downarrow_\uparrow) + v_\sigma(\Delta^c_\uparrow + \Delta^c_\downarrow) \right]$$  \hspace{1cm} (2.35)

from states with finite $\Delta N_s$ but vanishing $\Delta N_c = D_c = D_s = 0$, and using (2.10) and (2.11)

$$E(\Delta N_s, 0, 0, 0) - E_0 = \frac{2\pi}{N} v_\sigma \left( \frac{\Delta N_s}{2Z_{ss}} \right)^2.$$  \hspace{1cm} (2.36)

Its second derivative with respect to $\Delta N_s$ can then be identified to the inverse susceptibility of a Luttinger liquid and gives (2.34). To logarithmic accuracy in $h$, $K_\rho$ is unchanged, and one can use also the expressions for the (boundary) critical exponents of Luttinger liquids. A relation similar to (2.34) is also known for the 1D Heisenberg model\cite{32}, and a correction to the magnetic susceptibility of the 1D Hubbard model, logarithmic in $h$ and consistent with (2.34), has been derived by Kawano and Takahashi\cite{33}.

### III. A NEW UNIVERSALITY CLASS: BOUNDED LUTTINGER LIQUIDS

Universality classes of critical behavior are usually defined in terms of the scaling relations between the critical exponents. From the general expressions (2.12)–(2.14) above, it is clear
that these scaling relations on the boundary of a Luttinger liquid are different from those in the bulk. Luttinger liquids with open boundaries therefore realize a new universality class of (boundary) critical behavior which we propose to call *bounded Luttinger liquids*. More specifically, following Haldane’s statement for the periodic systems, we conjecture that one-dimensional quantum systems with gapless degrees of freedom and open boundaries form *bounded Luttinger liquids*. They comprise interacting electron systems, of which we discuss an example here, but also 1D bosons or spin chains. Bounded Luttinger liquids are boundary conformal field theories with central charge \( c = 1 \). Their nonuniversal exponents depend on one open coupling constant per degree of freedom \( K_\nu \) which is the same as in the bulk.

Here, we evaluate explicitly a variety of important boundary correlation functions. This will display the new set of scaling relations characterizing the bounded Luttinger liquids, and thus back our claim of a new universality class.

The single-electron Green’s function (spin-\( \uparrow \)) is

\[
G_\Psi(x_1, x_2, t) = \langle \Psi(x_1)\uparrow(t)\Psi(x_2)\uparrow(0) \rangle \sim \begin{cases}
t^{-2x_{\Psi,b}} & \text{if } t > 0 \\
 \sin(k_F x)b_{x-x_{\Psi,b}-d_{\Psi}} & \text{if } t < 0 \end{cases}
\]

where the last equality transforms our notation to the familiar Luttinger liquid notation with Green’s function exponents \( \alpha \). It involves the following excitations (both in terms of the Bethe ansatz for the Hubbard model, and in terms of a Luttinger liquid)

\[
\Delta N_c = 1, \quad \Delta N_s = 0, \quad \Delta I_c = \Delta I_s = 0
\]

\[
\Delta N_\rho = 1, \quad \Delta N_\sigma = 1, \quad \Delta I_\nu = 0
\]

In the absence of a magnetic field \( (Z_{cs} = 0) \), its boundary critical exponent is

\[
2x_{\Psi,b} = \frac{Z_{ss}^2 + Z_{sc}^2}{(\text{det } Z)^2}
\]

and

\[
x_{\Psi,b} + d_{\Psi} = \frac{1}{4} \left( 3 \frac{Z_{ss}^2 + Z_{sc}^2}{(\text{det } Z)^2} + Z_{cc}^2 + Z_{sc}^2 + Z_{ss}^2 - 2Z_{cs}Z_{sc} \right).
\]

Using (2.32), the Luttinger liquid notation obtains:

\[
\alpha_{\Psi,b} = \frac{1}{2K_\rho} - \frac{1}{2}
\]

and

\[
\alpha_{x,\Psi,b} = \frac{1}{8} \left( \frac{3}{K_\rho} + K_\rho - 4 \right).
\]

The same expressions are obtained, of course, when using directly Eq. (2.31). Photoemission experiments measure the Fourier transform of \( G_\Psi(t) \), the local spectral function
\[ \rho(x, \omega) = -\frac{1}{\pi} \text{Im} G(x, \omega + \mu) \sim |\omega|^{\alpha'_{\psi,b}}, \quad (3.8) \]

where \( \mu \) is the chemical potential. For repulsive interactions \( K_\rho < 1 \), we have

\[ \alpha'_{\psi,b} > \alpha_{\psi,p} = \frac{1}{4} \left( K_\rho + \frac{1}{K_\rho} - 2 \right) \quad (3.9) \]

which suggests that the pseudogap in the local density of states is *deepened* by the presence of boundaries. We will use these expressions in Section [V] below to discuss photoemission experiments in organic conductors.

Due to its relevance to photoemission experiments, the conformal field theory prediction (3.8) has been checked for the 1D Hubbard model. No exact calculation of the entire spectral function is available. Conformal field theory therefore provides the only exact prediction of properties of the spectral function, though only of its exponents. The question therefore is (i) to what extent other methods produce exponents consistent with conformal field theory, and (ii) if the deepening of the pseudogap in the local density of states is found, too. These issues were addressed recently, using perturbative Hartree and numerical DMRG calculations\[21\]. A surprising result of the Hartree calculations was an enhancement of the density of states, instead of a suppression, close to the chemical potential and close to the open boundary. DMRG was not able to calculate the frequency dependence of \( \rho(x, \omega) \). For the zero-frequency matrix elements, it asymptotically verified, however, a decay with system size as \( L^{-\alpha'_{\psi,b}} \), as expected from conformal field theory. Moreover, at finite \( L \), the matrix element approached the predicted power-law from below. Both facts suggest that the depth of the pseudogap is increased by the presence of open boundary conditions. However, that work also suggests a word of caution: for small \( U \), the asymptotic power-laws were approached only on very large lattices (\( L > 100 \) sites)\[2\] implying very small energy scales for (3.8) to be observed. How these scales depend on the interaction strength or range, and if the pseudogap is over- or underestimated at smaller \( L \) (the DMRG data seem to suggest the second possibility\[2\]), deserves further study. It could also be interesting to perform an exact calculation of the entire spectral function at \( U = \infty \) as has been done successfully for periodic systems\[34\].

The boundary critical exponent of the Green’s function also determines the temperature dependence of the tunneling conductance \( G \) through a weak link between two Luttinger liquids (LL) or between a Luttinger liquid and a normal metal (FL)

\[ G(T) = G_{\psi}^{\text{left}}(T) G_{\psi}^{\text{right}}(T) \sim \left\{ \begin{array}{ll}
T^{4x_{\psi,b} - 2} = T^{\frac{1}{K_\rho} + \frac{1}{K_\sigma} - 2}, & (LL - LL) \\
T^{2x_{\psi,b} - 1} = T^{\frac{1}{K_\psi} + \frac{1}{K_\sigma} - 1}, & (LL - FL)
\end{array} \right. \quad (3.10) \]

In magnetic fields, and for OBC, the exponents controlling these temperature dependences depend *in first order* on \( \ln(h_c/h) \), unlike periodic systems where the dominant dependence of the Green’s function exponent is of second order in \( \ln(h_c/h) \). This also holds for the related situations where particles scatter off a weak impurity in a periodic ring\[25\] because here, the temperature dependence of the conductance is controlled by the \( 2k_F \)-part of the density correlations,

\[ G(T) = G_0 \left[ 1 - \text{const.} \ T^{K_\rho + K_\sigma - 2} \right]. \quad (3.11) \]
Here, a finite $h$ will increase the exponent while in the tunneling case, the exponent will be decreased. If $K_{\rho} < 1$, in both cases the effect of a finite magnetic field will be to offset the interaction effects on the exponents contained in $K_{\rho}$, and to produce conductance variations more similar to free electrons. Precisely this effect has apparently been observed in semiconductor quantum wires in magnetic fields. Notice that in such structures, $E_{F}$ is small, typically some $\text{meV}$. Consequently, $h_c$ is also small and the magnetic field effect on $K_{\sigma}$ could well be big.

The density-density correlation function

\[ G_n(x_1, x_2, t) = \langle n(x_1, t)n(x_2, 0) \rangle , \]  

involves the following excitations

\[ \Delta N_c = \Delta N_s = 0, \quad \Delta I_c = 1, \quad \Delta I_s = 0 \quad \text{or} \quad \Delta I_c = 0, \quad \Delta I_s = 1, \]  
\[ \Delta N_{\rho} = 0, \quad \Delta N_{\sigma} = 0, \quad \Delta I_{\rho} = 1, \quad \Delta I_{\sigma} = 0. \]  

Notice that for open boundary conditions, there are no current excitations while in the bulk, the density operator can involve current excitations and therefore oscillate with wavevectors that are even multiples of $k_F$. Consequently, there is a single time behavior while the spatial dependence contains the usual $q \approx 0, 2k_F, 4k_F, \ldots$ components. We have

\[ x_{n,b} = 1 \]  

and

\[ G_n(0, 0, t) \sim t^{-2}, \]
\[ G_n(x, 0, 0) \sim x^{-2} + \sin(2k_Fx)x^{-\frac{3 + K_{\rho}}{2}} + \sin(4k_Fx)x^{-1 - 2K_{\rho}}. \]

In the bounded system, there is now a universal boundary critical exponent $x_{n,b} = 1$, while the time dependence was non-universal in the periodic system. The nonuniversal decay in $x$-direction, and the differences in the exponents of the various momentum components, are a consequence of the different bulk conformal dimensions of the $2k_F$-harmonics of the density operator.

Friedel oscillations appear in the system because of the breaking of translational invariance by the boundaries. They have been studied in detail by Bedürftig et al. We determine their spatial decay as

\[ \langle n(x) \rangle = n - A_1 \frac{\sin(2k_Fx)}{x^{\frac{K_{\rho} + 1}{2}}} - A_2 \frac{\sin(4k_Fx)}{x^{2K_{\rho}}} \]  

where we have used the Luttinger liquid language. Notice that they are governed not by boundary critical exponents but by the bulk exponents of the $2k_F$- and $4k_F$-parts of the density operator. The boundary exponents of the density correlations, are different from those of the Friedel oscillations, however. DMRG calculations of the Friedel oscillations are in impressive agreement with conformal field theory predictions both for spinless and spin-$1/2$ fermion systems.
The longitudinal and transverse spin-spin correlation functions involve the following excitations, respectively,

\[ G_z^{\sigma}(x_1, x_2, t) = \langle S_z(x_1, t)S_z(x_2, 0) \rangle, \]
\[ S_z(x, t) = \frac{1}{2}[n_\uparrow(x, t) - n_\downarrow(x, t)], \]
\[ \Delta N_c = \Delta N_s = 0, \quad \Delta I_c = 1, \quad \Delta I_s = 0 \quad \text{or} \quad \Delta I_c = 0, \quad \Delta I_s = 1, \]
\[ \Delta N_\rho = 0, \quad \Delta N_\sigma = 0, \quad \Delta I_\rho = 0, \quad \Delta I_\sigma = 1; \]

\[ G_{\perp}^{\sigma}(x_1, x_2, t) = \langle S_-^{\sigma}(x_1, t)S_+^{\sigma}(x_2, 0) \rangle, \]
\[ S_+^{\sigma}(x, t) = \Psi_\uparrow(x, t)\Psi_\downarrow(x, t), \]
\[ \Delta N_c = 0, \quad \Delta N_s = 1, \quad \Delta I_c = \Delta I_s = 0, \]
\[ \Delta N_\rho = 0, \quad \Delta N_\sigma = 2, \quad \Delta I_\rho = 0, \quad \Delta I_\sigma = 0. \]

In the absence of a magnetic field, they decay with the same exponents as the long-wavelength and the \(2k_F\)-components of the density correlations. The enhancement of magnetic over density correlations which we expect in the \(U > 0\)-Hubbard model, in the bulk is due both to logarithmic corrections and to prefactors. A similar enhancement in the correlation functions, is expected close to the boundary. Notice, however, that the static Friedel oscillations in the density will dominate there, and the importance of the magnetic correlations in the system will be limited either to dynamical measurements, or to the bulk region. It is also important to notice that, in the Luttinger liquid picture, it is the special value \(K_\sigma = 1\), embodying spin-rotation invariance, which makes the boundary critical exponents of the longitudinal and transverse spin correlations identical. Formally, we have

\[ x_{S, b}^\parallel = 1 \quad \text{and} \quad x_{S, b}^\perp = 1/K_\sigma. \]  

Finally pairing correlations are important. The singlet pairing correlations are

\[ G_{SS}^{(0)}(x_1, x_2, t) = \langle \Psi_\uparrow(x_1, t)\Psi_\downarrow(x_1, t)\Psi_\downarrow(x_2, 0)\Psi_\uparrow(x_2, 0) \rangle, \]
\[ \Delta N_c = 2, \quad \Delta N_s = 1, \quad \Delta I_c = \Delta I_s = 0, \]
\[ \Delta N_\rho = 2, \quad \Delta N_\sigma = 0, \quad \Delta I_\rho = 0. \]

Their boundary critical exponent is

\[ x_{SS, b} = \frac{2}{\xi_0^2(k)} = \frac{1}{K_\rho}, \]

so that they decay as

\[ G_{SS}^{(0)}(0, 0, t) \sim t^{-2/K_\rho}, \]  

\[ G_{SS}^{(0)}(x, 0, 0) \sim x^{-2K_\rho^{-1}}. \]

They will dominate for attractive interactions (\(K_\rho > 1\)) only. Then, however, the presence of a boundary will enhance them over their bulk values.

Triplet pairing correlations have three components \((S^z = 1, 0, -1)\) involving the following operators and excitations
Using the quantum numbers of the excitations, we find for $S_z$ this is different from the value of $S_z$ we propose to call "bounded Luttinger liquids". As we have shown earlier, the singlet correlations are not affected by this argument and (3.24) continues to hold. In a periodic Luttinger liquid, the triplet pairing operators with spin projection inconsistent with the model Hamiltonian. The solution of the puzzle is contained in Eq. (3.24). Superficially, this would imply a breaking of spin-rotational invariance which is inconsistent with the model Hamiltonian. The solution of the puzzle is contained in Eq. (3.24). Superficially, this would imply a breaking of spin-rotational invariance which is inconsistent with the model Hamiltonian. The solution of the puzzle is contained in Eq. (3.24). Superficially, this would imply a breaking of spin-rotational invariance which is inconsistent with the model Hamiltonian. The solution of the puzzle is contained in Eq. (3.24). 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from bulk Luttinger liquids. With bulk Luttinger liquids, they share the fact that the scaling relations between the nonuniversal critical exponents are parametrized by one renormalized coupling constant $K_\nu$ per degree of freedom $\nu$. These coupling constants are characteristic of the underlying Hamiltonian and the same irrespective of the boundary conditions. Unlike bulk Luttinger liquids, bounded Luttinger liquids have no current excitations. This gives universal boundary critical exponents to correlation functions of operators involving current excitations in the bulk, where they had nonuniversal exponents. Examples are the $2k_F$- and $4k_F$-components of the density correlations. This should also apply to the $3k_F$-Green’s function which would be another interesting example that might be worked out. Also, as we have shown, the linear dependence of right- and left-moving fermions introduced by the boundary, may produce different boundary critical exponents for operators which have the same bulk scaling dimensions.

Finally, while charge-spin separation may be present in a bounded Luttinger liquid, it will be exceedingly difficult to observe it: all excitations are localized by the boundaries, and there are no propagating solutions.

When expressed in terms of $K_\rho$, $K_\sigma$, our single-particle Green’s function takes the same form as those found elsewhere. The suggestion that a new universality class is realized by correlated fermions with open boundaries, was also made by Mattsson et al.

**IV. APPLICATION: THE PHOTOEMISSION PUZZLE IN THE BECHGAARD SALTS**

Here, we discuss one way in which these results can be put to use. The family of organic conductors $(TMTSF)_2X$ (where TMTSF stands for the molecule tetramethyltetraselenafulvalene, and X typically is $PF_6$, $ClO_4$, $ReO_4$, etc., the “Bechgaard salts”) is one of the candidates for the realization of a Luttinger liquid in quasi-1D electron systems. There is general experimental evidence for strong anisotropy of the electronic properties and strong electron-electron interactions. More specifically, several experiments have produced evidence in favor of Luttinger liquid behavior:

1. The NMR spin-lattice relaxation is consistent with a Luttinger form $T_1^{-1} \sim T + T^{K_\rho}$. Values $K_\rho \sim 0.15$ were suggested.

2. Optical conductivity does not directly probe the Luttinger liquid but its leading irrelevant operators which can relax momentum to the lattice. Assuming that these stem from electron-electron Umklapp scattering in a quarter-filled band, theory predicts $\sigma(\omega) \sim \omega^{16K_\rho-5}$ on the high-frequency tail of a mid-infrared peak. Experiments observe power-law behavior in this region, leading to $K_\rho \sim 0.23$.

3. Under a pressure of 9 kbar, the resistivity perpendicular to the chains shows power-law behavior in temperature. Theoretically, the exponent is related to that of the single-particle Green’s function, giving values $K_\rho \sim 0.25 \ldots 0.3$.

Although the values of $K_\rho$ suggested by the experiments do not agree precisely, the properties probed apparently are consistent with a Luttinger liquid. There is, however, one type of
measurement whose results systematically disagree with Luttinger liquid predictions: photoemission.

The spectral function of a Luttinger liquid generically exhibits two dispersing signals, due to charge-spin separation, whose singularities depend on \( K_{\rho} \). For \( K_{\rho} \approx 1/3 \ldots 1/4 \), one expects a divergence dispersing with the charge velocity and an exponent \(-1/3 \ldots -7/32 \approx -1/4\). While the singularity dispersing with the spin velocity has a smaller exponent \(-1/6 \ldots +1/16\). This is not observed. The result of the experiment on \((TMTSF)\textsubscript{2}ClO\textsubscript{4}\) can be summarized briefly: no charge-spin separation, no dispersion, not even low-energy peaks. Instead, there is a broad peak at -1 eV whose tail reaches down to zero intensity at the chemical potential.\(^2^3\) The leading edge of the spectra is independent of the wavevector \( k \) of the photoelectrons, and well fitted by a power law, \( \sim (-\omega)^{\alpha} \), with exponents \( \alpha \geq 1 \) over a wide range of energies. Moreover, the appearance of the momentum-resolved spectral functions is strikingly similar to that of an earlier experiment with low (or no) angular resolution.\(^2^2\)

We now discuss the possibility that this may be due to impurities on the sample surface. The argument involves three main steps which we develop in the following: (i) ARPES probes intrinsic properties of the surfaces of the Bechgaard salts; (ii) the surface states from which the photoelectrons are ejected, are localized; (iii) if these states are described as bounded Luttinger liquids, the \( K_{\rho} \)-values suggested by the bulk measurements together with Eq. (3.8) give a good description of the photoemission spectra.

Very similar lineshapes are observed in the insulating compound \((TMTTF)\textsubscript{2}PF\textsubscript{6}\) (sele-

nium substituted by sulfur) which is believed to be a 1D Mott insulator. In photoemission, the important difference to \((TMTSF)\textsubscript{2}X\) is that a gap of about 100 meV is observed, consistent with the values of the charge gap deduced from other experiments. Very new experiments on \((TMTSF)\textsubscript{2}ReO\textsubscript{4}\) which undergoes a metal-insulator transition due to anion ordering, observe lineshapes similar to \((TMTSF)\textsubscript{2}ClO\textsubscript{4}\) in the metallic phase and to \((TMTTF)\textsubscript{2}PF\textsubscript{6}\) in the insulating phase, and furthermore can monitor the gap opening as a function of temperature. Photoemission therefore is sensitive to spectral changes at the Fermi surface, and observes intrinsic properties of the surfaces of the Bechgaard salts.

The absence of dispersion in the experimental data then implies that the photoelectrons are ejected out of localized states. Then, even an angle-resolved photoemission experiment will measure the local density of states, \( \rho(x, \omega) = \int dk p(k; \omega) \), i.e. the momentum-resolved spectral function integrated over a wide range of momenta. The surface sensitivity of photoemission spectroscopy restricts this conclusion to the sample surface only. In the bulk, there may well be the propagating charge and spin excitations which are believed to underly the experiments discussed above. (Notice, though, that apart the longitudinal DC resistivity not discussed here, many experiments do not require them explicitly to be propagating.) The origin of the localization at the surface is not clear, although impurities, perhaps introduced by cleaving the samples, and/or the enhanced one-dimensionality, provide plausible causes.

If the bulk is assumed to be a Luttinger liquid, and if we approximate the impurities at the surface by open boundaries, then the chains at the surface consist of finite segments which must be described as bounded Luttinger liquids with the same \( K_{\rho} \) as the bulk. Provided the conditions underlying Eqs. (2.12) and (3.8) are fulfilled, the local spectral function is obtained as
The result for $K_\rho = 1/2$ has been obtained earlier by Eggert et al.\cite{Eggert1994}, who already speculated on the possible influence of surface impurities. In particular for values $K_\rho \approx 1/3 \ldots 1/4$ suggested by optics and DC-resistivity, the low-frequency photoemission weight is well described by (4.1) for a bounded Luttinger liquid. Notice moreover that, with photoelectrons emanating from localized states, the independence of the results of angular resolution finds a natural explanation.

The conditions on which Eq. (4.1) is based, imply that most of the ARPES intensity must come from states which are dominated by boundary effects. This energy range is widest when the impurities are rather closely spaced. In such a case, the discretization of the energy levels may no longer be negligible. However, these discreteness effects are likely washed out by averaging over many different segments, and one returns to the effective semi-infinite bounded Luttinger liquid underlying Eq. (2.12), as demonstrated by Mattsson et al.\cite{Mattsson1993} in the related problem of one small segment studied with a poor experimental resolution. A more detailed investigation of the spectral properties of a 1D correlated electron system with random impurities would, however, be useful.

We therefore come up with a picture of the Bechgaard salts as an inhomogeneous system where the bulk would be a standard Luttinger liquid with propagating charge and spin excitations, and impurities localizing these excitations at the surface.

\section{V. OPEN QUESTIONS}

As a consequence of broken translational invariance, a new set of boundary critical exponents appear in correlated 1D electron systems close to open boundaries. They define a new universality class which we proposed to call \textit{bounded Luttinger liquids}. In this paper, we explored these new scaling relations both by applying boundary conformal field theory to the 1D Hubbard model, and by using Luttinger liquid theory. Both methods can be implemented in a very similar way and, of course, lead to identical conclusions.

Our study leaves open a number of questions, however. We only investigated open boundary conditions. There is the possibility that the boundary critical exponents depend on type of boundary, e.g. additional boundary fields (magnetic or chemical potential, etc.), boundary operators (e.g. spins, relevant for the Kondo problem\cite{Kondo1964}), superconductors, etc., and that new scaling relations are associated with them. Such a possibility is suggested by a study of a Luttinger liquid coupled to a superconductor\cite{Mattsson1993} which finds a local density of states $\rho(x,\omega) \sim |\omega|^{(K_\rho - 1)/2}$, instead of our (3.8) and (3.9). One could then be left with a whole manifold of universality classes depending on the specific type of boundary conditions. The dressed charge matrices, and the Luttinger liquid coupling constants $K_\nu$ will, however, be independent of these details.

The bulk - boundary crossover has not been studied systematically yet. While this crossover has been studied for the \textit{local} single-particle density of states in a bounded Luttinger liquid by Mattsson et al.\cite{Mattsson1993}, the important question of how dispersion in a spectral
function appears when the length of a bounded electron system is varied from microscopic to macroscopic scales, has been left open. In the same way, one would like to understand, in terms of dispersion and critical exponents, how the open boundary condition effectively emerges in a correlated 1D electron system with an impurity. The extension to the spectral properties of systems with many random impurities would also be important.

We used the theory of a bounded Luttinger liquid to discuss the idea that impurities at the surface of organic conductors may lead to localized electronic states which would dominate the photoemission properties of such materials.\textsuperscript{23} Such an analysis, using the $K_\rho$-values suggested by experiments probing the propagating bulk excitations, gives a local density of states consistent with experiments. Of course, the picture of an inhomogeneous material, with localized states at the surface and propagating states in the bulk, is somewhat speculative. It would predict, however, a definite dependence of the results of an experiment on its probing depth. Such dependences should be searched for, and only if they are found, this idea should be taken serious. Finally, theoretical information on spectral weight distribution beyond the predictions of conformal field theory,\textsuperscript{21} and a clarification of the energy scales on which they are accurate, would be very important – even for the periodic systems.

ACKNOWLEDGMENTS

We wish to acknowledge useful discussions with B. Brendel, S. Eggert, H. Johannesson, V. Meden, M. Rother, K. Schönhammer and C. A. Stafford. J.V. is a Heisenberg fellow Deutsche Forschungsgemeinschaft, and received additional support from DFG under SFB 279-B4 in the early stages of this work.
REFERENCES

1 K. Binder, in *Phase transition and critical phenomena*, vol. 8, ed. by C. Domb and J. Lebowitz (Academic Press, London, 1983).
2 A. A. Belavin, A. M. Polyakov and A. B. Zamolodchikov, Nucl. Phys. B 241, 333 (1984); D. Friedan, Z. Qiu and S. H. Shenker, Phys. Rev. Lett. 52, 1575 (1984).
3 J. L. Cardy, J. Phys. A 17, L385 (1984); H. Blöte, J. L. Cardy and P. Nightingale, Phys. Rev. Lett. 56, 742 (1986); I. Affleck, ibid. 56, 746 (1986).
4 H. Frahm and V. E. Korepin, Phys. Rev. B 42, 10553 (1990).
5 J. Voit, Rep. Prog. Phys. 58, 977 (1995), for a review on Luttinger liquids and the properties of strongly correlated 1D electron systems.
6 F. D. M. Haldane, J. Phys. C 14, 2585 (1981).
7 F. D. M. Haldane, Phys. Rev. Lett. 45, 1358 (1980) and Phys. Lett. 81A, 153 (1981).
8 H. J. Schulz, Phys. Rev. Lett. 64, 2831 (1990).
9 J. L. Cardy, Nucl. Phys. B 241, 333 (1984).
10 Y. Wang, J. Voit, and F.-C. Pu, Phys. Rev. B 54, 8491 (1996).
11 S. Fujimoto and N. Kawakami, Phys. Rev. B 54, 5784 (1996).
12 M. Gaudin, Phys. Rev. A 4, 386 (1971).
13 H. Schulz, J. Phys. C 18, 581 (1985).
14 F. Woynarovich, Phys. Lett. 108A, 401 (1985); A. Foerster and M. Karowski, Nucl. Phys. B 396, 611 (1993); H. Asakawa and M. Suzuki, J. Phys. A 29, 225 (1996); G. Bedürftig and H. Frahm, J. Phys. A 30, 4139 (1997).
15 M. Fabrizio and A. O. Gogolin, Phys. Rev. B 51, 17827 (1995).
16 S. Eggert, H. Johannesson, A. Mattsson, Phys. Rev. Lett 76, 1505 (1996).
17 A. E. Mattsson, S. Eggert, and H. Johannesson, Phys. Rev. B 56, 15615 (1997).
18 G. Bedürftig, B. Brendel, H. Frahm, and R. M. Noack, Phys. Rev. B 58, 10225 (1998).
19 P. Schmitteckert and U. Eckern, Phys. Rev. B 53, 15397 (1996).
20 I. Affleck and S. Eggert, Phys. Rev. B 46, 10866 (1992).
21 K. Schönhammer, V. Meden, W. Metzner, U. Schollwöck, and O. Gunnarsson, cond-mat/9903121.
22 B. Dardel, D. Malterre, M. Grioni, P. Weibel, Y. Baer, J. Voit, and D. Jérôme, Europhys. Lett. 24, 687 (1993).
23 F. Zwick, S. Brown, G. Margaritondo, C. Merlic, M. Onellion, J. Voit, and M. Grioni, Phys. Rev. Lett. 79, 3982 (1997).
24 M. Grioni and J. Voit, to be published in “Electron spectroscopies applied to low-dimensional materials”, edited by H. Stanberg und H. Hughes, Kluwer Academic Publ. (1999).
25 C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. 68, 1220 (1992).
26 M. Rother, *et al.*, unpublished.
27 M. Bockrath, *et al.*, Nature 397, 598 (1999).
28 E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20, 1445 (1968).
29 We will also use the term “charge excitation” for particle addition, although these may occur both in the charge and spin sectors. From the context, it should be clear if “charge” refers to an excitation, or to a sector of the Hilbert space.
30 Charge and spin labels are used in a different sense in Bethe Ansatz and Luttinger liquid theory. We therefore use the subscripts $c$ and $s$ in a Bethe Ansatz context, and the greek
subscripts $\rho$ and $\sigma$ in a Luttinger liquid context. When we refer to the same quantities in both methods (e.g. the velocities $v_\rho, v_\sigma$), we prefer the Luttinger liquid notation.

31 H. Frahm and V. E. Korepin, Phys. Rev. B **43**, 5653 (1991).
32 I. Affleck and M. Oshikawa, cond-mat/9905002. N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, Nucl. Phys. B **275**, 687 (1986).
33 K. Kawano and M. Takahashi, J. Phys. Soc. Jpn. **64**, 4331 (1995).
34 K. Penc, K. Hallberg, F. Mila, and H. Shiba, Phys. Rev. B **55**, 15475 (1997).
35 R. Egger and H. Grabert, Phys. Rev. Lett. **75**, 3505 (1995).
36 J. Voit, J. Phys. C **21**, L-1141 (1988).
37 C. Bourbonnais, F. Creuzet, D. Jérôme, K. Bechgaard, and A. Moradpour, J. Phys. (Paris) Lett. **45**, L-755 (1984); P. Wzietek, F. Creuzet, C. Bourbonnais, D. Jérôme, and A. Moradpour, J. Phys. (Paris) I **3**, 171 (1993).
38 T. Giamarchi, Phys. Rev. B **44**, 2905 (1991).
39 A. Schwartz, M. Dressel, G. Gruner, V. Vescoli, L. Degiorgi, and T. Giamarchi, Phys. Rev. B**58**, 1261 (1998).
40 J. Moser, M. Gabay, P. Auban-Senzier, D. Jérôme, K. Bechgaard, and J.M. Fabre, Eur. Phys. J. B **1**, 39 (1998).
41 J. Voit, Phys. Rev. B **47**, 6740 (1993).
42 V. Meden and K. Schönhammer, Phys. Rev. B **46**, 15753 (1992).
43 This possibility can be investigated in *special* models for the Kondo effect in Luttinger liquids which produce “Fermi-liquid-like thermodynamics”, e.g. A. Schiller and K. Ingersent, Phys. Rev. B **51**, 4676 (1995); Y. Wang and J. Voit, Phys. Rev. Lett. **77**, 4934 (1996).
44 C. Winkelholz, R. Fazio, F. W. J. Hekking, and G. Schön, Phys. Rev. Lett. **77**, 3200 (1996).