Boundary Condition Changing Operators in Conformal Field Theory and Condensed Matter Physics *

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Boundary condition changing operators in conformal field theory describe various types of “sudden switching” problems in condensed matter physics such as the X-ray edge singularity. We review this subject and give two extensions of previous work. A general derivation of a connection between the X-ray edge singularity, the Anderson orthogonality catastrophe and finite-size scaling of energies is given. The formalism is also extended to include boundstates.

I. INTRODUCTION

Claude Itzykson has been an inspiring and supportive colleague to me, ever since I had the good fortune to spend a year as his neighbour at C.E.N. Saclay. He is sorely missed.

Conformal field theory with boundaries, a subject developed largely by John Cardy, has found applications to various quantum impurity problems in condensed matter physics. A particular branch of this subject involves boundary condition changing operators. They were used to obtain a new understanding of a class of problems in condensed matter physics where a local change in a Hamiltonian is made suddenly, for example by X-ray absorption in a metal. This article is mainly a review of work on this subject by Andreas Ludwig and the author with a few new insights presented. In the next section we review boundary condition changing operators in conformal field theory. In section III we discuss their application to the X-ray edge singularity and Anderson’s orthogonality catastrophe, giving some new results. In the final section we discuss X-ray edge singularities in the Kondo problem. Some of the new results were obtained in collaboration with Alex Zagoskin.

II. BOUNDARY CONDITION CHANGING OPERATORS IN CONFORMAL FIELD THEORY

Consider conformal field theory on the half-plane $z = r + i\tau, r \geq 0$. The requirement that the boundary of the half-plane, the real axis, remain fixed reduces the full group of conformal transformations, $z \rightarrow w(z)$, to those obeying $w(\tau) = w(\tau)$, an infinite subgroup. We will be interested in general conformally invariant boundary conditions on the strip which are consistent with

$$T(\tau, 0) = \overline{T}(\tau, 0), \quad (2.1)$$

where $T$, ($\overline{T}$), is the holomorphic (anti-holomorphic) part of the energy-momentum tensor. This corresponds to vanishing momentum density at the boundary, corresponding to conservation of quantum mechanical probability density. For a given bulk conformal field theory, the set of conformally invariant boundary conditions, $A$, $B$, ... can be determined.

In general the scaling dimensions of boundary operators can be related to the finite size scaling of energy levels on a strip, as shown in Figure (1). Under the conformal transformation $z = le^{\pi w/l}$ the correlation function of the primary boundary condition changing boundary operator $O$ transforms as:

$$\frac{1}{(\tau_1 - \tau_2)^2} \rightarrow \frac{1}{\left[\frac{2l}{\pi}\sinh\frac{\pi}{2l}(u_1 - u_2)\right]^{2x}} = \sum_n | <AA; 0|O|AB; n> |^2 e^{-|E_{n}^{AB} - E_{0}^{AA}|\Delta u}. \quad (2.2)$$

In the limit of large $\Delta u \equiv u_1 - u_2$, we see that:

$$\frac{1}{\left[\frac{2l}{\pi}\sinh\frac{\pi}{2l}(u_1 - u_2)\right]^{2x}} \rightarrow \left(\frac{\pi}{l}\right)^{2x} e^{-\pi x \Delta u}. \quad (2.3)$$

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Note that $O$ changes the boundary condition from $A$ to $B$ on the lower boundary. Since the finite size energies, $E_{n}^{AB}$, depend on the boundary conditions, $A$ and $B$, it follows that the dimensions of boundary operators depend on the boundary conditions:

$$x = \frac{l}{\pi}[E_{n}^{AB} - E_{0}^{AA}],$$

(2.4)

where $n$ labels the lowest energy state with a non-zero matrix element in the sum in Eq. (2.2). Depending on the operator, $O$, $n$ may equal 0, corresponding to the groundstate with boundary conditions $AB$, or possibly on excited state. We also see from Eq. (2.2) that this matrix element scales with system size as:

$$| < AA; 0|O|AB; n > | = \left( \frac{\pi}{l} \right)^{x}$$

(2.5)

FIG. 1. Conformal transformation from the infinite half-plane to the strip.

III. APPLICATION OF BOUNDARY CONFORMAL FIELD THEORY TO THE X-RAY EDGE SINGULARITY AND ANDERSON'S ORTHOGONALITY CATASTROPHE

Consider the electron energy levels in a metal. [See Figure (2).]

In addition to the partially filled conduction band there are also core levels in which the electron is tightly bound to a particular nucleus. X-ray absorption can either eject a core electron (photoemission) or raise it to the conduction band, as indicated in Figure (2). The resulting core hole produces a local electrostatic potential acting on the conduction electrons which affects the X-ray absorption probability producing a singularity at the threshold, as indicated in Figure (3). A very simple model was discussed by Nozières and De Dominicis.

$$H = \sum_{k} \epsilon_{k} c_{k}^{\dagger} c_{k} + b^{\dagger} b \sum_{k,k'} V_{k,k'} c_{k}^{\dagger} c_{k'} - E_{0} b^{\dagger} b.$$  

(3.1)

Here $\epsilon_{k}$ is the dispersion relation of the conduction band electrons, annihilated by $c_{k}$. $b$ annihilates the core electron. $V$ is the local potential. (Electron spin is ignored.) An essential observation is that:

$$[H, bb^{\dagger}] = 0.$$  

(3.2)
The Hilbert space consists of two sectors. In one $bb\dagger = 0$; the core level is filled and there is no potential. In the other $bb\dagger = 1$; the core level is empty and consequently the potential $V$ is exerted on the conduction electrons. In the simpler case of X-ray photoemission, the absorption intensity is:

$$I(\omega) \propto \int dt e^{i\omega t} <0|b(t)b(0)|0> \propto (\omega - \omega_0)^{-\alpha}.$$ (3.3)

Inserting the $b$ operator switches on the potential, $V$, at time 0. It is later switched off at time $t$. At low energies, turning on $V$ is equivalent to changing the boundary conditions. Thus $b$ is a boundary condition changing operator.

![FIG. 3. Schematic X-ray absorption intensity versus frequency.](image)

We will assume that both $\epsilon_\vec{k}$ and $V_{\vec{k},\vec{k}'}$ are spherically symmetric and consider only s-wave scattering. (It is straightforward to generalize the method to other cases.) Linearizing the dispersion relation around the Fermi surface, we obtain a low energy theory consisting of (1+1) dimensional Dirac fermions defined on the half-line $r > 0$, with the potential $V$ at the origin. See Figure (4). We integrate out all degrees of freedom except for electrons with energies very close to the Fermi energy, $E_F$. Thus the fields obey an effective boundary condition at the origin:

$$\psi_R(0) = e^{2i\delta(E_F)}\psi_L(0),$$ (3.4)

where $\delta(E_F)$ is the s-wave phase shift at the Fermi energy.

![FIG. 4. One-dimensional problem with potential at the origin.](image)

The state $b|0> \Rightarrow \text{core hole present but the conduction electrons filling the V=0 Fermi sea}$ In the infinite volume limit, this state is orthogonal to the groundstate with the core hole present, in which the electrons in the Fermi sea are rearranged by the potential. This is known as the “Anderson orthogonality catastrophe”. It is this rearrangement of the Fermi sea, produced by $V$, which leads to the X-ray edge singularity.

On a finite strip (corresponding to s-wave electrons inside a finite sphere):

$$<AB;0|b|AA;0> \neq 0.$$ (3.5)

Here $|AA;0>$ is the unperturbed filled Fermi sea and $|AB;0>$ is the state with the core electron absent and the filled Fermi sea perturbed by the presence of the core hole potential, $V$. From the conformal transformation of Eq. (2.2) we see that the X-ray exponent, the Anderson orthogonality exponent and the $1/l$ term in the groundstate energy difference are all given by the same number, $x$:

$$<b\dagger(t)b(0) > \approx \frac{1}{t^{2x}} \text{[X-ray exponent } \alpha = 1 - 2x]\]

$$|<AB;0|b|AA;0>| = \left(\frac{\pi}{4}\right)^x \text{[orthogonality exponent]}$$

$$E_0^{AB} - E_0^{AA} = \frac{\pi x}{l} \text{[finite size energy].}$$ (3.6)
The exponent, $x$, is most easily calculated from the finite size energy. It is instructive to calculate the complete expression for this energy difference, without making any low energy approximations, in order to ensure that the $1/l$ term, indeed only depends on the phase shift at the Fermi surface, $\delta(E_F)$, that is on the boundary condition in the low energy effective theory. For large $l$,

$$E_0 - E_0^V \approx l \int_0^{k_F} \frac{dk}{\pi} [\epsilon(\tilde{k}) - \epsilon(k)],$$

where $k_F$ is the Fermi wave-vector and the phase-shifted wave vector, $\tilde{k}$, is defined by the self-consistent equation:

$$\tilde{k} \equiv k - \frac{\delta(\tilde{k})}{l}. \quad (3.8)$$

Taylor expanding out to terms of $O(1/l)$,

$$\Delta E \approx -\int_0^{k_F} \frac{dk}{\pi} \left[ -\epsilon'(k)\delta(k) + \frac{1}{2} \epsilon''(k)\delta(k)^2 + \frac{1}{l} \epsilon'(k)\delta'(k)\delta(k) \right]$$

$$= -\frac{1}{\pi} \int_0^{E_F} d\epsilon \delta(\epsilon) + v_F \frac{1}{l} \left[ \frac{\delta(E_F)}{\pi} \right]^2. \quad (3.9)$$

Here $v_F = \epsilon'(k_F)$ is the Fermi velocity and we have integrated by parts to obtain the last line, using the fact that $\epsilon'(0) = 0$ which follows from analyticity of the dispersion relation. The first term in $\Delta E$ is $O(1)$ and depends on the phase shift throughout the conduction band. This formula is known as Fumi’s theorem. On the other hand, the second term, of $O(1/l)$, only depends on the phase shift right at the Fermi surface. Thus this term (although not the first one) is given correctly by the low energy theory which only keeps states near the Fermi surface. It is determined by the boundary condition of Eq. (3.4). Taking into account that we have set $v_F = 1$ in our previous equations, we see that the scaling dimension of the boundary condition changing operator, $b$ is given by:

$$x = \frac{1}{2} \left[ \frac{\delta(E_F)}{\pi} \right]^2. \quad (3.10)$$

Now suppose that the potential $V$ is attractive and produces a boundstate. In this case, the X-ray absorption intensity has 2 thresholds: a lower energy one corresponding to intermediate states in which the boundstate is occupied and a higher energy one corresponding to intermediate states in which it is empty. [See Figure 5.] These are separated by the binding energy of the boundstate, $E_B$. A crucial observation is that the boundstate wavefunction and energy decay exponentially and hence don’t contribute to the $O(1/l)$ terms in the energies. Hence the exponent at the first threshold is given by precisely the previous formulas, Eq. (3.10). To obtain the exponent at the second threshold, where the boundstate is empty, we just need to calculate the $1/l$ term in the energy. The calculation is precisely the same as before except that now there is one extra electron in the continuum, since it is not in the boundstate. The corresponding boundary condition changing operator in this case has no matrix element to the groundstate, $|AB:0 \rangle$ so the leading term in Eq. (2.3) comes from the excited state with one extra electron at the Fermi surface. The next available state at the Fermi surface has wave-vector $(\pi/2 - \delta(E_F))/l$, so:

$$\Delta E \rightarrow \Delta E + \epsilon \left[ k_F + \frac{\pi/2 - \delta(E_F)}{l} \right]$$

$$= \Delta E + E_F + v_F \frac{1}{l} \left( \frac{1}{2} \frac{\delta(E_F)}{\pi} \right)$$

$$= -\frac{1}{\pi} \int_0^{E_F} d\epsilon \delta(\epsilon) + E_F + v_F \frac{1}{l} \left[ \frac{\delta(E_F)}{\pi} - 1 \right]^2. \quad (3.11)$$

Hence the scaling dimensions for the filled and empty boundstate thresholds, $x_f$ and $x_e$ are:

$$x_f = \frac{1}{2} \left[ \frac{\delta(E_F)}{\pi} \right]^2, \quad x_e = \frac{1}{2} \left[ \frac{\delta(E_F)}{\pi} - 1 \right]^2. \quad (3.12)$$
These results for the X-ray exponent were all obtained earlier by Nozières and De Dominicis and Combescot and Nozières. An early calculation using bosonization was given by Schotte and Schotte. The result for the orthogonality exponent (ignoring boundstates) was obtained by Anderson. Nonetheless, the present approach, based on conformal transformation and calculation of the energy difference, has several advantages. Once the relationship to the energy difference is obtained, pages of complicated calculations reduce to a few lines. In particular, using previous approaches, it is only straightforward to obtain the relationship between exponents and phase shift in the Born approximation, where the phaseshift is proportional to the (weak) potential, \( V \). The simple derivation given above [Eq. (3.9)] establishes, via the connection with groundstate energies, that it is indeed precisely the phaseshift at the Fermi surface, \( \delta(\varepsilon_F) \), which determines the exponents, even when the potential is not weak. Furthermore, our new approach easily permits numerous generalizations to less trivial problems. For example, it can be used to calculate X-ray and orthogonality exponents in an interacting one-dimensional electron gas (Luttinger liquid). As long as the bulk interactions leave the electrons gapless, the low energy theory is a conformal field theory (free massless boson). While backscattering from the core hole potential leads to highly non-trivial renormalization, in the end the low-energy physics is governed by a simple conformally invariant boundary condition, for which the value of the scaling dimension, \( x \), can be determined from the finite-size energies, Eq. (2.4). Recent density matrix renormalization group work confirms the prediction for the exponent, \( x \), from both the finite-size energy and the matrix element, in Eq. (3.6). On the other hand, a direct numerical simulation of the Green’s function in Eq. (3.6) is a much more formidable task. We review another non-trivial application of this approach in the next section.

### IV. THE KONDO PROBLEM AND THE X-RAY EDGE SINGULARITY

Now we endow both conduction electrons and core electrons with a spin index, \( \alpha, c_{k\alpha}, b_{\alpha} \). As well as potential scattering there could also be a spin-spin interaction between core and conduction electrons:

\[
H \rightarrow H + b \frac{\sigma}{2} b^\dagger \sum_{k, k'} J_{k, k'} c^\dagger_k \sigma^\dagger_{k'} c_{k'}. \tag{4.1}
\]

(A sum over spin indices is implied.) As before, \([H, b b^\dagger] = 0\). When the core hole is present, it acts like an \( s=1/2 \) impurity spin:

\[
\vec{S}_{\text{imp}} = b \frac{\sigma}{2} b^\dagger. \tag{4.2}
\]

When it is absent the core level is spinless. Thus the X-ray absorption turns on a Kondo interaction, \( J_{k, k'} \). This problem appears considerably more difficult than the potential scattering case, discussed in the previous section, because the Kondo Hamiltonian contains non-trivial physics even without sudden switching. Assuming \( J \) is antiferromagnetic \( (> 0) \), it renormalizes to large values in the infrared. However, it has been shown that the infrared stable fixed
point corresponds to a conformally invariant boundary condition. From this solution of the Kondo problem we can determine X-ray edge and orthogonality exponents.

The conformally invariant boundary condition giving the infrared fixed point can be specified in terms of the finite size spectrum. We begin with free boundary conditions on both sides of a finite strip. This leads to a trivial spectrum. It is convenient to express this in terms of a (trivial) conformal embedding. Beginning with two Dirac fermions (one for each spin) we bosonize and introduce charge and spin bosons. The finite size spectrum can be expressed in terms of SU(2) Kac-Moody conformal towers with highest weight states of spin $j = 0, 1/2$. The reason for two SU(2)'s is that the underlying theory of 2 free Dirac fermions is equivalent to 4 free Majorana fermions and hence has SO(4) symmetry. Expressed in terms of SU(2) characters, the spectrum is:

$$Z_{\text{free, free}} = \chi_0 \chi_0 + \chi_{1/2} \chi_{1/2},$$

(4.3)

where the first and second factor come from the spin and charge sector respectively. The infrared Kondo fixed point corresponds to fusion with the $j = 1/2$ primary field in the spin sector. This fusion process is a conformal field theory representation of screening of the (s=1/2) impurity by the conduction electrons. The resulting spectrum is:

$$Z_{\text{Kondo, free}} = \chi_{1/2} \chi_0 + \chi_0 \chi_{1/2}.$$  

(4.4)

The energies of highest weight states, or scaling dimensions of primary operators, for spin $j$ and $SU(2)_k$ Kac-Moody algebra are given by:

$$x_{j,k} = \frac{j(j+1)}{2 + k}.$$  

(4.5)

The core hole operator, $b_\alpha$, takes the groundstate into the state with spin 1/2 and charge 0. (Only the charge of conduction electrons is relevant.) It has scaling dimension

$$x_{1/2,1} = \frac{1}{4}.$$  

(4.6)

So far we have only considered photoemission in which the core electron is ejected from the metal. Now we consider the case where instead the core electron is excited into the conduction band. Ignoring the eventual decay back into the core level (which occurs incoherently) the X-ray absorption intensity in this case is given by:

$$I(\omega) \propto \int dt e^{i\omega t} < b^\dagger_{\alpha}(t)c_{\delta}(t)c_{1/2}(0)b_\alpha(0) >.$$  

(4.7)

In principle (not worrying about possible selection rules in the X-ray absorption process), the core hole and extra conduction band electron can be in a singlet or triplet state. Different exponents are obtained for these two cases. We must calculate the dimension of the boundary condition changing operators $c^\dagger \partial b$ and $c^\dagger b$. These change the groundstate into a state with Kondo boundary conditions and quantum numbers $Q = 1, j = 1$ and $Q = 1, j = 0$ respectively. (We only count the charge of the conduction electrons.) The exponent $x$ is obtained from the lowest energy state with the right quantum numbers in the $Z_{\text{Kondo, free}}$ partition function. $Q = 1, j = 0$ corresponds to a primary field, of dimension

$$x_0 = \frac{1}{4},$$  

(4.8)

from Eq. (4.3), since $Q = 1$ corresponds to the $j = 1/2$ primary of a second $SU(2)_1$ KM algebra associated with charge. On the other hand, their is no primary with $j=1$ for $SU(2)_1$. This state is a descendent in the $Q = 1, j = 0$ product of conformal towers, with dimension:

$$x_1 = \frac{1}{4} + 1 = \frac{5}{4}.$$  

(4.9)

(It is a Mac-Moody descendent but a Virasoro primary, so Eq. (2.2) still applies.) The corresponding X-ray edge exponents are obtained from the usual formula, $\alpha = 1 - 2x$.

This calculation can be generalized to the k-channel Kondo problem in which the conduction electrons carry an additional flavour index, $c_{\alpha i}$, $i = 1, 2, 3, ... k$. The Kondo interaction with the core spin (which doesn’t carry a flavour index) is as in Eq. (4.1) with a diagonal sum over the flavour of the conduction electrons. The infrared fixed point for the multichannel Kondo problem has also been indentified as a conformally invariant boundary condition.

A
key step in this identification is a conformal embedding of $2k$ Dirac fermions. One first uses non-abelian bosonization to represent the $2k$ fermions by a charge boson and a $SU(2k)_1$ Wess-Zumino-Witten model. Then one uses the conformal embedding:

$$SU(2k)_1 \to SU(2)_k \times SU(k)_2,$$

which was worked out by Altshuler, Bauer and Itzykson. [The $SU(k)_2 \times U(1)$ theory is actually equivalent to $SP(k)_1$, but we won’t use this result here.] The finite size spectrum with Kondo-free boundary conditions is again obtained by fusion with the $j=1/2$ conformal tower in the $SU(2)_k$ theory. The photoemission exponent is given by the dimension of $b_\alpha$, with $j=1/2$, $Q=0$. From Eq. (4.10), this is:

$$x = \frac{3/4}{2 + k}. \quad (4.11)$$

The operators giving the X-ray exponents for the case where the core electron goes into the conduction band, $c_i^{\dagger} \sigma b$ and $c_i b$ have $j=1$ or 0 respectively, $Q=0$ and transform under the fundamental representation of $SU(k)$. From the fusion transformation on the free fermion spectrum, expressed using the conformal embedding, it can be checked that the corresponding primaries occur in the $Z_{Kondo}$, free spectrum. The scaling dimensions are:

$$x = \frac{1}{4k} + \frac{k^2 - 1}{2(2 + k)} + \frac{j(j + 1)}{2 + k}, \quad (j = 0 \text{ or } 1). \quad (4.12)$$

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