X-Ray Singularities and Boundary Conformal Field Theory

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I discuss a few points regarding the use of conformal field theory to study quantum impurity problems. In particular, I examine the problem of x-ray adsorbtion in metals using a boundary conformal field theory approach.

INTRODUCTION

The x-ray absorption spectrum of metals displays a singularity as a function of the energy of the incident x-ray. At a first glance, this should seem pretty reasonable; the x-ray kicks a core electron from a lower filled shell into the conduction band, which costs some energy E_0. So naively we may expect that the absorption intensity will be zero for $E < E_0$, and to suddenly jump to a finite value for $E \geq E_0$. For $E > E_0$, power law decay is observed. Schematically, we can write [1]

$$I(E - E_0) \propto \frac{\theta(E - E_0)}{(E - E_0)^{\alpha}} \tag{0.1}$$

Explaining this power law and obtaining the x-ray edge exponent is the goal of this paper.

There are a few things going on in the x-ray absorption process which we need to understand to write down an effective model. We will essentially consider the conduction electrons to be a free-fermion gas, so we neglect the interactions. This can be justified from the point of view that normal metals are described by fermi liquid theory, so many of their properties are similar to the free fermi gas with some renormalized couplings. However it is not clear to me to what extent the interactions in any real system will spoil this picture. At the very least it seems that on long time scales the decoherence will play an important role. Perhaps the results here should be considered a good approximation within some window $t_\epsilon \ll t \ll t_{\text{decoherence}}$ where t_ϵ is the (very short) time scale associated with the 'switching on' of the impurity potential and the decoherence time is inversely proportional to the interaction strength between different angular momentum channels.

When the x-ray kicks out the core electron, it leaves behind a hole which creates a potential felt by the conduction electrons. The physical quantity of interest is therefore the response of the conduction electrons to the sudden switching on of this impurity potential. A simple model introduced by Nozieres *et.al.* [2] to study this problem is to describe the conduction electrons by the following Hamiltonian

$$H = \sum_k \epsilon_k a_k^\dagger a_k + E_0 b^\dagger b + \sum_{k,k'} V_{k,k'} a_k^\dagger a_{k'} b b^\dagger \tag{0.2}$$

Here ϵ_k is the dispersion relation for free electrons, E_0 is the (constant) energy associated with the presence of the core electron, and b is the core electron annihilation operator. The last term describes the interaction between the conduction electrons and the core hole. A crucial fact is that the *core electron number* $b^\dagger b$ commutes with H, so the Hilbert space separates into two sectors where the core electron is either present or absent. In the former case the conduction electrons are completely free, and in the latter case they experience the scattering potential $V_{kk'}$.

The absorption intensity is given by the dynamical structure factor $S(q, \omega)$ (see *e.g.* [3]), which in this case is the fourier transform of the two point function of the operator which simultaneously creates the core hole and a conduction electron

$$S(k - k', \omega) = \int dt\ e^{i\omega t} \langle T a_k^\dagger(t) b(t) b^\dagger(t') a_{k'}(t') \rangle \tag{0.3}$$

The main point of this paper is to show that the behavior of this function is related to the difference of ground state energies of a finite size system with boundary conditions determined by the presence or absence of the core electron. The following techniques were developed mostly by Affleck and Ludwig in a series of papers, here we follow [4]

GENERALITIES OF CONFORMAL MAPPINGS AND BOUNDARY CONDITIONS

A fundamental role in quantum impurity problems is played by operators which change the boundary conditions, which we shall see applies to the core hole-conduction electron creation operator. Therefore, we first develop the general formalism to calculate scaling dimensions of such operators. First we expand in spherical harmonics to formulate the problem in one (half) spatial dimension ($r \geq 0$) and one time dimension; for simplicity we keep only the s-wave, although in general we have multiple angular momentum channels. In terms of the complex coordinate $z = t + ir$, our system lives in the upper half of the complex plane.

Recall that for a scale invariant system, correlation functions decay algebraically

$$\langle O(t_1) O^\dagger(t_2) \rangle \propto \frac{1}{(z_1 - z_2)^{2x_O}} \tag{0.4}$$

where x_O is the scaling dimension of the operator O. Under a conformal transformation, the correlation functions are multiplied by the Jacobian of the transformation [5]

In particular, under the transformation which maps the upper half plane to an infinite strip $z = le^{\frac{\pi w}{l}}$ with $w = u + iv, 0 \leq v \leq l$ we can find

$$\langle O(u_1)O^\dagger(u_2)\rangle = \frac{1}{\left[\frac{2l}{\pi}\sinh\frac{\pi}{2l}(u_1-u_2)\right]^{2x_O}} \tag{0.5}$$

There is one important thing missing from these expressions. In view of the hints that the boundary conditions will play an important role, we should also specify with respect to which boundary condition we are taking the ground state expectation value. If we denote the grond state for a particular boundary condition as $|A\rangle$, then what we really want to calculate are quantities $\langle A|O(u_1)O^\dagger(u_2)|A\rangle$. Actually since we are working in a strip geometry, there are two boundary conditions corresponding to the top and the bottom of the strip.

In addition to expression 0.5, we can calculate this two point function by inserting a complete set of states and using the fact that $O(t) = e^{iHt}Oe^{-iHt}$ to obtain

$$\langle AA|O(u_1)O^\dagger(u_2)|AA\rangle = \sum_n |\langle AA|O|n\rangle|^2 e^{-E_n(u_2-u_1)} \tag{0.6}$$

where the sum over n includes states with all possible boundary conditions and E_n is the energy of state n relative to the ground state energy E^0_{AA}.

Now *if* O is an operator which changes the boundary condition on the bottom of the strip from A to B (note that the conformal transformation maps the real axis to the real axis, so these operators always lie on the bottom of the strip), then we will have

$$\langle AA|O(u_1)O^\dagger(u_2)|AA\rangle \propto e^{-(E^0_{BA}-E^0_{AA})(u_2-u_1)} \tag{0.7}$$

However by expanding 0.5 for $u_1 - u_2 \gg l$ we obtain

$$\langle AA|O(u_1)O^\dagger(u_2)|AA\rangle \propto e^{-\pi x(u_2-u_1)/l} \tag{0.8}$$

Therefore we can identify the scaling dimension of the operator O with the difference in ground state energies corresponding to the different boundary conditions

$$x = \frac{l}{\pi}(E^0_{BA} - E^0_{AA}) \tag{0.9}$$

One last caveat: this equation is valid if the operator O produces the ground state with b.c. BA from AA. In general though it may produce the j'th excited state of the system with b.c. BA, in which case 0.9 is modified to

$$x = \frac{l}{\pi}(E^j_{BA} - E^0_{AA}) \tag{0.10}$$

X-RAY EDGE EXPONENT

Now that we have set up the general formalism, we need to show that the x-ray problem falls into this class of categories and determine the energy difference. This involves some theoretical machinery known as bosonization, for which there are many references available (also discussed in [3]). We will only need a few results, which I quote here. The key identity is that the fermion field ψ can be represented in terms of a bosonic field ϕ as

$$\psi \propto e^{i2\sqrt{\pi}\phi} \tag{0.11}$$

Near the Fermi surface, the kinetic part of the Hamiltonian becomes (with v_f set to 1)

$$-i\psi^\dagger\partial_x\psi \to (\partial_x\phi)^2 \tag{0.12}$$

The interaction term is bosonized as

$$\delta(x)V\psi^\dagger\psi bb^\dagger \to -\delta(x)\frac{V}{\sqrt{\pi}}\partial_x\phi bb^\dagger \tag{0.13}$$

so that the Hamiltonians with the core hole absent or present can be written respectively as

$$\begin{aligned} H_0 &= (\partial_x\phi)^2 \\ H_1 &= \left(\partial_x\phi - \frac{V}{2\sqrt{\pi}}\delta(x)\right)^2 \end{aligned} \tag{0.14}$$

We see that H_1 can be written in the same form as H_0 in terms of a shifted field $\tilde{\phi} = \phi - \frac{V}{4\sqrt{\pi}}\text{sgn}\,(x)$ [8]. Then from 0.11 we see that adding the interaction produces a constant phase shift $\psi_{\text{out}} = e^{2i\delta}\psi_{\text{in}}, \delta = -V/2$, which is a boundary condition on the field ψ.

One way to calculate the correlation function in 0.3 is to find a unitary operator which satisfies $U^\dagger H_0 U = H_1$. People [6] have done this, and they obtain:

$$\langle b^\dagger(t)\psi(t,0)\psi^\dagger(0,0)b(0)\rangle \propto \frac{1}{t^{(1-\delta/\pi)^2}} \tag{0.15}$$

The integral 0.3 is a little tricky but we can see that the dependence on the energy (frequency) yields the exponent in 0.1: $\alpha = 2(\delta/\pi) - (\delta/\pi)^2$.

We would like to use the formalism of Section II to obtain these results. Due to the slightly technical nature of the calculations, I just sketch the main ideas and present the reuslts. To calculate the energy levels we put the system in a finite length $x \in [-l, l]$ and calculate the spectrum for a given choice of boundary conditions. Here it seems that the important thing is the difference in energies when the boundary conditions change, so that we are free to choose the starting boundary conditions. We choose a boundary conditions for the fermions such that the boson field satisfies

$$\phi(-l) - \phi(l) = \sqrt{\pi}n, n = 0, \pm1, \pm2, \ldots \tag{0.16}$$

This boundary condition has a simple interpretation: the bosonized form of the normal ordered density field $:\psi^\dagger(x)\psi(x):$ is just $-\frac{1}{\sqrt{\pi}}\partial_x\phi$. The total number of fermions is then

$$-\frac{1}{\sqrt{\pi}}\int_{-l}^{l} dx\ \partial_x\phi(x) = \frac{1}{\sqrt{\pi}}\left(\phi(-l)-\phi(l)\right) \qquad (0.17)$$

Thus we see that n just counts the number of number of electrons ($n<0$ counts holes) relative to the filled fermi sea.

The free bosonic fields ϕ have mode expansions in terms of creation and annihilation operators, however there is a subtle yet crucial necessity of including the zero modes. When taken properly into account, the spectrum of the finite size system is found to be

$$E^n_{AA} = \frac{\pi}{l}\left(-\frac{1}{24}+\frac{1}{2}n^2+\sum_{m=1}^{\infty} m n_m\right) \qquad (0.18)$$

where n is the n appearing in the b.c. 0.16 and n_m is the occupation number for the m'th mode. We can understand this spectrum heuristically without knowing the technical details: particle-number-conserving excitations of a one dimensional fermion system can always be written in terms of density excitations, which correspond to the boson modes m. Raising the total fermion number by one also costs energy, which is counted by n. To obtain the constant term, we would need to actually do the calculation. This yields a ground state energy $E^0_{AA} = -\pi/24l$.

Now we act with the b.c. changing operator which creates the phase shift δ. This modifies the boundary condition on the boson field to $\phi(-l)-\phi(l) = \sqrt{\pi}(n-\delta/\pi)$. The spectrum in this case is the same as 0.18 with the replacement $n \to (n-\delta/\pi)$.

$$E^n_{BA} = \frac{\pi}{l}\left(-\frac{1}{24}+\frac{1}{2}(n-\delta/\pi)^2+\sum_{m=1}^{\infty} m n_m\right) \qquad (0.19)$$

To obtain the final result, we observe that the boundary changing operator $b\psi^\dagger$ adds an extra electron. Hence we take $n=1$ to obtain the energy difference and thus the scaling dimension

$$x_{b\psi^\dagger} = \frac{l}{\pi}(E^1_{BA}-E^0_{AA}) = \frac{1}{2}(1-\delta/\pi)^2 \qquad (0.20)$$

Then since $\langle b^\dagger(t)\psi(t,0)\psi^\dagger(0,0)b(0)\rangle \propto t^{-2x_{b\psi^\dagger}}$ we recover the result promised earlier. Again, to make a connection with experiment recall that this exponent is exactly that which appears in x-ray absorption intensity measurements.

CONCLUSION

We have learned that the scaling dimension of an operator which changes the boundary conditions in a conformally invariant theory is related to the difference in ground state energies in the different boundary conditions. We argued that this formalism is applicable to x-ray absorption in metals using a simple model Hamiltonian and bosonization. Finally, we 'calculated' the finite size spectrum to show that the results obtained by this method agree with known results obtained in other ways.

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[7] I. Affleck, "Quantum Impurity Problems in Condensed Matter Physics," 0809.3474, http://arxiv.org/abs/0809.3474.

[8] $\partial_x \mathrm{sgn}\ x = 2\delta(x)$