The Fermi edge singularity in the SU(N) Wolff model

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The low temperature properties of the SU(N) Wolff impurity model are studied via Abelian bosonization. The path integral treatment of the problem allows for an exact evaluation of low temperature properties of the model. The single particle Green’s function enhances due to the presence of local correlation. The basic correlation function such as the charge or spin correlator are also influenced by the presence of impurity, and show local Fermi liquid behaviour. The X-ray absorption is affected by the presence of local Hubbard interaction. The exponent is decreased (increased) for repulsive (attractive) interactions.

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I. INTRODUCTION

Local interactions have played an important role in explaining the behaviour of localized impurities, and in understanding the effect of electron correlation in lattice theories. The most studied magnetic impurity models are the Anderson and Kondo model, including their various generalizations. Their local Fermi or non-Fermi liquid behaviour in the low temperature regime is inferred from Bethe ansatz method, but dynamical properties are still very difficult to be calculated. Beyond the reliable renormalization group calculations, one is left with bosonization to gain insight into the low energy properties of such models.

One of the simplest description of a single impurity in a non-magnetic metal is based on the Wolff model, where electron correlation is still present. Also it is the basis of studying the effect of Coulomb interaction on resonant tunneling through a single quantum level. The model consists of conduction electrons interacting with each other solely at the origin through the Hubbard interaction. It is related to the Hubbard model in the same way as the single impurity Anderson model is related to its periodic version.

Several extensions of this model are possible including extended interactions or by changing the properties of conduction electrons. In the present work we study a most natural generalization of the usual Wolff model: we consider fermions with SU(N) spin index or alternatively we take the ensemble of spin and orbital degrees of freedom into account by the N index instead of the usual two-valued spin index. The additional degrees of freedom can be realized through orbital degeneracy, for example, as in Mn oxides. As a result, the additional degrees of freedom can be called flavour or color index. In similar models, the inclusion of orbital or flavour index led to non-Fermi liquid behaviour, such as the two channel Kondo model, or enriched our picture concerning the Mott-Hubbard transition as in the SU(N) Hubbard model.

The purpose of the present investigation is to see, how the interaction between N different species of electrons at a single site influence the low energy properties of the system. In the SU(N) Hubbard model with one particle per site, the Mott phase is reached at a finite value of the Hubbard interaction for N>2, as opposed to the zero critical interaction for the SU(2) case. In the SU(2) Wolff model, the crossover to strong coupling region is predicted to be symmetric with respect to the sign of U. Here we shall see how this condition is modified for SU(N) symmetry. The use of Abelian bosonization allows for an exact evaluation of the basic correlation functions, which show the instability toward local magnetic moment formation (i.e. Kondo regime), as the interaction parameter is increased. The critical interaction for repulsive U is independent of the value of N, but for attractive interaction its value is suppressed by 1/(N-1). The low energy behaviour of the system is characterized by a local Fermi liquid, obeying the well-known Fermi liquid relations (such as the Korringa relations) of the Anderson impurity model.

The X-ray response of the SU(N) Wolff model is evaluated with the use of boundary condition changing operators and is qualitatively similar to a system with correlated electrons over the whole lattice (namely the Hubbard model). The exponent characterizing the scaling dimension of the deep level electrons decreases with increasing Hubbard interaction.
II. FORMALISM, MODEL HAMILTONIAN

The Hamiltonian describing \( N \) different species of electrons interacting only at the origin is given by:

\[
H = \sum_{m=1}^{N} \left[ -iv \int_{-\infty}^{\infty} dx \Psi_m^+(x) \partial_x \Psi_m(x) + E : \Psi_m^+(0) \Psi_m(0) : + \frac{U}{2} \sum_{n=1, n \neq m}^{N} : \Psi_n^+(0) \Psi_n(0) : : \Psi_m^+(0) \Psi_m(0) : \right],
\]

and only the radial motion of the particles is accounted for by chiral (right moving) fermion fields. The model can be bosonized via

\[
\Psi_m(x) = \frac{1}{\sqrt{2\pi}} e^{i\sqrt{4\pi} \Phi_m(x)},
\]

and the bosonized Hamiltonian takes the form as

\[
H = v \int_{-\infty}^{\infty} dx \sum_{m} (\partial_x \Phi_m(x))^2 + \frac{E}{\sqrt{\pi}} \sum_{n} \partial_x \Phi_n(0) + \frac{U}{2\pi} \sum_{m,n=1, n \neq m}^{N} \partial_x \Phi_m(0) \partial_x \Phi_n(0).
\]

By introducing charge and spin fields as

\[
\Phi_c(x) = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} \Phi_m(x),
\]

\[
\Phi_{n,s}(x) = \frac{1}{\sqrt{n(n+1)}} \left( \sum_{m=1}^{n} \Phi_m(x) - n \Phi_{n+1}(x) \right),
\]

\( n = 1 \ldots N - 1 \), the Hamiltonian separates into different sectors: the spin sector is described by \( N - 1 \) identical decoupled bosonic modes, and the charge sector transforms into a similar massless bosonic mode as

\[
H_s = \sum_{m=1}^{N-1} \left[ v \int_{-\infty}^{\infty} dx (\partial_x \Phi_{m,s}(x))^2 - \frac{U}{2\pi} (\partial_x \Phi_{m,s}(0))^2 \right],
\]

\[
H_c = v \int_{-\infty}^{\infty} dx (\partial_x \Phi_c(x))^2 + E\sqrt{\frac{N}{\pi}} \partial_x \Phi_c(0) + \frac{(N-1)U}{2\pi} (\partial_x \Phi_c(0))^2.
\]

Since the Hamiltonians describe scattering of massless bosons on a point-like “impurity”, the bosonic correlation functions can readily be calculated. Hence in the followings it suffices to study the single Hamiltonian

\[
H = v \int_{-\infty}^{\infty} dx (\partial_x \Phi(x))^2 + E\partial_x \Phi(0) + U(\partial_x \Phi(0))^2\]

\( \Phi(x) \) the “space coordinate” with \( \Phi(x) \) and the momentum conjugate to \( \Phi(x) \) from the commutation relation of the \( \Phi \) field with itself \((\Phi(x), \Phi(y)) = i\text{sgn}(x - y)/4\). The obtained action is for chiral bosons, similar to the one investigated during the study of edge states. Then the generating functional is obtained as

\[
Z \sim \int D\Phi \exp(S(\Phi))
\]

with

\[
S = \int_{0}^{\beta} d\tau \left[ -i \int_{-\infty}^{\infty} \partial_x \Phi(x, \tau') \partial_x \Phi(x, \tau') - v \int_{-\infty}^{\infty} dx (\partial_x \Phi(x, \tau'))^2 - E\partial_x \Phi(0, \tau') - z(\tau')^2 - 2z(\tau') \sqrt{-U} \partial_x \Phi(0, \tau') \right] +
\]

\[ + i\mu(\Phi(0, \tau) - \Phi(0, 0)), \]
where the interaction term was decoupled by a time dependent Hubbard Stratonovich field $z(\tau)$. For $\mu = 0$, it gives the partition function, for $\mu = \sqrt{4\pi/N}$ it equals to the local Green’s function at the impurity site ($G(\mu) = Z(\mu)/Z(0)$) coming from either the charge or one of the spin sectors. After Fourier transforming the fields as

$$
\Phi(x, \tau) = \sum_{m,q} \exp(-i\omega_m \tau - iqx) \Phi(m,q),
$$

(11)

$$
z(\tau) = \sum_m \exp(-i\omega_m \tau) z(m),
$$

(12)

$\omega_m = 2m\pi T$ is the bosonic Matsubara frequency, the action is transformed to

$$
S = \sum_p \left( -iQ - viq^2 \right) \Phi(0,q) - \sum_p z(-m)z(m) + 2i\sqrt{-U} \sum_p z(-m)q \Phi(p) + \sum_p i\mu (\exp(-i\omega_m \tau) - 1) \Phi(p),
$$

(13)

where $p = \{m,q\}$. The $\Phi$ field can be integrated out, and the effective action reads as

$$
S_{eff} = -\sum_m z(-m)z(m) + \frac{1}{2} \sum_p \eta(0) G\eta(p),
$$

(14)

where

$$
G^{-1} = vq^2 + iq\omega_m,
$$

(15)

$$
\eta(p) = iEq\delta_{m,0} + 2i\sqrt{-U} z(-n)q + i\mu (\exp(-i\omega_m \tau) - 1).
$$

(16)

Integrating over the $z$ field gives for the free local Green’s function (where one has to substitute $\mu = \sqrt{4\pi/N}$) in the large $\tau$ limit

$$
G(\tau, 0) \sim \exp \left( -\frac{\mu^2 T}{2} \sum_p \frac{1 - \cos(\omega_m \tau)}{vq^2 + iq\omega_m} \right) \sim \left( \frac{T}{\sin(\pi T \tau)} \right)^{2/4\pi}.
$$

(17)

As to the $U$ dependent part, it is obtained as

$$
G_{corr}(\tau, 0) \sim \exp \left( -U\mu^2 T \sum_m |\gamma(\omega_m)|^2 \frac{1 - \cos(\omega_m \tau)}{1 + UL(\omega_m)} \right) \sim \left( \frac{U_0}{U_0 + 2\pi U} \right)^{\mu^2/2\pi}
$$

(18)

in the large $\tau$ limit with

$$
\gamma(\omega_m) = \sum_q \frac{2}{i\omega + vq},
$$

(19)

$$
L(\omega_m) = \sum_q \frac{2q}{i\omega + vq},
$$

(20)

$U_0 = \pi v/2n_0$, $n_0$ is the average density per spin channel in the homogeneous case. For $\mu = 0$, the change of the free energy of Eq. (8) in the presence of $U$ is evaluated as

$$
F = T \sum_m \ln(1 + UL(\omega_m)) - \frac{1}{4} \frac{E^2 L(0)}{1 + UL(0)},
$$

(21)

which gives for the total specific heat

$$
C(T) = \frac{\pi T}{6v} \frac{U_0}{U_0 + 2\pi U}.
$$

(22)

The presence of local Hubbard $U$ enhances the Sommerfeld coefficient for attractive interaction, and decreases it for repulsive one.

Another way to derive the same results would have been to follow the diagrammatic approach. Due to the presence of a single scattering center, the determinations and solution of the corresponding Dyson equation would have led to the same exact expressions for the Green’s function and free energy.
III. CORRELATION FUNCTIONS OF THE SU(N) WOLFF MODEL

By inserting the appropriate parameters into these results, we are able to determine the low temperature-low energy properties of Eq. (1). First of all, the specific heat including the impurity contribution reads as

\[ C_W(T) = \frac{\pi T}{6v} \left( \frac{U_0}{U_0 + (N-1)U} + \frac{(N-1)U_0}{U_0 - U} \right), \]

as opposed to its normal state value \( C(T) = \frac{N\pi T}{6v} \). In Fig. 1, we show the Sommerfeld coefficient, \( C_W(T)/C(T) \) as a function of \( U \). The main quantity of interest is the local electron propagator. Putting the above results together, one finds for the single particle electron Green’s function at the impurity site in the \( 0 \ll \tau \ll 1/T \) limit

\[ G_m(\tau) = -\langle \Psi_m(\tau,0)\Psi_m^+(0,0) \rangle = -\frac{T}{\sin(\pi T\tau)} \frac{U_0^2}{(U_0 + (N-1)U)^{2/N} (U_0 - U)^{2-2/N}}, \]

where \( U_0 = \pi v/2n_0 \) is the critical Hubbard interaction in the SU(2) Wolff impurity model, \( n_0 \) is the average density in the homogeneous system. For general \( N>2 \), however, the critical value of \( U \) is suppressed by \( 1/N \) as seen from the denominator of Eq. (24). When \( U \) exceeds this value, we expect local magnetic moment formation, and bosonization breaks down\(^{5,6}\). The one-body potential, \( E \) does not appear in Eq. (24) to leading order in \( \tau \), only renormalizes the \( \tau^{-2} \) correction. The \( \tau \to \infty \) limit determines the low energy behaviour of the local density of states. It remains constant, i.e. Fermi liquid like, but enhances due to the presence of local Hubbard \( U \), as can be seen in Fig. 1.

![FIG. 1: The Sommerfeld coefficient (left panel) and the density of states at the Fermi energy (right panel) are plotted as a function of local Hubbard \( U \) for \( N = 2, 3, 4 \) and \( 8 \) from edge to center. As is seen, the critical value of the interaction depends on its sign, namely \( U_c = U_0 \) for repulsion and \( -U_c = U_0/(N-1) \) for attraction.](image)

In the SU(2) case, the Sommerfeld coefficient and the local residual density of states have the same form, because the Hamiltonian splits into two sectors somehow corresponding to the original two species of electrons. For \( N>2 \), however, we have \( N \) different species, but only have two distinct sectors with different weights: \( N-1 \) for the spin sector as opposed to the single charge sector, resulting in different behaviour in the specific heat and Green’s function.

The other, \( \tau \to 0^+ \) limit determines the particle density as

\[ G_m(\tau \to 0^+) = n_0 - \frac{\sqrt{NE}}{U_0 + (N-1)U}. \]

The computation of the local density-density correlation function leads to

\[ \chi_{\text{charge}}(\omega) = \frac{N\chi_0(\omega)}{1 + (N-1)U\chi_0(\omega)}, \]

where \( \chi_0(\omega) \) is the local density correlation function in the homogeneous case, \( \chi_0(0) = 1/U_0 \). Due to Ward identity\(^{18}\), the exact susceptibility is identical to the RPA result in the SU(N) case as well\(^{16}\). The above result can further
be verified by the fluctuation-dissipation theorem. Namely, the charge response function is related to the charge correlator by $\langle n^2 \rangle - \langle n \rangle^2 = T \chi_{\text{charge}}$. Here $n$ is the charge density, and its momenta can be obtained by deriving the partition function with respect to $E$. At low frequency, where bosonization is expected to be valid, it is well approximated by

$$\chi_{\text{charge}}(\omega) \approx \frac{N}{U_0 + (N - 1)U} + i \frac{\omega}{2\pi v^2 (U_0 + (N - 1)U)^2}. \quad (27)$$

Its frequency dependence is shown in Fig. 2 for $N=4$ and for various values of $U$. As is seen, the low frequency part is influenced more significantly for attractive interactions. As $U$ decreases below zero, its imaginary part becomes a Dirac delta function at the origin, signaling the breakdown of bosonization. Similarly, the susceptibility in the spin sector can be evaluated as

$$\chi_{\text{spin}}(\omega) = \frac{(N - 1)\chi_0(\omega)}{1 - U\chi_0(\omega)}, \quad (28)$$

which again reduces to the RPA results. This is $N$-1 times the spin susceptibility of the SU(2) Wolff model, stemming from the N-1 massless bosonic modes in the spin sector. The low energy spin response is evaluated as

$$\chi_{\text{spin}}(\omega) \approx \frac{N - 1}{U_0 - U} + i \frac{\omega}{2\pi v^2 (U_0 - U)^2}. \quad (29)$$

Compared to Eq. (27), for repulsive interaction the spin response increases faster in energy than the charge one due to the denominator Eq. (29), as can be checked directly in Fig. 2. Similar results were found in the SU(2) case. Exactly at the critical $U$ deduced from the Green’s function, the charge or spin susceptibility diverges, signaling a possible transition or crossover to strong coupling case.

IV. X-RAY ABSORPTION

The basic Hamiltonian describing our previously studied system and deep level electrons ($d$) is given by

$$H_{\text{deep}} = H + E_0 \sum_{n=1}^{N} d_n^+ d_n + V \sum_{m,n=1}^{N} \Psi_m^+(0) \Psi_m(0) d_n^+ d_n,$$  

(30)
and the coupling of the metal to the X-ray field, describing the transfer of a deep level electron to the conduction band is given by

\[ H_X = W \sum_m \Psi_m^+(0)d_m e^{-i\omega t} + h.c. \]  

(31)

The quantity of interest is the X-ray scattering rate, which is written in the form of the Fermi golden rule as

\[ I(\omega) = 2|W|^2 \text{Im} S(\omega), \]

(32)

\[ S(t) = \langle d_m^+(t)\Psi_m(t,0)\Psi_m^+(0,0)d_m(0) \rangle. \]

(33)

As is well known, the number of d electron is conserved ([d^+d, H_{deep}]), it is not a truly dynamic quantity, so one can reformulate the problem in terms of time dependent core-hole potential. After bosonization, the core level electron couples solely to the charge sector as

\[ H_{deep} = H + E_0 \sum_m d_m^+d_m + V \sqrt{\frac{N}{\pi}} \sum_m d_m^+d_m \partial_x \Phi_c(0). \]

(34)

From now on we focus on the excitation of a single d_m electron, and forget about the presence of the other deep level particles. They can only renormalize the threshold frequency but not the exponent what we are interested in. Following the strategy of Schotte and Schotte, we introduce two Hamiltonians, one when there is no hole (H_I = H) and another, when conduction electrons feel a scattering potential (H_F = H + E_0 + V \sum_m \Psi_m^+(0)\Psi_m(0)). Similarly to the case of a normal Fermi liquid, there exist a unitary transformation (the boundary condition changing operator) relating the two Hamiltonians as

\[ H_F = U^+ H_I U, \]

(35)

\[ U = \exp\left(\frac{2\delta}{\sqrt{\pi}} \Phi_c(0)\right), \]

(36)

where

\[ \delta = \frac{\sqrt{NV}}{2v} \frac{U_0}{U_0 + (N-1)U}. \]

(37)

With the use of these, the d electron Green’s function can be calculated from

\[ D(t) = -\langle d_m(t)d_m^+ \rangle = \langle U^+(t)U \rangle. \]

(38)

Its time dependence can easily be determined from the asymptotics of the correlator of the charge sector using Eqs. 17 and 18 as

\[ D(t) \sim t^{-(\delta/\pi)^2}. \]

(39)

As is seen, the time decay implies non-Fermi liquid behaviour, characteristic to the X-ray problem. The Fourier transform of the deep level electron can be obtained, from which the d-electron density of states follows as

\[ -\text{Im} D(\omega) \sim \frac{\sin(\pi(1 - (\delta/\pi)^2))}{|\omega - E_0|^{1-(\delta/\pi)^2}}. \]

(40)

The original Dirac delta density of states situated at E_0 transforms into a power-law divergence with a finite tail. Compared to that of a normal metal without Wolff impurity, the exponent δ decreases for large number of channels, while in a normal metal the exponent grows with \(\sqrt{N}\). Also at fixed N, repulsive (U > 0) interaction suppresses δ, while in the attractive case the exponent increases rapidly. It is worth mentioning, that since only the charge channel is involved in the X-ray Hamiltonian, the singularity present in the Green’s function (Eq. 24) is absent here for repulsive interactions. The two-particle Green’s function, S(t) can be calculated similarly to D(t), namely

\[ S(t) = \langle U(t)\Psi_m(t,0)\Psi_m^+(0,0)U^+ \rangle. \]

(41)

Using the asymptotic formula for the correlator of the Φ field, it reads as

\[ S(t) \sim t^{-((1-\delta/\pi)^2+N-1)/N}. \]

(42)

Since only the charge degree of freedom is involved in the conduction-deep level electron interaction, the scattering phase shift comes with an additional factor of 1/N, overwhelmed by the spin degrees of freedom with zero phase shift.

Similar phenomenon occurs in the X-ray edge absorption, when we extend the local correlation of our model to the whole lattice, namely in the SU(2) Hubbard model. The X-ray exponent was found to decrease for repulsive interaction, and increase for attractive one. We believe, that the qualitative dependence of local quantities on electron correlation is well described by the single impurity Wolff model.
V. CONCLUSIONS

We have studied the low energy properties of the SU(N) Wolff impurity model via Abelian bosonization and the path integral treatment of the generating functional. The system decouples into N-1 identical spin sectors and one single charge sector, involving only chiral bosonic fields. The single particle Green’s function possesses Fermi liquid type asymptotics, but its weight can strongly be modified by the local Hubbard interaction. The spin and charge sectors become inequivalent, signaling a transition to the strong coupling phase at \(-U_0/(N-1)\) for attraction and at \(U_0\) for repulsion. For small interaction, the system exhibits local Fermi liquid behaviour\(^2\) in all evaluated quantities.

When interaction with deep level electrons is considered, the X-ray response of the model can be explored. It can be formulated similarly to the original work of Schotte and Schotte\(^{19}\), exploiting the fact, that the number of deep level electrons is a conserved quantity. The deep level electron Green’s function can be obtained using the boundary condition changing operators\(^{14}\), reflecting the influence of both the local Hubbard interaction and the presence of N species of electrons. The X-ray exponent is decreased (increased) for repulsive (attractive) Hubbard interaction.

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