Toulouse Points and Non-Fermi Liquid States
in the Mixed Valence Regime of the Generalized Anderson Model

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We study the mixed valence regime of a generalized Anderson impurity model using the bosonization approach. This single impurity problem is defined by the $U = \infty$ Anderson model with an additional density-density interaction, as well as an explicit exchange interaction, between the impurity and conduction electrons. We find three points in the interaction parameter space at which all the correlation functions can be calculated explicitly. These points represent the mixed valence counterparts of the usual Toulouse point for the Kondo problem, and are appropriately named the Toulouse points of the mixed valence problem. Two of the Toulouse points exhibit the strong coupling, Fermi liquid behavior. The third one shows spin-charge separation; here, the spin-spin correlation functions are Fermi-liquid-like, the charge-charge correlation functions and the single particle Green function have non-Fermi-liquid behaviors, and a pairing correlation function is enhanced compared to the Fermi liquid case. This third Toulouse point describes the novel intermediate mixed valence phase we have previously identified. In deriving these results, we emphasize the importance of keeping track of the anticommutation relation between the fermion fields when the bosonization method is applied to quantum impurity problems.

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I. INTRODUCTION

The mixed valence problem is a classic problem in condensed matter theory. It describes an impurity with three configurations, having both charge and spin degrees of freedom, coupled to a conduction electron bath. It differs from the Kondo problem in that low lying local charge fluctuations coexist with local spin fluctuations. The Kondo problem has been studied by a variety of techniques, and is by now well understood. As long as the effective Kondo coupling is antiferromagnetic, the low energy behavior is described by a strong coupling, Fermi liquid fixed point. The mixed valence problem has also been studied extensively. A variational study by Varma and Yafet, and renormalization group studies of Haldane and Krishnamurthy et al. have all found that the low energy behavior of the mixed valence problem is described by a strong coupling, Fermi liquid fixed point. This fixed point is qualitatively similar to that of the Kondo problem, though quantities such as the Wilson ratio are modified. These works were followed by extensive studies on the proper description of the resulting Fermi liquid states of both the Anderson impurity and Anderson lattice problems. These later works used techniques ranging from Gutzwiller variational wavefunctions to the slave boson large N expansion. They have provided qualitative, and sometimes quantitative, understandings of the physical properties of the heavy fermion metals.

In a series of papers we have revisited the mixed valence problem in an attempt to identify metallic non-Fermi liquid phases in a two band extended Hubbard model. In the limit of infinite dimensions, this extended Hubbard model can be solved through a generalized Anderson impurity model with a self-consistent electron bath. This single impurity model is defined by the $U = \infty$ Anderson model with an additional density-density interaction, as well as an explicit exchange interaction, between the impurity and conduction electrons. Away from half-filling, the self-consistency condition implies that, the associated impurity problem is in the mixed valence regime over an extended range of densities. The persistence of the mixed valence behavior for the self-consistent impurity model associated with a lattice model in infinite dimensions is in fact quite general and is not restricted to the two band extended Hubbard model. For example, in the one band case, the average occupation of the impurity in the self-consistent
Anderson model is simply the lattice density, which is not very close to one (local moment regime) or zero (empty orbital regime) over a wide range of densities. This, together with our finding that away from half-filling the self-consistent conduction electron bath has a finite density of states at the Fermi level, imply that the classification of the fixed points in the mixed valence regime of the generalized Anderson impurity model with a regular electron bath also specifies the possible metallic phases of the extended Hubbard model in infinite dimensions. Of course, in general, the couplings of the effective Anderson model at the cutoff energy scale of the universal regime can be different from the bare atomic interactions, just like the Coulomb pseudopotential at the Debye temperature scale is different from the bare Coulomb interactions.

We studied the generalized Anderson impurity model by extending Haldane’s renormalization group scheme such that the local charge fluctuations and local spin fluctuations are treated on an equal footing. In the mixed valence regime, we found three, and only three, kinds of fixed points, which we termed the strong coupling, weak coupling, and intermediate phase, respectively. The strong coupling and weak coupling phases are the direct analogs of their counterparts in the Kondo problem. The intermediate phase is entirely new and occurs only in the mixed valence regime. Its existence came as a surprise. In this new phase, spin and charge excitations are separated. From the renormalization group analysis, it is expected that the spin-spin correlation functions remain to have the Fermi liquid form, while the charge-charge correlation functions and single particle Green function have an algebraic behavior with interaction-dependent exponents.

The renormalization group procedure is based on a Coulomb gas representation for the single impurity problem. As usual, the Coulomb gas analysis uses a dilute instanton expansion. In the strong coupling and intermediate phases, some of the fugacities flow towards strong coupling, and the behaviors of the correlation functions can only be inferred through “extrapolating” the scaling trajectories beyond the dilute instanton regime. For the intermediate phase, this procedure does not allow an explicit determination of the exponents. Finally, it is in principle possible that additional fixed points, not captured by the dilute instanton expansion, may occur. An example for the latter arises in the related, though qualitatively different, problem of tunneling through a point contact in a Luttinger liquid.

To address these issues, here we study the mixed valence regime of the generalized Anderson model at some particular values of the interactions where the model is exactly soluble (in the sense that will be made precise below). These points in the interaction parameter space are the mixed valence counterparts of the usual Toulouse point of the Kondo problem, and are naturally called the Toulouse points of the mixed valence problem. We identify all the possible Toulouse points using the bosonization approach. We construct an effective Hamiltonian, and determine the single particle, spin-spin, and charge-charge correlation functions, at each of these Toulouse points. There are two subtle aspects associated with these Toulouse points. First, at the Toulouse points some of the interactions are larger than the conduction electron bandwidth. This makes the interpretation of these Toulouse points subtle. We clarify this issue through a comparison with an atomic expansion of the original impurity Hamiltonian. Second, when applying the bosonization method to the mixed valence problem, it turns out to be essential to keep track of the anticommutation relation between the fermion fields. When properly understood, the solutions to the generalized Anderson model at these Toulouse points substantiate, and provide a simple physical picture for, the mixed valent phases we have identified through the renormalization group analysis.

Parallel to our previous works, an impurity problem defined by the $U = \infty$ Anderson model with additional screening channels have been studied using the numerical renormalization group method. Recently, two other groups have studied an exactly soluble point of that impurity model. They have reached conclusions very different from ours, and we will comment on the origin of these differences.

The setup of this paper is the following. In Sec. I, we review the construction of the Toulouse points in a context where the physics is well understood, the Kondo model. In Sec. II, we summarize the main results of our Coulomb gas analysis of the mixed valence regime of the generalized Anderson model, and set up the formalism for our Toulouse-point analysis. The Toulouse points are discussed in detail in the following sections. The Toulouse points discussed in Sec. IV and Sec. V lie deep in the strong coupling limit. That of Sec. VI describes the non-Fermi liquid, intermediate phase. There is one more point, presented in Sec. VII, which has an effective Hamiltonian corresponding to a rank-2 generalization of the Emery-Kivelson resonant level model associated with the two-channel Kondo problem. This effective Hamiltonian is not exactly soluble. We conclude with a comparison of our results with those of related works, and a discussion about realizing the intermediate phase in other models of strongly correlated electron systems. Two appendixes are included. Appendix A summarizes the bosonization procedure relevant to our discussion, with an emphasis on the Klein factors that keep track of the anticommutation relation between fermions of different spins. Appendix B substantiates the bosonization results presented in the main text with those of an atomic analysis of the original Hamiltonian.
II. TOULOUSE POINTS OF THE KONDO MODEL

In this section, we introduce the notation, and review the bosonization method, in the context where the physics is well understood, the anisotropic one-channel spin-$\frac{1}{2}$ Kondo model. We show that there are two values of $J_z$, the longitudinal component of the Kondo exchange interaction, at which the problem is exactly soluble [13]. One of these is the well-known Toulouse point [14], for which the effective Hamiltonian is the resonant-level model [21]. The other occurs at the infinite value for $J_z$. The effective Hamiltonian for this second Toulouse point is the spin-boson Hamiltonian [22,23] close to a vanishing spin-boson coupling.

The anisotropic Kondo problem describes a bath of spin-$\frac{1}{2}$ conduction electrons coupled to an impurity which can fluctuate between two states, $|\uparrow\rangle$ and $|\downarrow\rangle$. The Hamiltonian is

$$\begin{align*}
H &= \sum_{k\sigma} E_k c_{k\sigma}^\dagger c_{k\sigma} + H_\perp + H_\parallel \\
H_\perp &= \frac{J_z}{2} \sum_k X_{\sigma\sigma} c_{k\sigma}^\dagger(0)c_{k\sigma}(0) \\
H_\parallel &= \frac{J_x}{4} \sum_k (\sigma X_{\sigma\sigma}) (\sum_{\sigma'} \sigma' \bar{c}_{\sigma'}(0)c_{\sigma'}(0)) 
\end{align*}$$

(1)

Here, $c_{k\sigma}^\dagger$ describes a free conduction electron bath with energy dispersion $E_k$, and $c_{k\sigma}(r) = \frac{1}{\sqrt{N_{\text{site}}}} \sum_k e^{i\mathbf{k}\cdot \mathbf{r}} c_{k\sigma}^\dagger$. The impurity is located at $\mathbf{r} = 0$, and is locally coupled to the conduction electrons through an exchange interaction. $J_x$ and $J_z$ are the transverse and longitudinal components of this exchange interaction, respectively, and are allowed to take different values. In Eq. (1), we have written the impurity spin operators in terms of the Hubbard operators, $X_{\sigma\sigma} = |\alpha > < \beta|$, where $\alpha, \beta$ describes the two impurity configurations, $|\uparrow\rangle$ and $|\downarrow\rangle$. The following constraint

$$X_{\uparrow\uparrow} + X_{\downarrow\downarrow} = 1$$

(2)

supplements Eq. (1).

A. Bosonization

Given that the interaction occurs at $\mathbf{r} = 0$ only, we need to keep only the $S$–wave component of the conduction electrons. This $S$–wave component is defined on the radial axis, $r \in [0, +\infty)$, and can be further decomposed into an outgoing and an incoming components. In a standard fashion, we extend to the full axis, $x \in (-\infty, +\infty)$, by retaining only one chiral component, which we denote by $\psi_\sigma(x)$. We can then introduce a boson representation for the $\psi_\sigma(x)$ field [23]. The details of this procedure is given in Appendix A. At the origin, $\psi_\sigma(0) = F_{\sigma}^\dagger \frac{1}{\sqrt{2\pi a}} e^{i\Phi_\sigma}$.

Here, $a$ is a cutoff scale which can be taken as a lattice spacing. $\Phi_\sigma$ is the shorthand notation for $\Phi_\sigma(x = 0)$. An important point is that, $\Phi_\sigma$ depends only on the $q \neq 0$ components of the Tomonaga bosons, $b_{\sigma}$ and $b_{\sigma}^\dagger$. The operator $F_{\sigma}^\dagger$, and its adjoint $F_\sigma$, are the so-called Klein factors. They should be thought of as acting on the $q = 0$ sector of the Hilbert space for the Tomonaga bosons. More precisely, they can be defined as the raising and lowering operators, respectively, in such a Hilbert space [26,27,28]. These operators are unitary, and anti-commute among the different spin species. Furthermore, they commute with $b_{\sigma}$ and $b_{\sigma}^\dagger$ for $q \neq 0$ and, hence, also with $\Phi_\sigma$.

The Kondo Hamiltonian can be rewritten in the bosonized form, $H = H_o + H_\perp + H_\parallel$, with,

$$\begin{align*}
H_o &= \frac{v_F}{4\pi} \int dx [(\frac{d\Phi_\uparrow}{dx})^2 + (\frac{d\Phi_\downarrow}{dx})^2] \\
H_\perp &= \frac{J_z}{4\pi a} (X_{\uparrow\uparrow} F_\uparrow F_\downarrow e^{-i\Phi_\sigma} \sqrt{2} + H.c.) \\
H_\parallel &= \frac{\sqrt{2\pi}}{\pi \rho_o} (X_{\uparrow\downarrow} - X_{\downarrow\uparrow}) (\frac{d\Phi_\uparrow}{dx})x=0 \frac{1}{2\pi} 
\end{align*}$$

(4)

where $\delta^s = \tan^{-1}(\pi \rho_o l_F^2)$ is the phase shift associated with the potential $\frac{\sqrt{2}}{2\pi}$. $v_F$ the Fermi velocity, and $\rho_o = \frac{1}{2\pi v_F}$ the conduction electron density of states at the Fermi level. In Eq. (1), we have also introduced the charge and spin boson fields, $\Phi_\sigma(x) = \frac{1}{\sqrt{2}} (\Phi_\uparrow(x) + \Phi_\downarrow(x))$ and $\Phi_\sigma(x) = \frac{1}{\sqrt{2}} (\Phi_\uparrow(x) - \Phi_\downarrow(x))$.

To construct soluble limits, we apply the following canonical transformation to the Hamiltonian,

$$U = e^{-i\alpha \Phi_\sigma(\sum_\sigma \sigma X_{\sigma\sigma})}$$

(5)

Using

$$U^+ \frac{d\Phi_\sigma}{dx} U = \frac{d\Phi_\sigma}{dx} - \alpha 2\pi \delta(x)(\sum_\sigma \sigma X_{\sigma\sigma})$$

$$U^+ X_{\uparrow\downarrow} U = e^{i2\alpha \Phi_\sigma(o)} X_{\uparrow\downarrow}$$

(6)

the transformed Hamiltonian, $H_{eff} = U^+ H U$, is

$$H_{eff} = H_o + H_j + \Delta H$$

$$H_j = \frac{J_z}{4\pi a} (X_{\uparrow\downarrow} F_\uparrow F_\downarrow e^{-i(\sqrt{2}-2\alpha)\Phi_\sigma} + H.c.)$$

$$\Delta H = \frac{\delta^s}{\pi \rho_o} (X_{\uparrow\downarrow} - X_{\downarrow\uparrow}) (\frac{d\Phi_\uparrow}{dx})x=0 \frac{1}{2\pi}$$

(7)

where $\delta^s = \sqrt{2\pi} - \pi \alpha$. We choose an $\alpha$ such that what remains as the conduction electron part in $H_j$ either has the form of a canonical fermion, or disappears entirely. The Toulouse points correspond to the bare values of the interactions such that $\delta^s = 0$, so that the residual interaction $\Delta H$ vanishes.
B. Toulouse Point I of the Kondo Problem

The effective Hamiltonian assumes a simple form when \( \delta^* \) is close to \( \delta^*_1 = (\frac{1}{2} - \frac{\Delta}{\pi})\pi \), i.e., \( J_z/4 = J^2_z/4 = \frac{1}{\pi} \tan^{-1}(\frac{1}{2} - \frac{\Delta}{\pi^2})\pi \). Choosing \( \alpha = (\sqrt{2} - 1)/2 \) in Eq. \( [3] \) leads to the following transformed Hamiltonian,

\[
H^1_{\text{eff}} = H_o + \frac{J_z}{\pi \alpha} \sum_{\sigma} (d_l^\dagger \eta + H.c.) + \Delta H
\]

\[
\Delta H = \frac{\delta^*}{\pi \rho_o} \sum_{\sigma} \left\{ (d_l^\dagger d_l - 1/2) \frac{d \Phi}{dx} \right\}_{x=0} \frac{1}{2\pi}
\]

where \( \delta^* = \sqrt{2}(\delta^* - \delta^*_1) \) measures the deviation of the interaction \( J_z \) from the chosen value \( J^2_z \). Here \( \eta = \frac{\pi}{\alpha} e^{-\Phi_0(0)} F_\eta \) is a canonical spin-fermion field. \( d_l \equiv X_{\uparrow \downarrow} F^\dagger_{\eta} + F_{\eta} F^\dagger_{\eta} X_{\downarrow \uparrow} \), and its adjoint, \( d_l^\dagger \equiv F_{\eta} F^\dagger_{\eta} F^\dagger_{\eta} X_{\downarrow \uparrow} + F_{\eta} F^\dagger_{\eta} \), satisfy the commutation relations appropriate for a fermion, \( \{d_l, d_l^\dagger\} = X_{\uparrow \uparrow} + X_{\downarrow \downarrow} = 1 \), \( \{d_l, d_l^\dagger\} = \{d_l, d_l^\dagger\} = 0 \). The effective Hamiltonian, therefore, describes a resonant-level model [2]. The spin-spin correlation functions can be calculated using the transformed longitudinal and transverse spin operators,

\[
S^+_{\text{eff}} \equiv U^+ \left( \frac{1}{2} \sum_{\sigma} \sigma X_{\sigma \sigma} \right) U = \frac{1}{2} \sum_{\sigma} \sigma X_{\sigma \sigma} = d_l^\dagger d_l - \frac{1}{2}
\]

\[
\sum_{\sigma} F^\dagger_{\eta} \Phi_\eta X^\dagger_{\eta}
\]

and noting that \( X_{\uparrow \downarrow} \) has the same dimension as \( \frac{1}{2\pi} F^\dagger_{\eta} \Phi_\eta \). The results are [29],

\[
\langle T_\tau S^+ (\tau) S^- (0) \rangle = \langle \frac{1}{2} \sum_{\sigma} \sigma X_{\sigma \sigma} \rangle = \frac{1}{2 \pi} e^{-i \Phi \pi} F^\dagger_{\eta} F^\dagger_{\eta} (0) \sim \frac{\rho_o}{\tau}
\]

\[
\langle T_\tau S^z (\tau) S^z (0) \rangle = \langle (d_l^\dagger d_l - \frac{1}{2}) (\tau) \rangle
\]

\[
= \langle (d_l^\dagger d_l - \frac{1}{2}) \rangle \sim \frac{\rho_o}{\tau}
\]

This is the usual Toulouse point [10], which describes the strong coupling, Fermi liquid fixed point.

C. Toulouse Point II of the Kondo Problem

We now turn to the case of \( \delta^* \) close to \( \delta^*_2 = \frac{1}{2} \pi \). This corresponds to an infinitely strong antiferromagnetic interaction, \( J_z = +\infty \). Choosing \( \alpha = \sqrt{2}/2 \) leads to the following terms for the transformed Hamiltonian, \( H^2_{\text{eff}} = \frac{J_z}{4 \pi \alpha} \sum_{\sigma} (d_l^\dagger \eta + H.c.) + \Delta H \)

\[
\Delta H = \frac{\delta^*}{\pi \rho_o} \sum_{\sigma} \left\{ (d_l^\dagger d_l - 1/2) \frac{d \Phi}{dx} \right\}_{x=0} \frac{1}{2\pi}
\]

In terms of \( b^\dagger_{\tau} \), the constraint given in Eq. \( [3] \) can be rewritten as \( \sum_{\sigma} b^\dagger_{\tau} b^\dagger_{\sigma} = 1 \). At \( \delta^* = \delta^*_2 \), \( H^2_{\text{eff}} \) describes a conduction electron bath decoupled from a spin degree of freedom on which a magnetic field of strength \( h \equiv -\frac{\Delta}{\pi} \) acts along the x direction in spin space. In general, \( H^2_{\text{eff}} \) describes the spin-boson Hamiltonian with an Ohmic bath introduced in Ref. [22], with \( \delta^* \) being proportional to the square root of the dissipation parameter \( \alpha \) defined in the macroscopic quantum coherence (MQC) context [23].

Using the transformed spin operators,

\[
S^+_{\text{eff}} = \frac{1}{2} \sum_{\sigma} (b^\dagger_{\sigma} b^\dagger_{\sigma} - b^\dagger_{\sigma} b^\dagger_{\sigma})
\]

\[
S^z_{\text{eff}} = -e^{i \Phi} \pi \rho_o F^\dagger_{\eta} F^\dagger_{\eta} (0)
\]

the transverse spin-spin correlation function is given by

\[
\langle T_\tau S^+ (\tau) S^- (0) \rangle \sim \frac{\rho_o}{\tau}
\]

The calculation of the longitudinal spin-spin correlation function is somewhat more subtle. At \( \delta^* = \pi/2 \), there is only an oscillatory piece (in real time), with period \( 2\pi \). Expanding around this point, the leading non-vanishing non-oscillatory term has the following long time behavior (\( \tau \gg \frac{1}{\rho_o} \))

\[
\langle T_\tau S^z (\tau) S^z (0) \rangle \sim \frac{\rho_o}{\tau}
\]

In addition, the oscillatory piece damps out [23], beyond a time scale of \( \sim \frac{1}{\rho_o} \pi \). Therefore, the asymptotic long-time behavior of the longitudinal spin-spin correlation function has the Fermi liquid, \( \frac{1}{2} \sigma^2 \), form. This is the same form as that of the transverse spin-spin correlation function. Such a long-time behavior of the correlation functions is consistent with the physical picture that, at long times the impurity spin degrees of freedom is “merged” with those of the conduction electron bath. The \( \frac{1}{2} \sigma^2 \) long-time behavior for the longitudinal spin-spin correlation function in the spin-boson problem is already known in the literature [23,22,24].

Given that this last Toulouse point occurs at an infinitely strong antiferromagnetic interaction, one might worry about the validity of the bosonization approach. In Appendix B, we carry out an atomic-expansion analysis for the Kondo Hamiltonian in the limit \( J_z \gg J_\perp, W \). The procedure is to first diagonalize the \( J_z \) coupling, taking \( J_\perp = W = 0 \). The lowest energy atomic configurations are...
effective spin operators, the same canonical transformation also leads to the following

generating out all the high energy configurations via a canonical transformation leads to the following effective Hamiltonian,

\[ H_{\text{eff}} = H'_o + J'_z (X_{12} + X_{21}) \]
\[ + \sum_{\sigma} \sigma c_{1\sigma}^\dagger c_{1\sigma} \]  

where \( c_{1\sigma}^\dagger \) creates a Wannier orbital of the conduction electrons at the site nearest to the origin, and \( J'_z \sim \frac{\omega^2}{2} \). The same canonical transformation also leads to the following effective spin operators,

\[ (S^z)_{\text{eff}} \sim \frac{1}{2} (X_{11} - X_{22}) \]
\[ (S^+)_{\text{eff}} \sim c_{1\uparrow}^\dagger c_{1\downarrow} X_{12} \]  

These results from the atomic expansion, Eqs. (17) and (18), are the direct analogs of the bosonization results, Eqs. (12) and (13).

To summarize, we have emphasized two aspects associated with the Toulouse points in the Kondo problem. First, we have explicitly retained the Klein factors in the bosonization representation of the fermion operators to keep track of the anticommutation relations satisfied by fermions with different spins. For the Kondo problem per se, the single fermion operators do not come into the Hamiltonian directly; only the fermion bilinear operators do. Therefore, identical results could have been derived without retaining these Klein factors. This is not true for the mixed valence problem, where the single fermion operators do appear in the hybridization term. And, as will be shown in detail in the following sections, it turns out to be essential to keep the Klein factors explicitly when applying the bosonization method to the mixed valence problem. Second, we discussed in detail a second Toulouse point that occurs at the infinite value for the longitudinal component of the Kondo exchange interaction. Through a comparison with the results of an expansion of the atomic limit of the Kondo Hamiltonian, we established that, even in this limit, bosonization can be applied. We also demonstrated that the correct behaviors of the longitudinal spin-spin correlation functions at this second Toulouse point can be derived by expanding around the Toulouse point. These insights turn out to be quite useful to properly understand the Toulouse points of the mixed valence problem.

III. THE GENERALIZED ANDERSON MODEL

In this section we define the generalized Anderson model, summarize our earlier scaling results, and set up the bosonization formalism for the Toulouse-point analysis appropriate for the generalized Anderson model. The Hamiltonian of the generalized Anderson model is

\[ H = \sum_{k\sigma} E_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} E_{d\sigma} d_{\sigma}^\dagger d_{\sigma} + \frac{U}{2} d_{\uparrow}^\dagger d_{\uparrow} d_{\downarrow}^\dagger d_{\downarrow} + \sum_{\sigma} t(d_{\sigma}^\dagger c_{\sigma} + h.c.) + V \sum_{\sigma,\sigma'} d_{\sigma}^\dagger d_{\sigma'}^\dagger c_{\sigma} c_{\sigma'} + V_p \sum_{\sigma} e_{I\sigma}^\dagger e_{I\sigma} \]
\[ + \frac{J}{4} \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_4} \tau_{\sigma_1,\sigma_2} \tau_{\sigma_3,\sigma_4} d_{\sigma_1}^\dagger d_{\sigma_2} c_{\sigma_3}^\dagger c_{\sigma_4} \]  

Here \( \tau \) label the Pauli matrices, and \( \sigma = \uparrow, \downarrow \). To study the mixed valence regime, we focus on \( U = \infty \). The double occupancy configuration of the impurity is then excluded. The three remaining configurations, \( |0\rangle > \) and \( |\sigma >= d_{\alpha}^\dagger |0\rangle > \), have energies \( E_0 = 0 \) and \( E_\sigma = E_{d\sigma} \), respectively. The hybridization \( t \), the density-density interaction \( V \), and the explicit spin exchange interaction \( J \) describe the couplings between the impurity and the electron bath. Anticipating the intrinsic particle-hole asymmetry in the mixed valence regime, we have also allowed for a potential scattering, \( V_p \). This Hamiltonian is general enough for the purpose of studying the interplay between the local spin and charge fluctuations in the mixed valence problem.

Following the procedure outlined in the previous section and given in more detail in Appendix C, we can reduce the problem to that of an impurity coupled to a one-dimensional non-interacting conduction electron bath, with one chiral component for each spin species, \( \psi_{\sigma}(x) \). For the purpose of the Coulomb gas as well as the Toulouse-point analyses, we also allow the longitudinal and transverse components of the exchange interaction, \( J_z \) and \( J_\perp \), to take different values. The Hamiltonian can be rewritten as

\[ H = H_o + E_{d\sigma} \sum_{\sigma} X_{\sigma\sigma} + H_{\perp\perp} + H_{\perp j} + H_V \]
\[ H_{\perp t} = t \sum_{\sigma} (X_{\sigma\sigma} \psi_{\sigma} + H.c) \]
\[ H_{\perp j} = \frac{J}{2} (X_{\uparrow\downarrow} \psi_{\uparrow}^\dagger (0) \psi_{\downarrow} (0) + H.c) \]
\[ H_V = \sum_{\alpha\sigma} V^\sigma_{\alpha} X_{\alpha\sigma} \psi_{\sigma}^\dagger (0) \psi_{\sigma} (0) \]  

Here, the impurity configuration \( |\alpha > \) runs over \( |0\rangle > \) and \( |\sigma > \). This requirement amounts to the following constraint,

\[ X_{\uparrow\uparrow} + X_{\downarrow\downarrow} + X_{\sigma\sigma} = 1 \]  

\( V^\sigma_{\alpha} \) denotes the local potential that the conduction electron of spin \( \sigma \) experiences when the impurity is frozen.
at the configuration $|\alpha \rangle$. In terms of the parameters of Eq. (19),
\begin{align*}
V_{\sigma}^\alpha &= V + \frac{J_z}{4} + V_p \\
V_{\sigma}^\beta &= V - \frac{J_z}{4} + V_p \\
V_{\sigma}^\alpha &= V_p
\end{align*}

(22)

A. The Coulomb Gas Representation and the Scaling Results

The physics of this model can be understood by focusing on the impurity degrees of freedom and tracing out the conduction electrons. The partition function is then a sum over all the histories of the impurity, each history being characterized by a sequence of transitions of the impurity configurations among $|0\rangle$ and $|\sigma\rangle$. This has been extensively discussed in our earlier papers [1,2,3]. For completeness, we summarize the main results in this subsection.

The partition function has the following Coulomb gas form,
\[ Z = \sum_{n=0}^{\infty} \sum_{[\alpha_1, ..., \alpha_n; \tau_1, ..., \tau_n]} \exp(-S[\alpha_1, ..., \alpha_n; \tau_1, ..., \tau_n]) \] (23)

where
\[ S[\alpha_1, ..., \alpha_n; \tau_1, ..., \tau_n] = \sum_{i<j} [K(\alpha_i, \alpha_j) + K(\alpha_{i+1}, \alpha_{j+1})] \\
- K(\alpha_i, \alpha_{j+1}) - K(\alpha_{i+1}, \alpha_j) ln(\frac{\tau_j - \tau_i}{\xi}) \\
- \sum_i ln(y_{\alpha_i, \alpha_{i+1}}) + \sum_i h_{\alpha_{i+1}}(\tau_{i+1} - \tau_i) \] (24)

Here, $[\alpha_1, ..., \alpha_n; \tau_1, ..., \tau_n]$ labels a history, with the impurity hopping quantum mechanically from one local state, $|\alpha_i\rangle$, to another, $|\alpha_{i+1}\rangle$, at the (imaginary) time $\tau_i$. The logarithmic interaction between the hopping events reflects the reaction of the electron bath towards the changes of the impurity configurations. Here, $\xi$ is the ultraviolet inverse energy cutoff, and the strength of the logarithmic interaction is characterized by the stiffness constants, $\epsilon_t = -K(0, \sigma)$ and $\epsilon_j = -K(\sigma, \sigma' \neq \sigma)$ which in turn are determined by the bare interaction strength of the original Hamiltonian. Specifically,
\begin{align*}
\epsilon_t &= \frac{1}{2} \left[ (1 - \frac{\delta_{\sigma}^2 - \delta_{\sigma'}^2}{\pi})^2 + (\frac{\delta_{\sigma}^2 - \delta_{\sigma'}^2}{\pi})^2 \right] \\
\epsilon_j &= (1 - \frac{\delta_{\sigma}^2 - \delta_{\sigma'}^2}{\pi})^2
\end{align*}

(25)

where
\[ \delta_{\alpha}^n = \tan^{-1}(\pi \rho \sigma V_{\alpha}^n) \] (26)

is the phase shift that the conduction electron bath of spin $\sigma$ experiences when the impurity configuration is $|\alpha\rangle$. The fugacities $y_{\alpha, \beta}$ describe the amplitudes for a quantum hopping between the configurations $|\alpha\rangle$ and $|\beta\rangle$. More specifically, the charge fugacity corresponds the hopping amplitude between two local states with different charge quantum numbers and is proportional to the hybridization amplitude, $y_{0, \sigma} \equiv y_{t} = \xi \epsilon_t$. Similarly, the spin fugacity describes the hopping amplitude between two local states with different spin quantum numbers and is given by the transverse component of the exchange coupling, $y_{\sigma, \sigma'} \equiv y_{j} = \frac{1}{2} \xi$ for $\sigma \neq \sigma'$. Finally, the fields $h_{\alpha}$ describe the energy splittings among the local configurations. In the absence of an external magnetic field, $h_0 = -\frac{1}{2} E_d^0 \xi$ and $h_{\sigma} = \frac{1}{2} E_d^0 \xi$.

The physical content of this Coulomb gas representation is as follows. $y_j$ and $\epsilon_t$ are the dimensionless quantities associated with the transverse and longitudinal couplings of the usual spin Kondo problem. $y_t$ and $\epsilon_t$, on the other hand, can be thought of as the analogous dimensionless quantities associated with the transverse and longitudinal couplings in a charge Kondo problem. And the difference between $h_0$ and $h_\sigma$, or rather the impurity level, $E_d^\sigma$, controls how “soft” the local charge fluctuations are; when $E_d^\sigma$ is tuned through the conduction electron Fermi level from far below to far above, the system evolves from a local moment regime, through a mixed valence regime, to the empty orbital regime. In the mixed valence regime, Kondo-like processes in the spin channel and charge channel are coupled together. The partition function given in Eq. (23) is the proper generalization of Haldane’s Coulomb gas representation of the mixed valence problem such that the interplay between the spin and charge channels are incorporated systematically.

Our renormalization group analysis of this partition function establishes the existence of three, and only three, mixed valence phases: 1) the usual strong coupling phase. Both the spin and charge Kondo problems are in the strong coupling regime; rapid fluctuations between all three local configurations take place and the conduction electrons quench both the charge and spin degrees of freedom of the impurity; 2) a weak coupling phase where neither the local charge nor the local spin degrees of freedom is quenched. Both the spin and charge Kondo problems are in the weak coupling regime, and all three atomic configurations decouple asymptotically at low energies; 3) an intermediate phase where the local spin degrees of freedom is quenched, but the local charge degrees of freedom is not. Here, the charge Kondo problem is in the weak coupling regime despite of the fact that the spin Kondo problem is in the strong coupling regime. There are two local configurations carrying different charges which are decoupled asymptotically. The phase diagram is properly given in terms of the $\epsilon_t - \epsilon_j$ parameter space. The strong coupling phase occurs when $\epsilon_t < 1$, as well as over a range of $\epsilon_j < 1$ when $\epsilon_t > 1$. The weak coupling phase can occur only when both $\epsilon_t > 1$ and $\epsilon_j > 1$. From Eq. (23) this condition means that the effective
exchange interaction has to be ferromagnetic. The weak coupling phase is, therefore, very likely to be of only academic value. The intermediate phase arises over a range within \( \epsilon_i > 1 \) and \( \epsilon_j < 1 \). For the model Hamiltonian [13] this means an antiferromagnetic exchange interaction, and a finite attractive density-density interaction, \( V \), between the impurity and conduction electrons. As will be further discussed in Sec. VIII B, taking \( V \) as an effective parameter this condition can be satisfied in a variety of realistic models. The transition between the different regimes is analogous to the localization phase transition studied in the context of MQC [23] and more recently in the context of transport through constrictions in interacting quantum wires [13].

B. Construction of the Toulouse Points of the Mixed Valence Problem

We now proceed to derive the Toulouse points. Bosonizing the conduction electrons, and making a canonical transformation using

\[
U = e^{-i\Phi_T} \sum_\sigma \sigma X_\sigma e^{-i\beta \Phi_T} e^{-i\Phi_T} X_\sigma e^{-i\gamma \Phi_T} \tag{27}
\]

we arrive at the effective Hamiltonian, \( H_{eff} = U^+ H U \),

\[
H_{eff} = H_0 + E_\delta \sum_\sigma X_\sigma + H_I + H_J + \Delta H
\]

\[
H_I = \frac{t}{\sqrt{2\pi a}} \sum_\sigma \left[ X_\sigma F_\sigma e^{-i \Phi_\sigma} e^{-i \beta \Phi_T} + H.c. \right]
\]

\[
H_J = \frac{J_{\perp}}{4\pi a} \left[ X_{\perp} e^{-i(\Phi_\sigma - \alpha \Phi_T) + H.c.} \right]
\]

\[
\Delta H = \sum_\alpha \frac{X_{\alpha} \sigma}{\pi \rho_0} \left[ \delta_{\sigma}^a \frac{d\Phi_\sigma}{dx} \right]_\sigma \frac{1}{2\pi} + \delta_{\sigma}^c \frac{d\Phi_\sigma}{dx} \frac{1}{2\pi} \tag{28}
\]

The notations are the same as in the previous section, \( \delta_\sigma^a = \delta_\sigma - \pi \sigma \), \( \delta_\sigma^c = \delta_\sigma + \pi \beta - \gamma \), and \( \delta_\sigma^c = \delta_\sigma - \pi \beta + \gamma \). Here, \( \delta_{\sigma}^a = \frac{1}{\sqrt{2}} \sum_\sigma \delta_{\sigma}^a \) and \( \delta_{\sigma}^c = \frac{1}{\sqrt{2}} \sum_\sigma \sigma \delta_{\sigma}^c \), where \( \delta_{\sigma}^c \) is defined in Eq. (28); more specifically,

\[
\delta_{\sigma}^a = \sigma (\delta_{\sigma}^c - \delta_{\sigma}^c)/\sqrt{2}
\]

\[
\delta_{\sigma}^c = (\delta_{\sigma}^c + \delta_{\sigma}^c)/\sqrt{2}
\]

\[
\delta_{\sigma}^c = (\delta_{\sigma}^c + \delta_{\sigma}^c)/\sqrt{2} = \sqrt{2} \delta_{\sigma}^c \tag{29}
\]

The last equality of the last equation holds in the absence of an external magnetic field. The latter also ensures that \( \delta_{\sigma}^c \neq 0 \).

To construct a Toulouse point, we choose the parameters \( \alpha \) and \( \beta \) such that the the conduction electron operators appearing in the transformed \( H_i \) and \( H_J \) have simple forms. The Toulouse point then corresponds to choosing the bare values of the interactions such that the transformed \( \Delta H \) vanishes. This means taking \( \delta_{\sigma}^a = 0 \), \( \delta_{\sigma}^c = \pi (\beta + \gamma) \), and \( \delta_{\sigma}^c = \pi (\gamma - \beta) \). From Eq. (29), these conditions are equivalent to requiring that the phase shifts \( \delta_{\sigma}^c \) take the following values,

\[
\delta_{\sigma}^a = \frac{1}{\sqrt{2}} (\beta + \gamma + \alpha) \pi \]

\[
\delta_{\sigma}^c = \frac{1}{\sqrt{2}} (\beta + \gamma - \alpha) \pi \]

\[
\delta_{\sigma}^c = \frac{1}{\sqrt{2}} (\gamma - \beta) \pi \tag{30}
\]

According to Eq. (28), the Coulomb gas stiffnesses at the Toulouse point are

\[
\epsilon_i = \frac{1}{4} (\alpha + 2\beta - \sqrt{2})^2 + (\alpha - 2\beta)^2 \]

\[
\epsilon_j = (\sqrt{2} \alpha - 1)^2 \tag{31}
\]

Eq. (30), together with Eqs. (22) and (26), allow us to determine the parameters of the generalized Anderson model at the Toulouse points. In terms of the phase shifts, they are

\[
\delta(J_z/4) = \tan^{-1} \left[ \frac{1}{2} \tan(\delta_{\sigma}^c - \frac{1}{2} \tan(\delta_{\sigma}^c) \right]
\]

\[
= \tan^{-1} \left[ \frac{1}{2} \tan(\beta + \gamma + \alpha) \right] - \frac{1}{2} \tan(\beta + \gamma - \alpha) \right] \}

\[
\delta(V) = \tan^{-1} \left[ \frac{1}{2} \tan(\delta_{\sigma}^c - \frac{1}{2} \tan(\delta_{\sigma}^c) - \tan(\delta_{\sigma}^c) \right]
\]

\[
= \tan^{-1} \left[ \frac{1}{2} \tan(\beta + \gamma - \alpha) \right] - \frac{1}{2} \tan(\beta + \gamma - \alpha) \right] \}

\[
= \frac{\gamma - \beta}{\sqrt{2}} \tag{32}
\]

At a Toulouse point, the correlation functions can be calculated in terms of the single particle, off-diagonal spin, diagonal spin, and density operators in the transformed basis,

\[
(d_{\sigma}^a)^{\dagger}_{eff} = U_{\sigma}^\dagger X_{\sigma} U = e^{i\alpha \Phi} e^{2i\beta \Phi} X_{\sigma} \]

\[
S_{\sigma}^+ = U_{\sigma}^\dagger X_{\sigma} U = e^{2i\alpha \Phi} X_{\sigma} \]

\[
S_{\sigma} = U_{\sigma} X_{\sigma} U = \frac{1}{2} \sum_{\sigma} X_{\sigma} \]

\[
\rho_{\sigma} = U_{\sigma} X_{\sigma} U = \sum_{\sigma} X_{\sigma} \tag{33}
\]

We found that only three independent points exist where the transformed Hamiltonian is exactly soluble, and one more point where the effective Hamiltonian assumes a simple form but is not exactly soluble. Before proceeding to analyze each of these points, we end this section with a comment on the role of the \( \gamma \) term in the canonical transformation and, likewise, the role of the potential scattering term in the generalized Anderson model. In general, Eq. (30) may require that, at
the Toulouse points, one or several of the phase shifts, \( \delta^o \), be outside the range specified by the unitarity limit, \([-\frac{\pi}{2}, \frac{\pi}{2}]\). While bound states can lead to the violation of the unitarity bounds of the coupling constants \( \Delta \), in our case we can take advantage of the freedom of varying the strength of the potential scattering term to make all the phase shifts in Eq. (30) to fall in the range \([-\frac{\pi}{2}, \frac{\pi}{2}]\). This will be seen to be especially convenient for the purpose of demonstrating the consistency of the bosonization results with those of the atomic expansions shown in Appendix B. The physics is independent of the potential scattering term, as can be clearly seen from the \( \gamma \)-independence of the effective Hamiltonian, Eq. (13), as well as the \( \gamma \)-independence of the Coulomb gas stiffnesses at the Toulouse points, Eq. (11).

IV. STRONG COUPLING TOULOUSE POINT I

The first Toulouse point arises with the choice of \( \alpha = \sqrt{\tau} \) and \( \beta = \sqrt{2\tau} \). At this point, Eq. (13) gives \( \epsilon_t = 0 \) and \( \epsilon_j = 0 \). The Coulomb gas analysis implies that we are deep in the strong coupling regime. The requirement that all the phase shifts \( \delta^o_e \) are within the range \([-\frac{\pi}{2}, \frac{\pi}{2}]\) leads to a unique choice for \( \gamma = -\sqrt{\tau} \). With this choice of \( \gamma \), \( \delta^o = \pi/2 \), \( \delta^o_\pi = -\pi/2 \), and \( \delta^o_\sigma = -\pi/2 \). Equivalently, \( \delta(J_e/4) \) and \( \delta(V) \) are both equal to \( \pi/2 \), while \( \delta(V_\pi) = -\pi/2 \). This corresponds to an infinite antiferromagnetic exchange interaction and an infinite repulsive density-density interaction.

In this case, \( H_t = \sum_{\sigma} (\sigma \delta^o) \sum (X_{\sigma \sigma} F_{\sigma} + H.c.) \), and \( H_j = \frac{J_j}{4\pi a} (X_{\uparrow \downarrow} F_{\uparrow} F_{\downarrow} + H.c.) \). We now introduce pseudofermion creation and annihilation operators \( f_{\sigma}^\dagger \) and \( f_{\sigma} \), and pseudoboson creation and annihilation operators \( b_{\sigma}^\dagger \) and \( b_{\sigma} \), as in Eq. (11). We further introduce the pseudoboson creation and annihilation operators \( b_{\sigma}^\dagger \) and \( b_{\sigma} \) such that \( X_{\sigma \sigma} = f_{\sigma}^\dagger b_{\sigma} \) and \( X_{\sigma \sigma} = b_{\sigma}^\dagger f_{\sigma} \). The effective Hamiltonian becomes

\[
H_{eff} = H_0 + E_d^0 \sum_{\sigma} b_{\sigma}^\dagger b_{\sigma} + \frac{t}{\sqrt{2\pi a}} \sum_{\sigma} (b_{\sigma}^\dagger b_{\sigma} + b_{\sigma}^\dagger b_{\sigma})
- \frac{J_j}{4\pi a} (b_{\pi}^\dagger b_{\pi} + H.c.) \quad \Delta H
\]

\[
\Delta H = \frac{J_j}{4\pi a} \sum_{\sigma} (b_{\sigma}^\dagger b_{\sigma} - b_{\sigma} b_{\sigma}) \frac{d\Phi_e}{dx} \bigg|_{x=0} \frac{1}{2\pi}
+ \frac{\kappa_{\pi}}{2\pi \rho_0} \sum_{\sigma} (\sigma b_{\sigma}^\dagger b_{\sigma} \frac{d\Phi_e}{dx} \bigg|_{x=0} \frac{1}{2\pi}) \quad (34)
\]

And the constraint Eq. (2) is rewritten as

\[
\sum_{\sigma} b_{\sigma}^\dagger b_{\sigma} + b_{\sigma}^\dagger b_{\sigma} = 1 \quad (35)
\]

In deriving the effective Hamiltonian, we have chosen \( \delta^o_0 \) such that the transformed potential scattering term vanishes. With this choice, \( \kappa_\pi \) and \( \kappa_\sigma \) can be explicitly written in terms of the original phase shifts as \( \kappa_\pi = \sqrt{2} (\delta^o_\pi + \delta^o_\sigma) \) and \( \kappa_\sigma = \sqrt{2} (\delta^o_\sigma - \delta^o_\pi - \pi) \). They vanish at the Toulouse point.

At the Toulouse point, the Hamiltonian describes a three-level system decoupled from the conduction electrons. It is the three-level analog of the two level spin-boson Hamiltonian with zero dissipation. The three-level system can be diagonalized exactly, with three eigenstates, \( |s0> = u|A> + v|o> \), \( |t> = |B> \), and \( |s1> = -|v|A> + u|o> \). Here, \( |A> = \frac{1}{\sqrt{2}} (b_{\pi}^\dagger + b_{\pi}^\dagger)|vac> \), \( |B> = \frac{1}{\sqrt{2}} (b_{\pi}^\dagger - b_{\pi}^\dagger)|vac> \), and \( |o> = b_{\pi}^\dagger |vac> \) (36)

define a new basis for the atomic states. In the absence of hybridization, these three configurations have energies \( E_A = E_d^0 - \frac{J_j}{4\pi a} \), \( E_B = E_d^0 + \frac{J_j}{4\pi a} \), and \( E_o = 0 \). The hybridization term mixes \( |A> \) and \( |o> \), leading to the bonding and anti-bonding states \( |s0> \) and \( |s1> \). \( u \) and \( v \) are the coherence factors, \( u^2 = 1 - v^2 = \frac{1}{2} \left( 1 - \frac{E_o - J_j/4\pi a}{(E_d^0 - J_j/4\pi a)^2 + 8(\pi/\sqrt{2}\pi a)^2} \right) \). The energies of the eigenstates are \( E_{s0} = \frac{(E_d^0 - J_j/4\pi a)^2 + 8(\pi/\sqrt{2}\pi a)^2}{2} / 2 \), \( E_{s1} = \frac{(E_d^0 - J_j/4\pi a)^2 + E_{s0}}{2} + (\pi/\sqrt{2}\pi a)^2 / 2 \). Given that \( J_j \) is antiferromagnetic, \( J_j \) should also be antiferromagnetic (positive). Therefore, irrespective of \( E_d^0 \), \( |s0> \) is always the ground state.

The ground state of the whole system is \( |gs> = U^+ |s0> |FS> \). The correlation functions can be calculated from the transformed single particle, spin and density operators

\[
(d_{\sigma})_{eff} = e^{i\sigma \Phi_e/\sqrt{\tau}} e^{i\Phi_e/\sqrt{\tau}} \: \frac{1}{\sqrt{2}} (X_{\sigma \sigma} + \sigma X_{\sigma \sigma}) F_{\sigma}^\dagger
\]

\[
S_{eff} = e^{i\Phi_e/\sqrt{\tau}} \frac{1}{2} (X_{\sigma \sigma} - X_{\sigma \sigma} - X_{\sigma \sigma} + X_{\sigma \sigma})
\]

\[
S_{eff}^2 = \frac{1}{2} (X_{\sigma \sigma} + X_{\sigma \sigma} - X_{\sigma \sigma} - X_{\sigma \sigma})
\]

\[
\rho_{eff} = (X_{\sigma \sigma} + X_{\sigma \sigma} - X_{\sigma \sigma} - X_{\sigma \sigma}) \quad (37)
\]

The single-particle and the transverse spin susceptibility are straightforward to calculate and have the Fermi liquid forms,

\[
< T_r d_{\sigma}(\tau) d_{\sigma}^\dagger(0) > \sim \frac{\rho_0}{\tau}
\]

\[
< T_r S^- (\tau) S^+ (0) > \sim \left( \frac{\rho_0}{\tau} \right)^2 \quad (38)
\]

At the Toulouse point, the longitudinal spin-spin correlation function and the density-density correlation function again have the oscillatory behaviors in real time at the Toulouse point. As for the longitudinal spin correlation
function near the Toulouse point II of the Kondo problem, a direct expansion in terms of the deviation from the Toulouse point leads to the following Fermi liquid behaviors for these two correlation functions,

\[ \langle T_\tau S^z(\tau)S^z(0) \rangle \sim \frac{\kappa_s}{2\pi\rho_s\hbar_s} \langle \frac{P_0}{\tau} \rangle^2 \]

\[ \langle T_\tau \rho(\tau)\rho(0) \rangle \sim \frac{\kappa_c}{2\pi\rho_c\hbar_c} \langle \frac{P_0}{\tau} \rangle^2 \]

(39)

where \( h_s = J_\perp/4\pi a \) and \( h_c = \tau/\sqrt{2\pi a} \). This Toulouse point, therefore, describes a strong coupling, Fermi liquid state.

Unlike for the Kondo problem, keeping track of the anticommutation relation between fermions of different spins in the boson representation plays an essential role. Failing to do that, the sign of \( H_\tau \) term would be reversed, leading to the atomic configuration \( |A> \) having energy \( E_o + E_d \) instead of \( E_o + E_d \), and \( |B> \) having energy \( E_o - E_d \) instead of \( E_o - E_d \). In that case, the spin-flip exchange interaction (\( J_\perp \)) would make the configuration \( |B> \) energetically more favorable than \( |A> \), while the hybridization (\( t \)) term, which mixes \( |A> \) with \( |o> \), would favor \( |s0> \) instead of \( |t> = |B> \). This competition between the spin-exchange and hybridization would then lead to a level-crossing as \( E_0 \) is varied: the ground state changes from \( |t> \) to \( |s0> \) as the \( d\) level varies from far below to far above the Fermi level. The level-crossing found in earlier works on related problems \([8][9]\) results from this failing to keep track of the anticommutation relation between the bosonized fermion fields.

We can gain much physical insights into our results by determining the quantum numbers of the respective impurity eigenstates. Within the bosonization approach, the meaning of the atomic configurations, \( |A> \), \( |B> \) and \( |o> \), is somewhat obscure. The physical content of these configurations becomes transparent once we compare them with the atomic configurations that appear in a perturbation expansion of the original Hamiltonian in terms of \( J_{\perp}/J_z, J_{\perp}/V, t/J_z, t/V, W/J_z, \) and \( W/V \). This atomic expansion is a natural procedure given that \( J_z, V \gg J_{\perp}, t \) at the Toulouse point. The details of this atomic expansion can be found in Appendix B. From Eqs. (B6) and (B7), \( |A>, |B> \) and \( |o> \) are identified with

\[ |A> = \frac{1}{\sqrt{2}}(|\uparrow> + |\downarrow>), |B> = \frac{1}{\sqrt{2}}(|\uparrow> - |\downarrow>), |o> = |0> \]

(40)

\( |A> \) is the local singlet formed between the impurity spin and the conduction electron spin at the impurity site, \( |B> \) the \( S_z = 0 \) state of the local triplet, and \( |o> \) the singlet with the impurity empty of electrons and the local conduction electron orbital doubly occupied. It is clear that both the exchange interaction (\( J_\perp \)) term and the hybridization (\( t \)) term favor the same singlet state \( |s0> := u|A> + v|o> \), for arbitrary values of \( E_o \). No level crossing occurs.

V. STRONG COUPLING TOLOUSE POINT II

We now choose \( \alpha = \frac{\sqrt{2}}{\sqrt{2+\pi}} \) and \( \beta = \frac{\sqrt{2-\pi}}{4} \). The corresponding Coulomb gas stiffnesses are \( \epsilon_t = 1/2 \) and \( \epsilon_j = 0 \), and the Coulomb gas analysis would again predict that the system is in the strong coupling phase. As in the previous section, the requirement that all the phase shifts fall in the range \([-\pi/2, \pi/2]\) leads to a unique choice for \( \gamma = \frac{1}{2} - \frac{\sqrt{2}}{4} \). This choice corresponds to \( \delta_o^0 = \pi/2, \delta_o^0 = -\pi/2, \) and \( \delta_o^0 = \frac{\sqrt{2}-1}{\pi} \). Equivalently, \( \delta(J_z/4) = \pi/2, \delta(V) = \frac{\sqrt{2}-1}{\pi}, \) and \( \delta(V_o) = \frac{\sqrt{2}-1}{\pi} \). We have an infinite antiferromagnetic exchange interaction and a large, but finite, attractive density-density interaction.

In this case, \( H_t = \frac{t}{\sqrt{2\pi a}} \sum_{\sigma} (X_{\sigma}F_{\sigma}e^{-i\Phi_{\sigma}} + H.c.) \), and \( H_j = \frac{J_{\perp}}{\pi a} (X_{\sigma}F_{\sigma}F_{\sigma}^\dagger + H.c.) \). Introducing a fermion field, \( \eta_i = F_{\sigma}^\dagger \sqrt{\frac{\sqrt{2}}{2\pi a}} e^{i\Phi_{\sigma}} \), and defining \( f_{\sigma}^\dagger = X_{\sigma}F_{\sigma}F_{\sigma}^\dagger \), we derive the following effective Hamiltonian,

\[ H_{\text{eff}}^{B} = \sum_{k} E_k \eta_k \eta_k^\dagger + E_{d} \sum_{\sigma} f_{\sigma}^\dagger f_{\sigma}^\dagger + t(\sum_{\sigma} f_{\sigma}^\dagger)(\sum_{\sigma} \eta_{\sigma}) + H.c. \]

\[ \frac{J_{\perp}}{4\pi a} (f_{\uparrow}^\dagger f_{\downarrow}^\dagger + H.c.) \]

(41)

It is convenient to introduce a new basis for the atomic configurations, \( |A> = \frac{1}{\sqrt{2}}(f_{\uparrow}^\dagger + f_{\downarrow}^\dagger)|0> \), \( |B> = \frac{1}{\sqrt{2}}(f_{\uparrow}^\dagger - f_{\downarrow}^\dagger)|0> \), and \( |o> \). The corresponding atomic levels are \( E_A = E_d^0 - \frac{J_{\perp}}{4\pi a}, E_B = E_d^0 + \frac{J_{\perp}}{4\pi a}, \) and \( E_o = 0 \). In this new basis, the constraint becomes

\[ X_{AA} + X_{BB} + X_{oo} = 1 \]

(42)

and the effective Hamiltonian can be rewritten as

\[ H_{\text{eff}}^{B} = \sum_{k} E_k \eta_k \eta_k^\dagger + \sqrt{2t}(X_{Ao}\eta + H.c.) \]

\[ + E_o - \frac{J_{\perp}}{4\pi a} X_{AA} + E_d^0 + \frac{J_{\perp}}{4\pi a} X_{BB} \]

(43)

Among the three impurity configurations \( |A>, |B>, \) and \( |o> \), \( |A> \) and \( |o> \) hybridize with the conduction electrons, while \( |B> \) is decoupled. Therefore, this Hamiltonian can be diagonalized exactly. The Hilbert space factorizes into two sectors. Again, since \( J_z \) is antiferromagnetic, \( J_{\perp} \) should also be taken as antiferromagnetic. It is clear that, the low lying excitations lie in the sector in which the ground state is

\[ \phi = |o> \phi_o + |A> \phi_A \]

(44)
where \( \phi_0 \) and \( \phi_A \) are the conduction electron wave functions such that \( \phi \) is the ground state of a resonant level model with \( X_{\phi_0} \) treated as a free fermion operator. The ground state energy (relative to a free Fermi sea) is that of the resonant-level model with a resonance width \( 2\pi\rho_o\tau^2 \) and an effective \( d \)-level \( E_d^0 = -J_{4\pi\alpha} \).

Using \( d^+_d = e^{i\sqrt{2\pi}t,\sigma/2}e^{i(\sqrt{2} - 2)\phi_0/2}X_{\sigma_0} \), \( S^+ = e^{i\sqrt{2\pi}t,\sigma/2}X_{\perp 1} \), \( S^z = (X_{AB} + X_{BA})/2 \), and \( \rho = (X_{A\sigma} + X_{B\sigma} - X_{\sigma_0}) \), noticing that \( X_{\sigma_0} \) has the dimension of \( \sqrt{2\pi}e^{i\phi_0} \), we find that all the correlation functions have the Fermi liquid form,

\[
\begin{align*}
< T_{\tau}d_\sigma(\tau)d^\dagger_\sigma(0) > & \sim \frac{\rho_0}{\tau} \\
< T_{\tau}S^-(\tau)S^+(0) > & \sim \left( \frac{\rho_0}{\tau} \right)^2 \\
< T_{\tau}S^z(\tau)S^z(0) > & \sim \left( \frac{\kappa_s}{2\pi\rho_0} \right)^2 \left( \frac{\rho_0}{\tau} \right)^2 \\
< T_{\tau}\rho(\tau)\rho(0) > & \sim \left( \frac{\rho_0}{\tau} \right)^2
\end{align*}
\tag{45}
\]

where \( \kappa_s \) is again the deviation from the Toulouse point. This establishes the strong coupling, Fermi liquid nature of this Toulouse point.

Except for the change of sign in \( J_\perp \), the effective Hamiltonian (41) is identical to that of Refs. [18] and [19]. The sign change for \( J_\perp \) occurs. The bosonization results are consistent with our previous renormalization group results.

VI. A TOULOUSE POINT FOR THE INTERMEDIATE PHASE

In Refs. [10,11] we found a new mixed valence phase, which we called the intermediate phase. It is a non-Fermi liquid with quasiparticle-like spin excitations and incoherent charge excitations. In this section, we present a Toulouse point which clearly exhibits the physics of the intermediate phase. It occurs with the choice of \( \alpha = \frac{\sqrt{2}}{2} \) and \( \beta = -\frac{\sqrt{2}}{2} \). The corresponding Coulomb gas stiffnesses are \( \epsilon_i = 1 \) and \( \epsilon_j = 0 \). While it is not possible to determine the precise boundary between the intermediate phase and the strong coupling phase, it is not inconsistent with the Coulomb gas results that these values of the Coulomb gas stiffnesses lie close to such a boundary.

Taking \( \gamma = \frac{\sqrt{2}}{2} \) specifies the phase shifts at the Toulouse point: \( \delta_o^\alpha = \frac{\pi}{2} \), \( \delta_o^\beta = -\frac{\pi}{2} \) and \( \delta_o^\gamma = \frac{\pi}{2} \). Equivalently, \( \delta(J_2) = \frac{\pi}{2} \), \( \delta(V) = -\frac{\pi}{2} \), and \( \delta(V_o) = \frac{\pi}{2} \). These parameters correspond to an infinite antiferromagnetic exchange interaction and an infinite attractive density-density interaction.

In the canonicallly-transformed Hamiltonian, \( H_i = \frac{1}{\sqrt{2\pi\alpha}} \sum_{\sigma} \frac{1}{2} \sigma \phi_0^\dagger \phi_0 e^{-i\phi_0} \sqrt{2} + H.c. \), \( H_j = \frac{J_{4\pi\alpha}}{2\pi\rho_0} (X_{A\parallel}F_\parallel + F_\parallel + H.c.) \). The effective Hamiltonian can be written as

\[
H_{eff}^C = \sum_{\sigma} E_{\sigma} c^\dagger_{\sigma} c_{\sigma} + \frac{D}{\pi\rho_0} \sum_{\sigma} \sigma X_{\phi_0} c_{\sigma} + H.c. + \frac{\kappa_c}{2\pi\rho_0} (X_{AB} + X_{BA})(c^\dagger_{\uparrow} c_{\uparrow} + c^\dagger_{\downarrow} c_{\downarrow})
\tag{46}
\]

Here, \( |A\rangle > = -\frac{1}{\sqrt{2}} \sum_{\sigma} (-\sigma \phi_0 F_{\parallel}^\dagger) \) and \( |B\rangle > = \frac{1}{\sqrt{2}} \sum_{\sigma} (-\phi_0 F_{\parallel}^\dagger) \). Again, with the requirement on \( \delta_o^\sigma \) such that the transformed potential scattering term vanishes, \( \kappa_c \) and \( \kappa_s \) can be written explicitly as \( \kappa_c = \sqrt{2}(\delta_o^\sigma + \delta_o^\parallel) \) and \( \kappa_s = \sqrt{2}(\delta_o^\parallel - \delta_o^\gamma - \pi) \), and are non-zero only away from the Toulouse point.

In this effective Hamiltonian, the charge sector is described by a genuine charge Kondo model. \( |A\rangle > \) and \( |\rangle > \) play the role of \( |\uparrow\rangle > \) and \( |\downarrow\rangle > \) of the spin Kondo problem and should be thought of as objects carrying charge 2 and 0, respectively. The transformed hybridization term is the direct analog of the spin-flip term in the spin Kondo problem, with a change of the charge quantum number by two replacing a change of the spin quantum number by 1 in the latter. The residual interaction in the charge sector, \( \frac{\kappa_c}{2\pi\rho_0} \), is the analog of the longitudinal exchange interaction in the spin Kondo problem, with the density playing the role of the spin in the latter. In the conventional notation, \( \frac{1}{2} J_{\parallel}^{\text{charge}} = 2\pi\sqrt{\alpha} \) and \( \frac{1}{2} J_{\parallel}^{\text{charge}} = \frac{k_c}{2\pi\rho_0} \). The essential difference between the charge Kondo problem in this mixed valence context and the spin Kondo problem lies in the symmetry-breaking field. In the latter, the spin symmetry guarantees that no explicit magnetic field term will be generated in the absence of an applied field. In our charge Kondo problem, the particle-hole symmetry is explicitly broken, and the symmetry-breaking field \( h^{\text{charge}} = E_{\parallel}^d - \frac{\kappa_c}{2\pi\rho_0} \) is in general non-zero. For the impurity problem, the condition that the renormalized \( h^{\text{charge}} \) vanishes can be achieved only through fine-tuning the bare \( d \)-level \( E_{\parallel}^d \) to a critical value \( E_{\parallel}^d \).

When \( h^{\text{charge}} = 0 \) is enforced, a zero temperature quantum phase transition takes place as \( \kappa_c \) is increased through zero. The transition is characterized by a Kosterlitz-Thouless transition in the charge sector; the spin sector is not critical. The phenomenology of the intermediate phase is recovered on the negative \( \kappa_c \) side, to which the remaining of this section is devoted. Here, the charge sector is described by the weak coupling fixed point of the charge-Kondo problem, while the spin excitations by the strong coupling, Fermi liquid-like fixed
point of the Kondo problem. A spin-charge separation takes place.

Within the charge sector, the impurity configuration in the ground state is entirely \( |o> \) for \( K_{\text{charge}} < 0 \), and \( |A> \) for \( K_{\text{charge}} > 0 \). This is the result of infinite charge susceptibility in the corresponding ferromagnetic charge Kondo problem. Exactly at \( K_{\text{charge}} = 0 \), namely, when \( E_0^a \) is tuned to the critical value \( E_0^a = \frac{J}{4\pi\sigma} \), the impurity degrees of freedom in the ground state involve an equal, incoherent, mixture of \( |o> \) and \( |A> \). Schematically, the ground state wavefunction can be written as

\[
\phi = |A> + |o> \phi_o \tag{47}
\]

where \( \phi_A \) and \( \phi_o \) are the wave functions of the conduction electrons such that \( \phi \) solve a ferromagnetic Kondo model with zero magnetic field. With \( K_{\text{charge}} = 0 \), the intermediate mixed valence dynamics applies at all temperatures. When \( E_0^a \) is moved away from the critical value, a finite cross-over temperature \( T_{c0} \sim |E_0^a - E_0^s| \) emerges. The intermediate mixed valence dynamics continue to apply at \( T > T_{c0} \). At low temperatures \( (T < T_{c0}) \), however, the charge fluctuations become gapped out. Such a cross-over can already be inferred from the renormalization group trajectories in our previous work \[10\].

The correlation functions that describe the critical dynamics associated with the intermediate mixed valence phase can be calculated explicitly. Consider first the single particle Green function. Using \( \langle d^\dagger_{\sigma} \rangle = e^{i\Phi_\sigma/\sqrt{2}\pi e^{-i\Phi_\sigma/\sqrt{2}}(-\frac{1}{\sqrt{2}})(\sigma X_{Ao} + \sigma X_{Bo})F_\sigma \), we find that

\[
<T_r \rho(\tau) \rho(0) >_{\text{connected}} \sim \frac{\rho_0^2}{(-4\kappa_\sigma)^{(-4\kappa_\sigma)}} \tag{50}
\]

This algebraic piece, once again, has an interaction-dependent exponent. We note that, the fact that the exponent vanishes with \( \kappa_\sigma \) has already been noted before in related problems \[34,35\].

Other correlation functions in the charge sector also have an algebraic behavior with interaction-dependent exponents. For instance, the excitonic correlation function, using \( \langle d^\dagger_{\sigma} \rangle = e^{-i\Phi_\sigma}(\frac{1}{\sqrt{2}})(X_{Ao} + \sigma X_{Bo})F_\sigma \), has the following form,

\[
<T_r(\sum \sigma d^\dagger_{\sigma})(\tau)(\sum \sigma d^\dagger_{\sigma})G_\sigma > \sim \frac{\rho_0^2(1-\frac{1}{\sqrt{2}})^2}{(-4\kappa_\sigma)^{(-4\kappa_\sigma)}} \tag{51}
\]

Finally, we consider the pairing susceptibility. Following a similar procedure, we find that

\[
<T_r(\sum \sigma d_{\sigma})(\tau)(\sum \sigma d^\dagger_{\sigma})G_\sigma > \sim \frac{\rho_0^2(1-\frac{1}{\sqrt{2}})^2}{(-4\kappa_\sigma)^{(-4\kappa_\sigma)}} \tag{52}
\]

which is enhanced compared to the Fermi-liquid case. This makes it plausible that the ground state in the corresponding lattice model is superconducting. In that case, the intermediate mixed valence dynamics would describe the physics in the normal state, i.e., at temperatures between the transition temperature and some upper cutoff energy scale.

To summarize, the intermediate phase has spin-charge separation, a quasiparticle residue vanishing in a power-law fashion, self-similar local correlation functions with interaction-dependent exponents. These characteristics bear strong similarity to those of the Luttinger liquid in one dimensional interaction fermion systems \[24,25\].

VII. A POINT WITH SIMPLE, BUT NOT EXACTLY SOLUBLE, EFFECTIVE HAMILTONIAN

The three Toulouse points that we have discussed for the mixed valence problem is exactly soluble. In this section, we discuss one more point in the interaction parameter space which is described by a simple effective Hamiltonian. It arises from the choice of \( \alpha = -(1 - \sqrt{2}) \) and \( \beta = \frac{1}{2\sqrt{2}} \). The Coulomb gas stiffness are \( \epsilon_i = \frac{1}{2} \) and \( \epsilon_j = 2 \). In this case, there is a
range of $\gamma$, $-\sqrt{2}\pi \leq \gamma \leq \pi$, that satisfies the requirement that all the phase shifts $\delta^0_\sigma$ fall in the range $[-\pi, \pi/2]$: $\delta^0_\sigma = (3/4 - \sqrt{2}/2 + \sqrt{3}/2)\pi$, $\delta^0_\pi = (\sqrt{2}/2 - 1/4 + \sqrt{3}/2)\pi$, and $\delta^0_\eta = (-1/4 + \sqrt{3}/2)\pi$. This range corresponds to a large ferromagnetic $J_z$ and a large repulsive $V$ (and attractive $V_p$). For instance, choosing $\gamma = \gamma_{\text{min}} = -\sqrt{2}\pi/2$ corresponds to $\delta(J_z/4) = -\sqrt{2}\pi$, $\delta(V) = 0$, and $\delta(V_p) = -\pi$, while choosing $\gamma = \gamma_{\text{max}} = \sqrt{2}\pi$ corresponds to $\delta(J_z/4) = \sqrt{2}\pi$, $\delta(V) = \pi/2$, and $\delta(V_p) = -\sqrt{2}\pi$. Independent of the choice of $\gamma$, $H_t = \frac{1}{\sqrt{2\pi}a} \sum_\sigma (X_{\sigma o} F_\sigma e^{-i\Phi_\sigma} + H.c)$, $H_1 = \frac{1}{\sqrt{2\pi}a}[X_{1\uparrow} F_{\uparrow} e^{-i\Phi_{\uparrow}} + H.c]$. As $H_1$ is strongly irrelevant, we can take the $J_{\perp}$ term to be zero and consider $H_t$ as a perturbation later. Introducing a fermion field $\eta = F_{\eta} e^{-i\Phi_{\eta}}$, and $|\sigma/|=|\sigma > F_{\sigma} F_{\eta}$, the effective Hamiltonian has the following form,

$$H_{\text{eff}}^{D} = \sum_k E_k \eta_k^+ \eta_k + t((X_{1\uparrow} + X_{1\downarrow}) \eta + H.c) - E_o^D X_{oo} \quad (53)$$

This Hamiltonian has the same form as that investigated analytically and numerically in our earlier studies of a spinless two band model in large dimensions [36]. It has also been found [37] to arise within a particular rotation scheme in the bosonized form of the Anderson impurity model with additional screening channels. What distinguishes this effective Hamiltonian from those of the previous subsections is the fact that, the operator $(X_{1\uparrow} + X_{1\downarrow})$ is now a rank-2 matrix. In fact, $H_{\text{eff}}^{D}$ is a rank-2 generalization of the Emery-Kivelson resonant-level model for the Toulouse point of the two-channel spin-$-1/2$ Kondo problem [23]. The non-abelian nature of the phase space makes the problem non-adiabatic and not exactly soluble. In the following, we establish the nature of the solutions in the two limits, $-E_o^D >> |t|$, $W$, and $E_o^D >> |t|$, $W$.

Consider first the limit of $-E_o^D >> |t|$, $W$. Here, the configurations $|\uparrow>$ and $|\downarrow>$ lie at low energies, while $|o>$ should be treated as a high energy configuration. The hybridization $t$ term mixes the low energy and high energy configurations, and can be eliminated with a canonical transformation. This results in an effective Hamiltonian, $H_o + (-\frac{t^2}{|E_o^D|})(X_{1\uparrow} - X_{1\downarrow})(\eta^\dagger \eta - 1/2)$. The sign of the effective interaction makes the spin-flipping term even less relevant. The result is a ground state with a double degeneracy.

For the opposite limit, $E_o^D >> |t|$, $W$, $|o>$ alone lies at low energies, while $|\uparrow>$ and $|\downarrow>$ are high energy configurations that can be eliminated. The resulting low energy behavior is a potential scattering problem. The ground state is a singlet, and the low lying excitations have the Fermi liquid form. Therefore as the impurity level moves from far below to far above the Fermi level, the system evolves from a non-Fermi liquid with a doublet ground state to an empty-orbital Fermi liquid.

We can in fact understand the doublet character of the ground state in the limit of $-E_o^D >> |t|$, $W$ already from the renormalization group equations for the original Hamiltonian, Eq. (19). The relevant renormalization group equations are given in the Appendix B of Ref. (14). For a large negative $E_o^D$, the contribution to the scaling of the spin-flip $J_{\perp}$ term from the second order in hybridization $t$ term is small. The scaling of $J_{\perp}$ is then entirely determined by $J_z$, as in the Kondo problem. Given that $J_z$ is ferromagnetic, the system remains a spin doublet at the fixed point. As $E_o^D$ moves closer to the Fermi level, the contribution of the second order in $t$ term to the scaling of $J_{\perp}$ becomes more important, and eventually dominates the $J_z$ contribution. These conclusions are consistent with the numerical calculations we have performed on the Hamiltonian (53).

Yet one more line of reasoning leads us to the same physical picture of the phases of the Hamiltonian (53). We have shown earlier [36] that the Hamiltonian (53) maps onto the spinless resonant level model with particle-hole symmetry and in the limit of vanishing $W/V_{rl}$ and $W/t_{rl}$ (where $W$, $V_{rl}$ and $t_{rl}$ are, respectively, the conduction electron bandwidth, the interaction strength, and the hybridization of the resonant level model). In this mapping, the parameter $t$ of Eq. (53) is of the order of $W$, while $E_{rl}^D = V_{rl}/2 - t_{rl}$. For a fixed $t_{rl}$, increasing $E_{rl}^D$ in the Hamiltonian (53) is equivalent to increasing $V_{rl}$ in the resonant level model with particle-hole symmetry. When $t_{rl}/W$ is small, the resonant level model undergoes a phase transition from a doublet to a singlet as $V_{rl}$ increases from a strongly attractive value to a large repulsive one. The mixed valence regime of the Hamiltonian (53) is the strong coupling version of the critical regime associated with this phase transition of the resonant level model. Whether the physics of the resonant level model at large values of $t_{rl}/W$ and $V_{rl}/W$ is smoothly connected to the physics of the resonant level model at small $t_{rl}/W$ and $V_{rl}/W$, or a phase transition separates these two regimes, remain unclear and is a problem deserving further investigation.

VIII. CONCLUDING REMARKS

A. Related Works

The mixed valence problem is closely related to problems in the macroscopic quantum tunneling (MQT) and macroscopic quantum coherence (MQC) where a few local degrees of freedom are coupled to a bath of low energy excitations [23]. In the MQT and MQC literature, typically only two-level systems are considered. The mixed valence problem amounts to a three-level generalization.

The mixed valence problem has historically been studied in the context of impurities embedded in a metal. It was stressed early on that, in order to satisfy the Friedel
In the context of high temperature superconductivity, it has been suggested \[18,19\] that the mixed valence regime of an impurity model, with a repulsive impurity density-conduction electron density interaction and a large number of screening conduction electron orbitals, would be a local model exhibiting the novel non-Fermi liquid characteristics of the marginal Fermi liquid, i.e. logarithmically divergent charge and spin susceptibilities. The numerical results of Ref. \[17\] indicate divergent charge and spin susceptibilities near the mixed valence point. However, the numerical results are not conclusive because the susceptibility enhancement may be just due to a crossover to a local moment regime as the impurity level is varied. The divergence is especially difficult to see in the spin susceptibilities near the mixed valence point. How- ever, the numerical results are not conclusive because the susceptibility enhancement may be just due to a crossover to a local moment regime as the impurity level is varied. The divergence is especially difficult to see in the spin susceptibilities, as the susceptibility continues to increase when \(E_d^o\) is decreased through the transition regime \[17\].

Within the renormalization group analysis, the effect of screening channels is to modify the initial conditions of the renormalization group flow \[9\]. The additional screening channels are passive observers which slow down the response of the impurity degrees of freedom (hence increase the orthogonality) but do not participate in the formation of fixed points other than those within the renormalization group classification. This is consistent with the considerations of Giamarchi et. al. \[41\] and Guinea et. al. \[8\]. From this perspective, the Anderson model with additional screening channels has the same low energy behavior as the generalized Anderson model considered here as well as in our earlier works \[10,11\].

Recently, however, two groups \[18,19\] have sought to study an exactly soluble point of the Anderson model with additional screening channels. These works, using the bosonization method, have reached conclusions that would signal a novel fixed point unexpected from our previous renormalization group results. One of the major conclusions in this work – the arguments for which being detailed in Secs. \[14,15\] – is that the fixed points discussed in Refs. \[18,19\] are the result of using incorrect bosonization expressions for the fermion operators. What was missing are the Klein factors that keep track of the anticommutation relations of the fermions of different spin species. When the correct bosonization expressions are used, the results become compatible with our previous renormalization group results. We are therefore forced to the conclusion that, the only known generic solutions to the spin–\(\frac{1}{2}\) mixed valence problem in the generalized Anderson impurity models are the three phases identified within our previous renormalization group scheme.

**B. The Intermediate Phase in Realistic Models**

The intermediate mixed valence state that we have identified represents a new state of strongly correlated electron systems. It will therefore be interesting to explore the phenomenological consequences of this non-Fermi liquid state, and to search for such a state in other strongly correlated electron models. In this connection, two important issues need to be addressed.

First, within the generalized Anderson model that we have studied, the interaction parameter regime for this intermediate phase corresponds to a range of antiferromagnetic exchange interaction, and finite attractive density-density interaction, between the impurity and the conduction electrons [in addition to the large repulsive on-site Hubbard interaction]. It is important to address how this attractive density-density interaction between the impurity and conduction electrons can be generated from purely repulsive interactions in more realistic impurity and lattice models. Several directions have been explored along this direction. Additional screening channels enhance the orthogonality effects \[10\] and effectively play the role of attractive density-density interactions. Alternatively, dynamical screening effects that arise from integrating out high energy configurations in strongly correlated electron systems can generate effective attractive density-density interactions \[11\]. From the perspective of a local approach such as in the limit of infinite dimensions, this effect is especially important since the effective bandwidth of the self-consistent conduction electron bath is usually quite small \[14,15\]. The generation of attractive density-density interaction from purely repulsive interactions have also been discussed in a class of multi-band models \[33\].

Second, in general non-Fermi liquid states in impurity models can be realized only through fine-tuning parameters. For the intermediate mixed valence phase, there is one parameter that needs to be fine-tuned, namely the impurity level \(E_d^o\). This places constraints on the realization of the intermediate state in real materials displaying impurity physics. However, the situation becomes much better in real materials that are described by lattice models, as alluded to at the beginning of this paper. In lattice models, the mixed valence condition can be satisfied over a range of densities \[14,15\].

**C. Summary**

In this paper, we have studied several exactly soluble points in the mixed valence regime of the generalized Anderson model. We found three such points and clarified the physics of each. Two of these points have the strong coupling, Fermi liquid behavior. The third Toulouse point describes the novel intermediate mixed valence phase. Our explicit results about the correlation functions at this last Toulouse point clarified the exci-
tation spectra in this new phase of strongly correlated electron systems. Finally, we established that, once the anticommutation relations between the bosonized forms of the fermion fields are taken care of, the Toulouse-point results derived within the bosonization formalism become consistent with our previous renormalization group results.

From a more general perspective, our results clearly illustrate the importance of the competition between local charge and spin fluctuations in strongly correlated electron systems. In the intermediate phase, the competing low energy local charge and spin fluctuations lead to a spin-charge separation, Fermi-liquid-like spin susceptibilities, non-Fermi-liquid charge susceptibilities, non-Fermi liquid single particle spectral functions, and an enhanced pairing susceptibility. This represents a new route towards spin-charge separation alternative to what leads to the Luttinger liquid in the interacting fermion models in one dimension. In our case, the underlying physics is local in nature, while in one dimension, it is dominated by long wavelength fluctuations. Nonetheless, the characteristics of the correlation functions in the intermediate phase have strong similarities to those of the Luttinger liquid.

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APPENDIX A: BOSONIZATION FOR IMPURITY PROBLEMS

In this appendix, we summarize the bosonization procedure relevant to our discussion. For the purpose of studying an impurity problem with contact interaction at \( r = 0 \) only, the \( S \)-wave component of the conduction electrons alone needs to be kept. This \( S \)-wave component can in turn be written as a superposition of an incoming component and an outgoing one defined on the half-axis \( r \in [0, +\infty) \), with the boundary condition that these two components be equal at the origin \( r = 0 \). This boundary condition allows us to keep only one, say the incoming, component while simultaneously extending the problem to the full axis, \( x \in (-\infty, +\infty) \). Denoting this component as \( \psi_\sigma(x) \), discarding the uncoupled higher-than-\( S \)-wave components of the conduction electrons, and linearizing the energy dispersion about the Fermi level, we can rewrite the Hamiltonian for the non-interacting conduction electron bath, \( H_o \), as follows,

\[
H_o = \sum_\sigma v_F \int \, dx \psi_\sigma \frac{d\psi_\sigma}{dx}
\]

where \( v_F \) is the Fermi velocity. The linearized conduction electron dispersion assumes the form \( E_k = v_F (k - k_F) \). The density of states is \( \rho(\epsilon) = \sum_k \delta(E_k - \epsilon) = \frac{1}{2\pi v_F} \).

We can now introduce a boson representation of the \( \psi \)-field. To keep track of the anticommutation relation between the fermion fields, we write the boson representation of the fermion fields as follows,

\[
\psi_\sigma^\dagger(x) = F_\sigma^\dagger \frac{1}{\sqrt{2\pi a}} e^{i\Phi_\sigma(x)} e^{ik_F x}
\]

Here \( a \) is a cutoff scale which can be taken as a lattice spacing. \( \Phi(x) \) is defined in terms of the Tomonaga bosons,

\[
\Phi_\sigma(x) = \frac{2\pi x}{L} N_\sigma + \sum_{q>0} \sqrt{\frac{2\pi}{qL}} (-ib_\sigma^\dagger e^{iqx - qa/2} + ib_\sigma e^{-iqx + qa/2})
\]

In Eq. \( (A3) \), \( b_{q\sigma} \) and \( b_{q\sigma}^\dagger \) are the Tomonaga bosons,

\[
\begin{align*}
b_{q\sigma} &= \sqrt{\frac{2\pi}{qL}} \sum_k \psi_{k+q\sigma}^\dagger \psi_{k\sigma} \\
b_{q\sigma}^\dagger &= \sqrt{\frac{2\pi}{qL}} \sum_k \psi_{k\sigma}^\dagger \psi_{k+q\sigma}
\end{align*}
\]

Notice that \( \Phi_\sigma(0) \) involves only the \( q \neq 0 \) components of the Tomonaga bosons. \( L \) is the length of the dimension: \( x \in [-L/2, L/2] \). \( N_\sigma \) and \( F_\sigma \) represent the zero modes of the boson fields. \( N_\sigma \) is the deviation of the conduction electron occupation number from the ground state value. It represents the \( q = 0 \) counterpart of the finite \( q \) Tomonaga boson occupation number \( n_{q\sigma} \equiv b_{q\sigma}^\dagger b_{q\sigma} \). The boson Hilbert space is spanned by \( |N_\sigma, n_{q\sigma}\rangle \). Within this Hilbert space, the operator \( F_\sigma^\dagger \) raises \( N_\sigma \) by one, while its adjoint, \( F_\sigma \), lowers \( N_\sigma \) by one \( |27,28\rangle \). These are traditionally called the “Klein factors”. They satisfy the following relations,

\[
\begin{align*}
F_\sigma^\dagger F_\sigma &= F_\sigma F_\sigma^\dagger = 1 \\
F_\sigma^\dagger F_\sigma &= -F_\sigma F_\sigma^\dagger \\
F_\sigma F_\sigma &= -F_\sigma F_\sigma
\end{align*}
\]

They commute with \( b_{q\sigma} \) and \( b_{q\sigma}^\dagger \), for \( q \neq 0 \).

In this boson representation, the non-interacting Hamiltonian Eq. \( (A1) \) has the following form,

\[
H_o = \frac{v_F}{4\pi} \sum_\sigma \int_{-\infty}^{+\infty} \, dx \left( \frac{d\Phi_\sigma(x)}{dx} \right)^2
\]

and the density operator

\[
\rho_\sigma(x) \equiv \psi_\sigma^\dagger(x) \psi_\sigma = \frac{1}{2\pi} \frac{d\Phi_\sigma(x)}{dx}
\]

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APPENDIX B: ATOMIC EXPANSION

Consider first the Toulouse point II of the Kondo problem discussed in Sec. II C. Given that the vicinity of this Toulouse point corresponds to $J_z \gg J_{\perp}, W$, we can carry out an expansion in terms of $J_z, W$ and $W'/J_z$. For this purpose, we rewrite the original Kondo Hamiltonian as

$$H = W \sum_{i=0,\sigma}^N (c_i^\dagger c_{i+1\sigma} + H.c.) + \frac{J_z}{2} (S^z c_i^\dagger c_i + S^- c_i^\dagger c_i^-) + \frac{J_z}{4} S_z \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$$

where $c_{i\sigma}^\dagger$ creates a Wannier orbital at site $i$ in the Wilson basis [2]. To the leading order, we need simply to diagonalize an atomic problem defined in the Hilbert space of the impurity spin doublet and $c_{i\sigma}^\dagger$. The lowest energy atomic states are given

$$|1> = |\uparrow\uparrow\rangle |\downarrow\rangle$$
$$|2> = |\downarrow\rangle |\uparrow\downarrow\rangle$$

For finite $J_{\perp}$ and $W$, these low energy atomic states become coupled with the high energy atomic states, $|A\sigma> = |\sigma\rangle |\downarrow\uparrow\rangle$, $|B\sigma> = |\sigma\rangle |\downarrow\rangle |\uparrow\rangle$, and $|C\sigma> = |\sigma\rangle |\uparrow\rangle |\downarrow\rangle$. Integrating out these high energy states via a canonical transformation

$$S = \frac{W}{J_z} (-X_{A\uparrow\uparrow,1}c_{1\uparrow\uparrow} + X_{B\uparrow\downarrow,1}c_{1\uparrow\downarrow})$$

leads to an effective Hamiltonian

$$H_{eff} = H_{o} + J_{\perp} (X_{11} + X_{21}) + J'_z (X_{11} - X_{22}) \sum_\sigma c_{1\sigma}^\dagger c_{\sigma}$$

where

$$H_{o} = W \sum_{i=1,\sigma}^N (c_i^\dagger c_{i+1\sigma} + H.c.)$$

and $J'_z = W^2/J_z$.

The effective spin operators are, $S^z_{eff}$ = and $S^+_{eff}$ = are given by

$$S^z_{eff} = e^S z e^{-S} = \frac{1}{2} (X_{11} - X_{22})$$
$$S^+_{eff} = e^S z^+ e^{-S} = 2 (W/J_z)^2 c_{1\uparrow\uparrow}^\dagger c_{1\downarrow\downarrow} X_{12}$$

Eqs. (B3) and (B4) are the direct analogs of Eqs. (12) and (15).

We now turn to the strong coupling Toulouse point I of the mixed valence problem discussed in Sec. IV. The low energy atomic states are,

$$|1> = |\uparrow\uparrow\rangle |\downarrow\rangle$$
$$|2> = |\downarrow\rangle |\uparrow\downarrow\rangle$$
$$|O> = |\uparrow\rangle |\downarrow\rangle$$

The mixed valence condition amounts to the requirement on $E^o$ such that the energy difference between $|1>$, $|2>$ and $|O>$, $2E^o = E^o + V + |V_0| - \frac{W}{4}$, is small. The canonically-transformed Hamiltonian is

$$H_{eff} = H_{o} + E'_d (X_{11} + X_{22} - X_{00}) + J_{\perp} (X_{12} + X_{21})$$
$$+ t (X_{1O} - X_{2O} + H.c.) + J'_z (X_{11} - X_{22}) \sum_\sigma c_{1\sigma}^\dagger c_{\sigma}$$

where $V_0 = W^2/J_z$. The canonically-transformed operators are

$$(d_{\sigma}^\dagger)_{eff} \sim \sqrt{W/J_z} c_{1\uparrow\sigma} X_{1O}$$

and

$$(d_{\sigma}^\dagger)_{eff} \sim -\sqrt{W/J_z} c_{1\downarrow\sigma} X_{2O}$$

These expressions are the direct analogs of the expressions derived using the bosonization representation, Eqs. (B4) and (B5).

Finally, we consider the intermediate Toulouse point of Sec. VI. The low energy atomic states are,

$$|A> = \frac{1}{\sqrt{2}} \sum_\sigma |\sigma\rangle |\uparrow\rangle |\downarrow\rangle + |\downarrow\rangle |\downarrow\rangle |\uparrow\rangle$$
$$|B> = \frac{1}{\sqrt{2}} \sum_\sigma |\sigma\rangle |\uparrow\rangle |\downarrow\rangle$$
$$|O> = |\uparrow\rangle |\downarrow\rangle$$

The canonical transformed Hamiltonian is

$$H_{eff} = H_{o} + J_{\perp} [-X_{AA} + X_{BB}] + t' (X_{AO} c_{1\uparrow\sigma} + H.c.)$$
$$+ V' (X_{AA} + X_{OO}) \sum_\sigma c_{1\sigma}^\dagger c_{\sigma}$$

where $t' = -2W^2/J_z$ and $V' = -(1+\nu^2)W^2/4$. The canonically transformed $S^z_{eff}$, $S^+_{eff}$, and $\rho_{eff}$ are similar to those given in Eq. (B8), while
\[(d_{\sigma})_{\text{eff}} \sim - \frac{1}{\sqrt{2}} \frac{W}{J_z} + \frac{W}{|V|} c_{1\bar{\sigma}} (\sigma X_{AO} + X_{BO}) \]  \hspace{1cm} (B11)

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