Conserving many body approach to the fully screened, infinite $U$ Anderson model.

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Using a Luttinger Ward scheme for interacting gauge particles, we present a conserving many body treatment of a family of fully screened infinite $U$ Anderson models that has a smooth cross-over into the Fermi liquid state, with a finite scattering phase shift at zero temperature and a Wilson ratio greater than one. We illustrate our method, computing the temperature dependence of the thermodynamics, resistivity and electron dephasing rate and discuss its future application to non-equilibrium quantum dots and quantum critical mixed valent systems.

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The infinite $U$ Anderson model is a central element in the theory of magnetic moments, in their diverse manifestations within antiferromagnets, heavy electron systems and quantum dots. While the underlying physics of the Anderson impurity model is well understood, with a wide variety of theoretical techniques available for its description, there are many new realms of physics that relate to it, such as quantum critical mixed valent and heavy fermion materials or voltage biased quantum dots where our tools and understanding of equilibrium impurity physics are inadequate.

These considerations motivate us to seek new theoretical tools with the flexibility to explore the physics of the Anderson model in a lattice and non-equilibrium environment. One of the well-established tools of many body physics is the Luttinger Ward (LW) scheme. This scheme permits a systematic construction of many-body approximations which preserve important interrelationships between physical variables, such as the Luttinger sum rule, or the Korringa relationship between spin relaxation and spin susceptibility, that are implied by conservation laws. Recent work on the application of the LW scheme to gauge theories provides new insight into how such conserving approximations can be extended to encompass Fermi liquids in which ultra-strong interactions are replaced by constraints on the Hilbert space.

In this paper we show how these insights can be applied to the infinite $U$ Anderson model to obtain a description of the smooth cross-over from local moment to Fermi liquid behavior, in which the important conserving relationships between the physical properties of the ground-state, such as the Friedel sum rule and the Yamada-Yosida relationships between susceptibilities and specific heat, are preserved without approximation. Our method is scalable to a lattice, and can also be extended to non-equilibrium settings. To demonstrate the method we compute the temperature dependent thermodynamics, resistivity and electron dephasing rate in a single impurity model, and discuss how the method can be extended to encompass a non-equilibrium environment.

Our starting point is a Schwinger boson representation for the $SU(N)$ infinite $U$ Anderson model. Schwinger bosons can be used to describe magnetically ordered local moments, and in the limit of large $N$, this description becomes exact. Recent progress has shown how this scheme can be expanded to encompass the Fermi liquid physics of the Kondo effect, through the study of a family of “multichannel” Kondo model, in which the number of channels $K$ commensurate with $n_b = 2S$, ($K = 2S$), where $S$ is the spin of the local moment. The corresponding infinite $U$ Anderson model is

$$
\mathcal{H} = \sum_{k\nu\alpha} \epsilon_{k\nu} c_{k\nu\alpha}^\dagger c_{k\nu\alpha} + \frac{V}{\sqrt{N}} \sum_{k\nu\alpha} c_{k\nu\alpha}^\dagger \chi_{k\nu}^\dagger b_{\alpha} + H.c
\]

$$

Here $c_{k\nu\alpha}^\dagger$ creates a conduction electron with momentum $\vec{k}$, channel index $\nu \in [1, K]$, and spin index $\alpha \in [1, N]$. The bilinear product $b_{\alpha}^\dagger \chi_{k\nu}$ between a Schwinger boson $b_{\alpha}^\dagger$, and a slave fermion (or holon) operator $\chi_{k\nu}$ creates a localized electron in the constrained Hilbert space, which hybridizes with the conduction electrons. The $\sqrt{N}$ denominator in the hybridization ensures a well-defined large $N$ limit. The energy of a singly occupied impurity $\epsilon_0$ is taken to be negative. The conserved operator $Q = \sum_{\alpha} b_{\alpha} b_{\alpha} + \sum_{k\nu} \chi_{k\nu}^\dagger \chi_{k\nu}$ replaces the no-double occupancy constraint of the infinite $U$ Anderson model, where $Q = 2S = K$ is required for perfect screening.

The characteristic “Kondo scale” of our model is

$$
T_K = D \left( \frac{\Gamma}{\pi D} \right)^{K/N} \exp \left\{ -\frac{\pi |\epsilon_0|}{\Gamma} \right\},
$$

where $D$ is the conduction electron half bandwidth, $\Gamma = \pi \rho N^2$ is the hybridization width and $\rho$ is the conduction electron density of states. This relationship follows from general leading logarithmic scaling of the model. The non-trivial prefactor in the Kondo temperature depends on the third order terms in the beta function.
The next step is to construct the LW functional \( Y[G] \). The variation of \( Y[G] \) with respect to the full Green’s functions \( G_\zeta \) of the conduction, Schwinger boson and slave fermion fields, \( \Sigma_\zeta = \delta Y/\delta G_\zeta \), self-consistently determines the self-energies \( \Sigma_\zeta \) of these fields\(^5\). \( Y[G] \) is equal to the sum of all two-particle irreducible free energy Feynman diagrams, grouped in powers of \( 1/N \) (Fig. 1(a)). In our procedure we neglect all but the leading order \( O(N) \) term in the LW functional, and then impose the full self-consistency generated by this functional.

In the formal large \( N \) limit, the conduction electron self-energy is of order \( O(1/N) \), and at first sight, should be neglected. However, the effects of these terms on the free energy are enhanced by the number of channels \( K \) and spin components \( N \), to give a leading order \( O(N) \) contribution to the free energy: it is precisely these terms that produce the Fermi liquid behavior\(^10\). The complex issue of exactly when the conduction electron self-energies should be included is naturally resolved by using the leading order LW functional, subsequently treating \( 1/N \) as a finite parameter, using the conduction electron self-energies inside the self-consistency relations. The explicit expressions for the self-energies are then

\[
\begin{align*}
\Sigma_\chi(\tau) &= V^2 G_b(\tau) G_c(-\tau) \\
\Sigma_s(\tau) &= -(K/N)V^2 G_\chi(\tau) G_c(\tau) \\
\Sigma_c(\tau) &= (1/N) V^2 G_b(\tau) G_\chi(-\tau)
\end{align*}
\]

(3)

where \( G_b \), \( G_\chi \) and \( G_c \) are the fully dressed imaginary time Green’s functions of the boson, holon and conduction electrons respectively. Equations \( \Box \) are solved self consistently, adjusting the chemical potential \( \lambda \) to satisfy the averaged constraint \( \langle Q \rangle = K \).

A key step in the derivation of the Ward identities is the presence of a scale in the excitation spectrum, which manifests itself mathematically in our ability to replace Matsubara summations by integrals at low temperatures:

\[
T \sum_{\omega_n} \rightarrow \int \frac{d\omega}{2\pi}
\]

This transformation is the key to derivations of the Friedel sum rule, the Yamada-Yosida and Shiba relationships between susceptibilities, specific heat and spin relaxation rates\(^12\)\(^13\)\(^14\). There is long history of attempts to develop conserving approximations to the infinite U Anderson model\(^12\)\(^13\)\(^14\), but each has been thwarted by the development of scale-invariant X-ray singularities in the gauge or slave particle spectra for which the above replacement is illegal. In the multi-channel approach, the gauge particles - the formation of a stable Kondo singlet when \( 2S = K \) leads to the formation of a gap in the spinon and holon spectrum [see Fig. 1(b,c)], which permits a Fermi liquid spectrum to develop at lower energies. This feature permits all of the manipulations previously carried out on the finite U Anderson model to now be extended to infinite \( U \). Moreover, these relationships are all satisfied by the use of the leading LW functional.

There are many important conserving relationships that are preserved, provided the spinons and holons develop a gap. The first of these is the Friedel sum rule (or in the lattice, the Luttinger sum rule), according to which the sum of the conduction electron phase shifts must be equal to the total charge \( K - n_\chi \) on the impurity, whith \( n_\chi \) as the ground-state holon occupancy, so

\[
\delta_c = \pi \frac{K - n_\chi}{N} + O\left(\frac{T_K}{D}\right),
\]

(4)

Fig. 1. contrasts the dependence of phase shift obtained from the t-matrix in our conserving scheme, with that obtained using \( \Sigma_c \) from the leading order \( 1/N \) expansion. The relationship \( \Box \) is obeyed at each value of \( N \) in our approximation.

The quasiparticle spectrum in the Fermi liquid ground-state is intimately related to the conduction electron phase shifts via Nozières Fermi liquid theory\(^13\). The change in the scattering phase shift in response to an applied field, or a change in chemical potential, is directly related to the spin, charge and channel susceptibilities, which in turn, leads to a generalized “Yamada-Yosida identity”, distributing the \( N \) degrees of freedom among the spin, flavor and charge sectors:

\[
NK \frac{\gamma}{\gamma^0} = K \frac{N^2 - 1}{N} \chi_s + N \frac{K^2 - 1}{K} \chi_f + \frac{\chi_c}{\chi_c^0}.
\]

(5)

Here \( \gamma \) stands for the specific heat coefficient \( \gamma = C/T \), and \( \chi_s, \chi_f \) and \( \chi_c \) stand for the spin, flavor and charge susceptibilities. \( \chi_{s,f,c}^0 \) denotes the corresponding susceptibilities in the absence of the impurity. Our identity \( \Box \) reduces to the known results for the Wilson ratio in the
heat coefficient and entropy. The latter marks the saturation of the specific self-energy corrections that arise from the field-dependence of the self-energies. The single and double primes mark the real and imaginary part respectively. The impurity contribution to the spin susceptibility, we couple a small magnetic field to the magnetization, defined as

$$S = -\text{Tr}_c \int d\epsilon \frac{dn_c}{dT} \left[ \text{Im} \left( -G^{-1}_\zeta \right) + G'_\zeta \Sigma''_\zeta \right], \quad (6)$$

where the trace denotes a sum over the spin and channel indices of the various fields and \(n_\zeta\) is the distribution function (Fermi for \(\zeta = c, \chi\) and Bose for \(\zeta = b\)). \(G_\zeta\) and \(\Sigma_\zeta\) respectively denote the retarded Green functions and self energies. The single and double primes mark the real and imaginary part respectively. The impurity contribution to the entropy \(S_{\text{imp}} = S - S_0\), where \(S_0\) is the entropy of the bare conduction band, is shown in the upper panel of Fig. 2. An inspection of low temperatures shows a linear behavior of the impurity contribution to the entropy. The latter marks the saturation of the specific heat coefficient \(\gamma_{\text{imp}} = \partial S_{\text{imp}} / \partial T\) at low temperatures and the formation of a local Fermi liquid.

To calculate the spin susceptibility, we couple a small magnetic field to the magnetization, defined as

$$M = \sum_\alpha \text{sgn}(\alpha - \frac{N+1}{2}) (b_\alpha^d b_\alpha + \sum_{\vec{k}\nu} c_{\vec{k}\nu a}^d c_{\vec{k}\nu a}).$$

The impurity magnetization is obtained by subtracting the magnetization of the free conduction sea from \(M\). When we apply a field, we must keep track of the vertex corrections that arise from the field-dependence of the self-energies. These vertex functions are essential to maintain the conservation laws. We compute the magnetic field vertex functions by iterating the solutions to self-consistency in a small magnetic field. Figure 2 shows the impurity susceptibility \(\chi(T)\). The susceptibility is peaked slightly below the Kondo temperature and saturates to a constant at a lower temperature.

One of the important conservation laws associated with the conservation of spin, is the Korringa-Shiba relation between the dynamical and static spin susceptibility. On the assumption that the gauge particles are gapped, the LW derivation carried out by Shiba on the finite U Anderson model, some thirty years ago, can be simply generalized to the infinite U model, to obtain\(\chi''(\omega)/\omega_{\omega=0} = (N\pi/2K)(\chi/N)^2\). This relationship guarantees that the power-spectrum of the magnetization is linear at low frequencies, ensuring that the spin response function decays as \(1/t^2\) in time. Remarkably, a Fermi liquid, with slow gapless spin excitations is sandwiched beneath the spinon-holon continuum.

We now turn to a discussion of the electron scattering off the impurity, which is determined by the conduction electron t-matrix, \(t(z) = \sum_{\nu} G_{\nu}(z) = \sum_{\nu} (\epsilon - \epsilon_{\nu})^{-1}\) is the bare local conduction electron propagator. Various important physical properties, such as the impurity resistivity and the electron dephasing rate in the dilute limit can be related to this quantity. Figure 3 shows the imaginary part of \(t(\epsilon + i\eta)\): as temperature is lowered towards the Kondo temperature, a resonance peak starts to develop around the Fermi energy. The peak continues to evolve with temperature and finally saturates a decade below the Kondo temperature. The fully developed resonance is pinned to the Langreth sum-rule value of \(\sin^2\delta_\epsilon / \pi\rho_\epsilon\) at the Fermi energy presented by the dot in the inset of Fig. 3.

The impurity contribution to the resistivity \(R_i\) is related to a thermal average of the t-matrix,

$$R_i = \frac{3m^2 n_i}{2e^2 \rho k_F} \left\{ \int d\epsilon \left( -\frac{\partial f}{\partial \epsilon} \right) [\text{Im} (\epsilon + i\eta)]^{-1} \right\}^{-1}. \quad (7)$$
where $k_F$ is the Fermi wavelength and $f$ is the Fermi distribution function. Figure 4 shows $R_0(T)$. The resistivity increases as the temperature decreases, saturating at a value determined by the scattering phase shift.

As a final application of the t-matrix, we compute the electron dephasing rate $\tau_\phi^{-1}$ that controls the field dependence of weak electron localization. In the cross-over to the Fermi liquid state, the formation of the Kondo resonance gives rise to a peak in the inelastic scattering\cite{19} and the electron dephasing rate\cite{20}. In the dilute limit, the impurity contribution to the dephasing rate is given by $\tau_\phi^{-1} = 2n_i[-\text{Im} - \pi \rho |t|^2]$\cite{19,21,22}. Fig. 4 shows the dephasing rate on the Fermi surface computed from $\tau$, showing how the scattering scales with the Kondo temperature $T_K$ in the Kondo regime of the model.

Our calculation of the dephasing rate shows that our method captures the cross-over into the coherent Fermi liquid. However, it also highlights a shortcoming that we hope to address in future work. At low temperatures, the electron dephasing rate has a quadratic dependence on temperature. The electron-electron scattering diagrams responsible for these processes involve an internal loop of gauge particles, which only enters in the subleading $O(1)$ terms of the LW functional shown in Fig. 1(a), which are absent from the current work. On the other hand, the low temperature, on-shell value of the conduction electron vertex is directly related to $\gamma$ by Ward identities\cite{21}, providing a possible future simplification for treating these processes.

There are many directions for future development. We are particularly interested in the extension to nonequilibrium quantum dots\cite{4}. The theoretical understanding of the Kondo physics of quantum dots at finite voltage bias is still evolving. An extension of our method to a voltage biased infinite Anderson model can be made using a Keldysh generalization of the self-consistency equations\cite{24}. Many features of our approach, its conserving properties, its inclusion of scaling properties up to third order in the beta function, and its systematic incorporation of spin relaxation effects on the boson lines, suggest that this will be a robust method to examine how spin and electron dephasing effects evolve with voltage in quantum dots. These methods can also be used to study the voltage dependence\cite{24} of the distribution function and in noise in mesoscopically doped wires\cite{25}.

One of the striking features of the Schwinger boson approach to the Anderson and Kondo models, is the coexistence of a gapless Fermi liquid, sandwiched at low energies between a gapped spinon and holon fluid. The gap in the spin-charge decoupled excitations appears intimately linked to the development of the Fermi liquid Ward identities. The methods presented in this paper can be scaled up to describe the dense Anderson and Kondo lattice models, where the Friedel sum rule is replaced by the Luttinger sum rule\cite{7}. In the lattice, the $U(1)$ local symmetry of the impurity model will in general be replaced by a global $U(1)$ symmetry associated with the pair-condensed Schwinger bosons\cite{26}. In this setting, the gapped spinons and holons are propagating excitations, whose gap is fundamental to the large Fermi surface. It is this very gap that we expect to collapse at a quantum critical point. The current work, which includes the effects of valence fluctuations, provides a powerful framework for examining this new physics.

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