Extended Dynamical Mean Field Theory
for Correlated Electron Models

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An overarching question in strongly correlated electron systems is how the landscape of quantum phases emerges from electron correlations. The method of extended dynamical mean field theory (EDMFT) has been developed for clean lattice models of the correlated electrons. For such models, not only onsite Hubbard-like interactions are important, but so are intersite interactions. Importantly, the EDMFT method treats the interplay between the onsite and intersite interactions dynamically. It was initially formulated for models of the two-band Anderson-lattice type with intersite interactions, as well as for the one-band Hubbard type with intersite Heisenberg-like terms that are often called Hubbard-Heisenberg models. In the case of Kondo lattice models, the EDMFT method incorporates a dynamical competition between the local Kondo and intersite Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions. In these models, the EDMFT-based analyses led to the notion of Kondo destruction, which has played a central role in the understanding of quantum critical heavy fermion metals. In this article, we summarize the EDMFT method, and survey its applications, particularly for Kondo/Anderson lattice models. We also discuss the prospect for further developing the EDMFT method, as well as for applying it to address the correlation physics in a variety of new settings. Among the latter are the orbital-selective Mott physics that arises both in iron-based superconductors and in frustrated bulk systems with topological flat bands.
I. INTRODUCTION

A wide variety of bad metals form the bedrock of strongly correlated electron systems. Often, a bad metal is operationally defined in terms of the electrical resistivity at room temperature reaches or exceeds the Mott-Ioffe-Regel limit \([1, 2]\). This limit is defined in terms of the mean free path \(\ell\), corresponding to \(k_F\ell/2\pi \approx 1\) for each Fermi surface, which signifies a proximity to a Mott localized state \([2]\). A complementary criterion is based on a sizeable reduction of the optical Drude weight from its non-interacting-electron expectation \([3–5]\). Heavy fermion metals and metals that lie in the vicinity of a Mott insulator exemplify bad metals.

Quantum many-electron systems are traditionally studied in terms of a perturbative expansion of the interaction \([6]\). The assumption is that the noninteracting electrons are the building blocks for low-energy physics. A standard model is the one-band Hubbard model, which contains an electron band of width \(D\) and an onsite interaction – the Hubbard interaction – of strength \(U\). The Fermi liquid description applies in an order-by-order perturbative treatment of \(U/D\) to infinite orders. Here, coherent quasiparticles appear as a pole in the single-particle Green’s function \(G(k, \omega)\). When \(U/D\) becomes of order unity, non-perturbative effects may develop. The most famous case is the development of a Mott insulator for a half-filled band \([7]\), in which the electron correlations drive the quasiparticle weight to zero. Concurrently, a gap develops in the single-particle and charge excitation spectrum; the ground state is no longer a metal and is no longer adiabatically connected to its noninteracting counterpart.

In general, when the electron correlations reach and exceed the electron bandwidth, as is the case in bad metals, other degrees of freedom emerge as a part of the building blocks for the low-energy physics. A typical case involves spins, as seen from the notion of local moment formation of a correlated and deep orbital in a metallic matrix \([8]\). As a result, models of strongly correlated electrons may involve both local moments and itinerant electrons, as exemplified by heavy fermion metals \([1, 9–12]\). A similar set of building blocks develop once a Mott insulator \([7]\) is coupled to a metallic band.

When expressed in terms of the electron degrees of freedom, the correlation physics describes the effect of Coulomb repulsion between the electrons \([13, 14]\). However, if represented in terms of the emergent building blocks such as local moments, the competition between
different types of effective interactions becomes particularly explicit. A case in point is a Kondo lattice Hamiltonian, which contains an antiferromagnetic spin-exchange (Kondo) interaction between the local moments and spins of the conduction electrons on the one hand, and the RKKY interaction between the local moments on the other.

The EDMFT method was introduced to dynamically study this type of competition [15–17]. Consider the case of the Kondo lattice model. Here, the local Kondo interaction favors the formation of a Kondo singlet between the local moments and spins of the conduction electrons. Whereas the RKKY interaction, which often is also antiferromagnetic, promotes singlet formation among the local moments. To properly account for the amplified quantum fluctuations that develop when the two types of effects would produce comparable energy scales, the dynamical interplay between the two interactions is crucial; this interplay is captured by the EDMFT method. This is to be contrasted with the standard dynamical mean field theory [13, 14], in which the local interactions such as the Kondo couplings are treated in a dynamical way, while the intersite interactions such as the RKKY couplings are handled in terms of a static Hartree-Fock approximation.

The EDMFT method has played a central role in the elucidation of quantum phase transitions of heavy fermion metals [18]. Studies based on such a method have led to the advancement of the concept of Kondo destruction [19–23]. Qualitatively, the Kondo physics underlies the formation of (heavy) quasiparticles in such systems. The quasiparticles develop through the formation of the Kondo singlet, and appear in the form of a Kondo-driven composite fermion. These processes are captured by the local self-energy of the conduction electrons. As such, studying the dynamical competition between the RKKY and Kondo interactions provides a way of describing the reduction – and eventual destruction – of the Kondo singlet in the ground state and, by extension, the quasiparticles. In other words, the EDMFT approach is ideally suited to access how (heavy) quasiparticles are lost.

The concept of Kondo destruction has influenced the development of quantum critical metals in a profound way, particularly on the destruction of quasiparticles and dynamical Planckian ($\hbar \omega/k_B T$) scaling at the quantum critical point (QCP), and a sudden jump of a “large” to “small” Fermi surface across the QCP [18].

The present article is devoted to three topics:

- We describe the dynamical equations associated with the EDMFT method.
We illustrate the application of the EDMFT approach by focusing on the Kondo lattice models and summarizing i) the methodological aspect of the approach and ii) the results as pertaining to the heavy fermion quantum criticality. Further analyses that have been motivated by the result of such calculations are touched upon, especially in the form of a global phase diagram.

The prospect for further progress along this general direction is discussed.

II. EDMFT APPROACH

We illustrate the EDMFT approach in terms of the single-band Hubbard-Heisenberg-type model \[15–17, 24\]:

\[
H_{U-v} = \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{\langle ij \rangle} v_{ij} : n_i \lessdot n_j : \tag{1}
\]

The first two terms specify the Hubbard model for a spin-$\frac{1}{2}$ band. The onsite Hubbard interaction is $U$ and the hopping matrix is $t_{ij}$, whose Fourier transform corresponds to the band dispersion $\varepsilon_k$. The third term describes an intersite density-density ($v_{ij}$) interaction (a spin-exchange interaction, $J_{ij}$, can also be added, as originally done; see below), with $n_i$ being the density operator of the $c$-electrons and $: n \lessdot n - \langle n \rangle$ representing its normal-ordered form. For concreteness, we limit the intersite interactions to the nearest-neighbor ($\langle ij \rangle$) contributions, but this can be readily generalized.

The EDMFT approach amounts to the summation of an infinite series of diagrams as outlined in Fig. 1. The approach is systematic and conserving. Moreover, the EDMFT equations are generated by an effective action function of the Baym-Kadanoff type.

The EDMFT approach incorporates a local self-energy, $\Sigma$, for the single-electron Green’s function $G$ and a related irreducible quantity in the density channel, $M$, which is defined in terms of a cumulant that is $v_{ij}$-irreducible [15]; for notational convenience, it has been referred to as a (density) self-energy. The self-energies determine the dynamical density susceptibility and single-particle Green’s function as follows:

\[
\chi(q, \omega) = \frac{1}{M(\omega) + v_q}, \tag{2}
\]
FIG. 1. The single-site, two-site, and three-site diagrams for the Luttinger Ward potential in the extended DMFT [16, 20]. A shaded circle contains all the on-site diagrams fully-dressed by the fermion Green’s function (solid lines) as shown in the first diagram. The dashed lines further represent the intersite interactions; we have denoted them by $J_{ij}$, but they could also be interactions in other channels, such as $v_{ij}$ of Eq. (1).

together with

$$G(k, \epsilon) = \frac{1}{\epsilon + \mu - \epsilon_k - \Sigma(\epsilon)}. \quad (3)$$

These self-energies can be calculated from a local action, which can equivalently be expressed in terms of a local Hamiltonian:

$$\mathcal{H}_{\text{loc},U-v} = U n^\uparrow n^\downarrow + \sum_{k,\sigma} E_p c_{k\sigma}^\dagger c_{k\sigma} + g \sum_p : n : \left( \phi_p + \phi_p^\dagger \right) \quad (4)$$

Here the dispersion of the bosonic bath, along with its fermionic bath counterpart, are self-consistently determined. The set of nonlinear equations can be expressed as follows. The bath dispersion defines Weiss fields, $\chi_0$ and $G_0$, as follows:
\[ g^2 \sum_{\mathbf{p}} \frac{2w_p}{(i\nu_m)^2 - w_p^2} = -\chi_0^{-1}(i\nu_m), \]

(5)

\[ \sum_k \frac{1}{i\omega_n - E_k} = G_0(i\omega_n), \]

where \( \nu_m \) and \( \omega_n \) are bosonic and fermionic Matsubara frequencies, respectively. The Dyson equations for the density and electron self-energies take the following forms:

\[ M(\omega) = \chi_0^{-1}(\omega) + 1/\chi_{\text{loc}}(\omega), \]

(6)

and, as usual,

\[ \Sigma(\omega) = G_0^{-1}(\omega) - 1/G_{\text{loc}}(\omega). \]

(7)

The self-consistency equations can then be simply written to capture the translational invariance:

\[ \chi_{\text{loc}}(\omega) = \sum_{\mathbf{q}} \chi(\mathbf{q}, \omega), \]

(8)

\[ G_{\text{loc}}(\omega) = \sum_k G(\mathbf{k}, \omega). \]

(9)

It can be inferred from Eq. 2 that, for the intersite interactions \( v_{ij} \) or \( I_{ij} \) (for later reference), the following quantity,

\[ \rho_{\text{f}}(x) = \sum_{\mathbf{q}} \delta(x - \mathbf{I}_q), \]

(9)

comes into the self-consistency equation. In practice two particular forms have been used. In one form, \( \rho_{\text{f}}(x) \) has a constant onset at the lower edge of its support. In another, it has a square-root onset.

We stress that the dynamical susceptibility is defined in terms of connected correlation functions. As such, the density operator appears in the equations in the normal-ordered form. This point is also important when states with a conventional long-range order (such as charge or spin orders) are considered. We will write down the corresponding equations below, in the context of Anderson/Kondo lattice models. The importance of this normal ordering in the EDMFT formulation was stressed from the beginning [15, 16, 24]. When the normal ordering is not taken into account, the ordered state would yield an action that (unphysically) scales as \( \beta^2 \) [25].
III. KONDO LATTICE MODEL: EDMFT EQUATIONS AND SOLUTION METHODS

The Kondo lattice model represents the limit of the Anderson lattice model when the \(f\)-electron level lies sufficiently below the Fermi energy, and when the interaction \(U\) for the \(f\)-electrons is sufficiently large [26]. It features two competing interactions. The Kondo coupling/hybridization favors the formation of a Kondo singlet. Whereas the RKKY interaction leads to the development of quantum magnetism; the typical case corresponds to antiferromagnetic (AF) RKKY interactions, which promotes the formation of inter-moment spin singlets.

The vantage point of the Kondo effect provides a particularly clear physical picture. It is the development of the Kondo singlet in the ground state that supports heavy quasiparticles in the excitation spectrum. The dynamical competition brought on by the RKKY interactions is detrimental to the quasiparticles. This has led to the notion of Kondo destruction [1, 9–12, 19], which has played a central role in the elucidation of quantum critical heavy fermion systems.

In this section, we summarize the basic equations of the Kondo lattice model within the EDMFT approach, and discuss the corresponding solutions for the phases and quantum phase transitions.

A. Kondo lattice Hamiltonian

The Kondo lattice Hamiltonian takes the following form:

\[
H_{KL} = \sum_{ij} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{ij} I_{ij} S_i \cdot S_j + \sum_i J_K S_i \cdot c_{i}^{\dagger} \bar{\sigma} c_{i}.
\]  

It contains a conduction-electron band, \(c_{i\sigma}\), with hopping matrix \(t_{ij}\), and, correspondingly, band dispersion \(\varepsilon_k\). At each site \(i\), the spin of the conduction electrons, \(s_{c,i} = (1/2)c_{i}^{\dagger} \bar{\sigma} c_{i}\), is coupled to the spin of the local moment, \(S_i\), by a Kondo interaction, namely an AF Kondo exchange interaction \(J_K\). Here \(\bar{\sigma}\) represents the Pauli matrices. Meanwhile, the local moments are coupled to each other via an RKKY interaction \(I_{ij}\).
B. EDMFT equations

For the Kondo lattice Hamiltonian, the EDMFT approach calculates local correlation function in terms of the following local action [19, 20, 24, 27, 28]:

\[
S_{\text{loc}} = S_{\text{top}} + \int_0^\beta d\tau \int_0^\beta d\tau' \left[ \sum_\sigma c_\sigma^\dagger(\tau)G_0^{-1}(\tau - \tau')c_\sigma(\tau') \right] + \int_0^\beta d\tau h_{\text{loc}}S_z. \tag{11}
\]

Here, \( \beta = 1/k_B T \), \( S_{\text{top}} \) describes the Berry phase of the local moment, while \( G_0^{-1} \) and \( \chi_0^{-1} \) are the dynamical Weiss fields determined self-consistently by Eq. 8. Finally, \( h_{\text{loc}} \) is the static Weiss field determined by an additional self-consistent equation:

\[
h_{\text{loc}} = -I_\mathbf{Q}\langle S_z \rangle. \tag{12}
\]

The retarded interactions of the spin fields have been written with normal ordering. Equivalently, it could be expressed without using normal ordering:

\[
-\int_0^\beta d\tau \int_0^\beta d\tau' \frac{1}{2} : S : (\tau) \cdot \chi_0^{-1}(\tau - \tau') : S : (\tau') = -\frac{1}{2} S(\tau) \cdot \chi_0^{-1}(\tau - \tau')S(\tau') + \int_0^\beta d\tau \tilde{h}_{\text{loc}}S_z(\tau) + \text{const} \tag{13}
\]

\( \tilde{h}_{\text{loc}} = \int_0^\beta \chi_0^{-1}(\tau)m^z d\tau \) is the effective magnetic field from normal ordering and \( m^z = \langle S_z \rangle \). This action is equivalent to the following effective local Hamiltonian:

\[
H_{BFK} = \sum_k E_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_p \omega_p \phi_p^\dagger \phi_p + J_K S \cdot \frac{c_0^\dagger c_0}{2} + g : S : \sum_p (\phi_p^\dagger + \phi_p^\dagger) + h_{\text{loc}}S_z \tag{14}
\]

where \( E_k \) and \( \omega_p \) characterize the dispersion of the fermionic fields \((c_{k,\sigma})\) and bosonic fields \((\phi_p)\), and \( J_K \) \((g)\) is the coupling strength between the impurity and fermionic fields (bosonic fields). The relation between the dispersions and Weiss fields are given in Eq. 5.
C. Variants of the Kondo lattice model

The Kondo lattice Hamiltonian, Eq. (10), has an SU(2) symmetry. In heavy-fermion systems, the spin-orbit coupling can reduce the spin symmetry down to either easy plane (xy-anisotropic) or easy axis (Ising-anisotropic). This can be treated by making the interactions to depend on the spin component \( \alpha = x, y, z \). Because the flow towards the Kondo fixed point in systems with anisotropic Kondo interactions restores the SU(2) symmetry, in practice it suffices to incorporate the spin-anisotropy in the RKKY interaction, namely to replace the term \( \sum_{ij, \alpha=x,y,z} I_{ij} S_i \cdot S_j \) by \( \sum_{ij} I_{ij}^x S_i^x S_j^x \). Correspondingly, in the Bose-Fermi Kondo model, both the dispersion of the bosonic bath and the Bose-Kondo coupling \( g \) depends on the component \( \alpha = x, y, z \).

For large but finite values of the Hubbard interaction \( U \) and \( f \)-orbital-energy level separation from the Fermi level, the \( f \) electrons behave as correlated electrons instead of a pure quantum spin. The system in this case is described by an Anderson lattice model with explicit RKKY interactions:

\[
H_{AL} = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} I_{ij} S_i \cdot S_j + \sum_{i\sigma} V(f_{i\sigma}^c c_{i\sigma} + c_{i\sigma}^\dagger f_{i\sigma}) + \sum_{i} (U n_{i\uparrow}^f n_{i\downarrow}^f + \epsilon_d n_{i\sigma}^f).
\]  

Here, \( f_{\sigma}^c \) creates a correlated electron with spin \( \sigma \), \( n_{i\sigma}^f = f_{i\sigma}^c f_{i\sigma}^\dagger \) and \( S_i = \frac{f_{i\sigma}^c f_{i\sigma}^\dagger}{2} \) are the density operator and spin operators of the \( f \) electrons, \( \epsilon_d \) is the local energy scale, and \( V \) is the hybridization strength. Via EDMFT, the local correlators of the Anderson lattice model are determined by a Bose-Fermi Anderson model with the following action

\[
S_{loc,A} = -\int_0^\beta d\tau \int_0^\beta' d\tau' \sum_\sigma \left[ c_{\sigma}(\tau) G_0^{-1}(\tau - \tau') c_{\sigma}(\tau') + f_{\sigma}(\tau)(\partial_{\tau} - \epsilon_d) f_{\sigma}(\tau) \right]
+ \int_0^\beta d\tau \left[ U n_{i\uparrow}^f(\tau) n_{i\downarrow}^f(\tau) + V \sum_\sigma (c_{\sigma}(\tau) f_{\sigma}(\tau) + h.c.) + h_{loc} S_z(\tau) \right]
- \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' : S : (\tau) \cdot \chi_0^{-1}(\tau - \tau') : S : (\tau')
\]  

The corresponding Hamiltonian reads

\[
H_{BFA} = \sum_k E_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_p \omega_p \phi_p^\dagger \phi_p + h_{loc} S_z + U n_{i\uparrow}^f n_{i\downarrow}^f + \epsilon_d (n_{i\uparrow}^f + n_{i\downarrow}^f)
+ V \sum_{k,\sigma} (\epsilon_{k\sigma} f_{\sigma} + h.c.) + g : S : \sum_p (\phi_p^\dagger + \phi_p^\dagger)
\]  

where the relation between bath dispersions and bath functions are given in Eq. (5).
D. Bose-Fermi Kondo model

FIG. 2. The Kondo fixed point and its destruction of the Bose-Fermi Kondo model, described in terms of an RG flow based on an expansion in $\epsilon$ [20] (that is taken to be $> 0$).

The Bose-Fermi Kondo model contains a Kondo fixed point and, for a suitable form of the bosonic-bath spectrum, its destruction. This was first seen in an RG analysis based on an $\epsilon$-expansion in the Ising-anisotropic Bose-Fermi Kondo model [15], which was subsequently generalized to the SU(2)-symmetric version of the model [29, 30]. Here, $\epsilon$ is defined in terms of the power-law spectrum of the bosonic bath:

$$\rho_b(\omega) \equiv \sum_p \delta(\omega - w_p) \propto |\omega|^{1-\epsilon} \quad \text{for } |\omega| < \Lambda.$$  \hspace{1cm} (18)

When $\epsilon = 0$, the bosonic bath has an ohmic spectrum. For $\epsilon > 0$, the spectrum is sub-ohmic. The RG analysis was extended to two and higher loops [31, 32].

To one loop, the RG equations are

$$\beta(J_K) = J_K(J_K - g^2) \quad , \quad \beta(g) = g(\epsilon/2 - g^2).$$  \hspace{1cm} (19)
They yield a Kondo destruction (KD) quantum critical point as shown in Fig. 2. The KD quantum critical point describes a quantum phase transition between a Kondo-screened phase with $J_K \neq 0$ and a Kondo-destroyed phase with $J_K = 0$.

The Kondo fixed point features a spin-singlet ground state. An infrared Kondo energy scale is nonzero, which makes the local spin susceptibility to take a Pauli form. As the system approaches the separatrix of the RG flow, which is controlled by the critical KD fixed point, this infrared Kondo energy scale collapses to zero, and the local spin susceptibility diverges in the zero-frequency limit at $T = 0$. On the other side of the separatrix, the RG flow is towards a fixed point with zero Kondo coupling. Nonetheless, dynamical Kondo effect still takes place here when the bare Kondo coupling is nonzero.

In the SU(2) BFKM, a very recent study has analytically treated the model based on a large-$S$ expansion [33], where $S$ is the spin size. This analysis finds a slew of new fixed points for small $\epsilon$, beyond the ones that were identified in the aforementioned $\epsilon$-expansion RG method. With increasing $\epsilon$, the analysis identifies a sequence of fixed-point annihilation, which are consistent with – and extends – the results of quantum Monte Carlo calculations [34].

E. Solution methods

To analyze the self-consistent equations of the EDMFT approach, one needs to solve the Bose-Fermi Kondo/Anderson models. We have already discussed the $\epsilon$-expansion RG method. This analytical approach is accompanied by several numerical methods.

One is the numerical renormalization group (NRG) method [27, 35]. Within the framework of NRG, we first preform a logarithmic discretization of both the fermionic bath and bosonic bath and map both baths into semi-infinite chains where the local degrees of freedom are coupled to the first site. Subsequently, the model is solved by diagonalizing the Hamiltonian iteratively. In each step, we add new sites to both chains.

Another is the continuous-time Monte Carlo method. Both the SU(2)-symmetric Anderson model [34] and the Anderson model in the Ising limit [36, 37] can be solved via the quantum Monte Carlo method. For the model in the Ising limit, we first perform the unitary (Firsov-Lang) transformation $f \rightarrow \tilde{f}_\sigma = f_\sigma e^{-g/2\sigma \Phi^z}$, where $\Phi^z$ is a linear function of the bosonic fields corresponding to the bosonic bath. Then we can solve the model by
directly expanding the hybridization term $V(c^\dagger c + \tilde{f}^\dagger \tilde{f})$ and sampling the configuration via the Monte Carlo method. As for the SU(2)-symmetric Anderson model, besides expanding the hybridization term, we also need to expand the perpendicular coupling \cite{34,39} between spin impurity and bosonic fields $gS^x/\phi^x/y$.

IV. KONDO LATTICE MODEL: KONDO DESTRUCTION

A. Phase diagram

The EDMFT analysis led to a continuous zero-temperature transition between a Kondo-driven paramagnetic phase and an AF order, as illustrated in Fig. 3(a), for an Ising-anisotropic Kondo lattice \cite{28}. A $E^*_{\text{loc}}$ scale is defined in terms of the local responses of the effective Bose-Fermi Kondo model. Qualitatively, a vanishing $E^*_{\text{loc}}$ means that the Bose-Fermi Kondo model has reached the critical Kondo-destruction fixed point – the red fixed point shown in the RG flow of Fig. 2.

![FIG. 3. (a) The phase diagram for the Ising-anisotropic Kondo lattice model as determined by the EDMFT approach. The inverse static AF susceptibility as a function of $I/T_K^0$ from the paramagnetic (trial $h_{\text{loc}} = 0$) and AF (trial $h_{\text{loc}} \neq 0$) solutions \cite{40}. (b) The staggered magnetization (solid circle) and the Kondo-destruction energy scale $E^*_{\text{loc}}$ (open diamonds) as a function of $I/T_K^0$ \cite{41}.](image-url)
B. Kondo destruction

For the Ising-anisotropic Kondo lattice model, the scale $E_{\text{loc}}^*$ as a function of the tuning parameter $\delta$, defined as the ratio of the RKKY interaction ($I$) to the bare Kondo scale ($T_0^K$) is shown in Fig. 3(b) [24, 42]. The scale $E_{\text{loc}}^*$ is found to vanish at the QCP, signifying that the QCP is of the Kondo-destruction type. This feature has recently been shown to develop in the SU(2) Kondo lattice model [43].

Kondo destruction leads to the development of singular spin dynamics with a fractional exponent at the QCP. This is illustrated in Fig. 4(a) for the Ising-anisotropic Kondo lattice model [44] and in Fig. 4(b) for the SU(2)-symmetry Kondo lattice model [43].

![Graphs showing frequency dependence of the antiferromagnetic lattice spin susceptibility for (a) Ising-anistropic Kondo lattice at the QCP and (b) SU(2) Anderson lattice in the paramagnetic side.]

FIG. 4. Frequency dependence of the antiferromagnetic lattice spin susceptibility for (a) Ising-anistropic Kondo lattice at the QCP [44] and (b) SU(2) Anderson lattice in the paramagnetic side [43].

C. Dynamical Kondo effect

Kondo destruction in Kondo lattice models originates from the dynamical competition between the Kondo and RKKY exchange interactions. The exact marginality of the Kondo coupling inside the AF order phase has been demonstrated based on an RG analysis within a quantum nonlinear sigma model analysis [45, 46]. Indeed, the dynamical Kondo effect allows the gain of a Kondo exchange energy in the absence of static Kondo singlet formation, which is important to help stabilize a Kondo-destroyed phase and allows for the quantum
FIG. 5. Dynamical local spin susceptibility for SU(2) Anderson lattice model in the magnetic ordered side [43].

phase transition from Kondo phase to be second order. The dynamical Kondo effects is particularly pronounced in the Kondo destroyed phase, in which the amplitude of the static Kondo-singlet vanishes. Figure 5 shows the local dynamical spin susceptibility, $\chi_{\text{loc}}(\omega_n)$, as a function of frequency in the AF phase [43]. The monotonic increase of $\chi_{\text{loc}}(\omega_n)$ as $I/T_K^0$ is tuned towards the QCP reflects the growth of the dynamical Kondo effect. The match of the local dynamics from both sides at the quantum critical point demonstrates the second-order nature of the zero-temperature transition. The dynamical Kondo effect also implies that the quasiparticles near the small Fermi surface in the Kondo-destroyed phase have an enhanced mass, which is important to understand the enhancement of the Sommerfeld coefficient, cyclotron mass, and quadratic-in-$T$ coefficient of the electrical resistivity in the Kondo-destroyed phase implicated in YbRh$_2$Si$_2$ (Ref. [47]) and related systems.
In addition to the spin dynamics, Kondo destruction quantum criticality also involves the localization-delocalization of the $f$-electrons at the QCP. This partial Mott transition is accompanied by a sharp large-to-small Fermi surface reconstruction across the phase transition. Thus, the charge degree of freedom represents an integral part of the quantum criticality. A recent terahertz spectroscopy measurement in the quantum critical heavy fermion metal YbRh$_2$Si$_2$ have discovered a singular charge response [48]. This observation is inconsistent with conventional SDW QCP, where only the order parameter should be singular and the charge correlations are expected to be smooth. The EDMFT analysis is able to capture the singular charge response at the KD QCP [49]. As shown in Fig. 6(a), the charge-carrying hybridization B-field at the KD QCP follows dynamical Planckian scaling. This result is complemented by the corresponding calculation in a Bose-Fermi Kondo model within a dynamical large-$N$ approach, where the index $N$ appears in the spin channel, as shown in Fig. 6(b).

**FIG. 6.** (a) Singular charge response of the hybridization $B$-field in the lattice model at the KD quantum critical point, calculated by the EDMFT method. (b) Dynamical Planckian scaling of the charge response at the KD quantum critical point in the spectral function of the $B$-field in the dynamical large-$N$ limit. Both figures from Ref. [49] (see also Ref. [50]).
VI. FURTHER DEVELOPMENTS

We now turn to discussing the prospect for further developing the EDMFT method, as well as for applying it to new settings for correlation physics.

A. Cluster version of EDMFT

We first summarize the cluster extended dynamical mean field theory (CEDMFT) [51]. We first divide a $d$ dimensional lattice with size $L$ into several clusters, where each cluster has $N_c = (L_c)^d$ sites with size $L_c$. We therefore use $\tilde{x}$ to label the position of cluster and use $X$ to label the position of site within the cluster. Correspondingly, we let $K$ (or $P$) and $\tilde{k}$ (or $\tilde{p}$) to label the reciprocal spaces corresponding to the position vectors $X$ and $\tilde{x}$ respectively. Therefore, the original momentum vector $k$ can be written as $k = K + \tilde{k}$.

Then, via dynamical cluster approximation, we are able to map the original lattice model to a self-consistent impurity model, where the impurities are defined on a cluster. In the case of Kondo lattice model defined in Eq. 10, we obtain the following impurity model

\[
S_{\text{imp}} = S_c + S_\phi + S_I
\]

\[
S_c = -\int_0^\beta \int_0^\beta \sum_{K,\sigma} c_{K,\sigma}^\dagger(\tau) G_0^{-1}(\tau - \tau', K) c_{K,\sigma}(\tau') d\tau d\tau'
\]

\[
S_\phi = -\frac{1}{2} \int_0^\beta \int_0^\beta \sum_{P,\mu} S_\mu^P(\tau) \chi_0^{\mu-1}(\tau - \tau', P) S_\mu^{-P}(\tau') d\tau d\tau'
\]

\[
S_I = \int_0^\beta \sum_{P,K} \frac{J}{\sqrt{N_c}} S_P(\tau) \cdot c_{K+P,\sigma}(\tau) \frac{c_{K,\sigma}(\tau)}{2} d\tau d\tau + \int_0^\beta \sum_P \tilde{I}_P S_P(\tau) S_{-P}(\tau) d\tau
\]

\[
+ \int_0^\beta \sum_{P,\mu} h_\mu^P S_\mu^P(\tau) d\tau
\]

where the intra-cluster interactions are defined as $\tilde{I}_P = \frac{(L_c)^d}{L^d} \sum_{\tilde{p}} I_{P+\tilde{p}}$ with $I_P$ the Fourier transformation of RKKY interactions $I_{ij}$. $h_\mu^P$ corresponds to an effective magnetic field, which characterize the development of long-range magnetic order. $G_0(\tau, K)$ and $\chi_0^{\mu}(\tau, P)$ are the fermionic and bosonic bath functions respectively. The case with $N_c = 2$ is illustrated in Fig.7.

Via the Dyson equations, the self-energies of the single-particle Green’s function and
FIG. 7. Illustration of the two impurity Bose-Fermi Anderson model that arises from the CEDMFT approach.

Spin-spin correlation functions take the following forms

$$M_\mu(i\omega_n,P) = \chi_{_0}^{-1}(i\omega_n,P) - \bar{I}_P + \chi_{\text{loc}}^{-1}(i\omega_n,P)$$

$$\Sigma(i\omega_n,K) = G_0^{-1}(i\omega_n,K) - G_{\text{loc}}^{-1}(i\omega_n,K)$$

where the local correlation functions are defined as

$$\chi_{\text{loc}}^\mu(\tau,P) = \langle T_{\tau} : S_\mu^P : (\tau) : S_{-P}^\dagger : (0) \rangle_{S_{\text{imp}}}$$

$$G_{\text{loc}}(\tau,K) = -\langle T_{\tau} c_{K,\sigma}(\tau) c_{K,\sigma}^\dagger (0) \rangle_{S_{\text{imp}}}$$

where we introduce the normal ordering of spin fields : $S_\mu^P := :S_\mu^P : -m_P^\mu$ with the magnetization $m_P^\mu = \langle S_\mu^P \rangle_{S_{\text{imp}}}$. The bath functions and the effective magnetic fields are then defined self-consistently by requiring

$$\chi_{\text{loc}}^\mu(i\omega_n,P) = \left( \frac{L_c}{L} \right)^d \sum_{\tilde{P}} \frac{1}{I_{P+\tilde{P}} + M_\mu(i\omega_n,P)}$$

$$G_{\text{loc}}(i\omega_n,K) = \left( \frac{L_c}{L} \right)^d \sum_{\tilde{k}} \frac{1}{i\omega_n - \epsilon_{K+\tilde{k}} - \Sigma_c(i\omega_n,K)}$$

$$h_P^\mu = -m_P^\mu \left( \chi_0^\mu(i\omega_n = 0,P) + I_P^\mu - \bar{I}_P^\mu \right)$$

We note that, by adding the $h_P^\mu$ contributions, we have normal-ordered the retarded interactions induced by the bosonic bath $\chi_0^\mu(\tau,P)$. 

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The original lattice model are then solved by repeatedly solving the cluster model in Eq. 20 via quantum Monte Carlo until the self-consistent relations in Eq. 23 are satisfied. Comparing to the single-impurity formula, we are able to partially capture the momentum dependency of the self energies and describe the inter-site correlations in CEDMFT. The inter-site correlations would allow attractive interactions between two electrons from different sites and, thus, provide a route towards unconventional superconductivity. Therefore, CEDMFT provides a platform to study the unconventional superconductivity induced by electron correlations. This approach has allowed the study of how Kondo destruction quantum criticality drives unconventional and high-$T_c$ superconductivity [52].

B. Models with disordered exchange interactions

The EDMFT approach has some similarities with the dynamical mean field theory of random spin systems. The quantum Sherrington-Kirkpatrick model was considered by Bray and Moore in Ref. [53], where the spin-exchange interactions are infinite-ranged, random and have a Gaussian distribution whose mean vanishes and whose variance is $J^2/N_s$ where $N_s$ is the size of the system. A disorder averaging using the replica trick, as usual, gives rise to four-spin interactions, with each spin carrying a replica index. Because the exchange couplings on different bonds are not correlated, the four-spin interaction corresponds to two spins at two different times $\tau$ and $\tau'$, from any site, interacting with two other spins, at the same times $\tau$ and $\tau'$ and from every other site. Taking the limit of $N_s \to \infty$ yields a single-site problem with retarded spin-spin interactions. In the paramagnetic phase, the local correlators are determined by an effective local problem whose form is similar to the spin part of Eq. (11), with a self-consistency equation that corresponds to a semi-circular $\rho_1(x)$. When the spin symmetry is generalized from SU(2) to SU(N) and the limit of large-$N$ is taken, a spin liquid ground state is realized [54].

More recently, a $t-J$ model with such a random-Gaussian $J$ interactions between the spins of the fermions has been studied. The saddle-point equations are similar to the EDMFT equations as reviewed in this article, with a semi-circular $\rho_1(x)$. In this case, while the asymptotic low-temperature dynamics will ultimately be similar to what happens in an SDW QCP, at intermediate temperatures and energies the results [25, 55, 56] are similar to what we have surveyed.
C. Application to electronic structure calculations: the GW+EDMFT approach

The EDMFT approach has been combined with *ab initio* methods for electronic-structure calculations, incorporating non-perturbative effects in the GW-method (GW+DMFT). In the GW approach [57], the self-energies are derived by calculating the one-loop diagrams involving the screened Coulomb interaction, and are momentum- and frequency-dependent. The EDMFT method provides a non-perturbative approach for the local self-energies. In the GW+EDMFT approach [58–61], the two methods are combined where the local part of the GW self-energies are replaced by the EDMFT-derived local self-energies. Thus, the GW+EDMFT approach provides a non-perturbative and efficient method to perform electronic structure calculations from first principles.

D. EDMFT approach in new settings

The EDMFT method is uniquely suited to elucidate the correlation physics in a variety of new settings. Here we describe two issues as examples.

One issue concerns the orbital-selective Mott phase, in which certain orbitals are Mott localized while the others remain itinerant, which is of considerable current interest in the field of iron-based superconductors [5]. Such an orbital-selective Mott phase in the presence of kinetic inter-orbital hybridization has been demonstrated using certain auxiliary spin method but has yet to be shown in methods based on the dynamical mean field theory. Recent renormalization-group analysis [62] motivates an EDMFT-based examination of the interplay between the inter-orbital hybridization and intersite spin-exchange interactions, both of which are important to the physics of the iron-based superconductors.

Another issue deals with frustrated bulk systems with topological flat bands that are coupled to wide bands. Recent work has illustrated how an effective orbital-selective Mott transition can take place when an Anderson/Kondo lattice model is realized as an effective description [63]. The EDMFT approach is expected to shed considerable new light on this emerging topic.
VII. SUMMARY AND OUTLOOK

We have provided an overview of the extended dynamical mean field theory for correlated electron models. The method is especially suited for settings where the competing interactions arise from local and intersite terms, respectively. Our emphasis has been on models for which the method was initially formulated and developed, namely models of the multi-band Anderson-lattice type and those of the one-band Hubbard-Heisenberg kind.

A setting in which this method has been most extensively used is the Kondo/Anderson lattice models for heavy fermion systems, where the key issue is the dynamical competition between the local Kondo and intersite RKKY interactions. In elucidating how the amplitude of the Kondo singlet in the ground state and the weight of heavy quasiparticles are critically destroyed, these studies underline the notion of Kondo destruction. The associated physics includes a loss of quasiparticles and dynamical Planckian scaling at the quantum critical point and a large-to-small Fermi surface jump across the quantum critical point [18].

We have also discussed the prospect for further developing the method, including in the form that is suitable to study unconventional superconductivity. In the same spirit, we note that new settings have continue to arise for which the approach of the extended dynamical mean field theory is poised to clarify new physics. We have described two such issues. One concerns the orbital-selective Mott phase in the iron-based superconductors, and the other about the correlation physics of coupled topological flat-wide bands in kinetically-frustrated bulk systems. Given the versatility that the EDMFT approach has shown in elucidating the dynamical interplay between local and spatial correlations, we expect that other settings will also develop in which the approach will provide new insights into the underlying correlation physics.

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