Dynamical Mean Field Theory, Density-Matrix Embedding Theory and Rotationally Invariant Slave Bosons: a Unified Perspective

Thomas Ayral,1 Tsung-Han Lee,1 and Gabriel Kotliar1,2

1 Physics and Astronomy Department, Rutgers University, Piscataway, New Jersey 08854, USA
2 Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA

We present a unified perspective on Dynamical Mean Field Theory (DMFT), Density-Matrix Embedding Theory (DMET) and Rotationally Invariant Slave Bosons (RISB). We show that DMET can be regarded as a simplification of the RISB method where the quasiparticle weight is set to unity. This relation allows to easily transpose extensions of a given method to another: for instance, a temperature-dependent version of RISB can be used to derive a temperature-dependent free-energy formula for DMET.

Strong correlations count amongst the most challenging problems in condensed-matter physics. While the development of Dynamical Mean Field Theory (DMFT) [1] and its cluster [2–6] and diagrammatic [7] extensions has led to a better understanding of relatively simple strongly-correlated models and systems, there are still situations where the exact solution of the DMFT quantum impurity model becomes prohibitive due to the size of its Hilbert space and/or the Monte-Carlo negative sign problem. These situations range from the study of multiorbital systems to the exploration of low temperature phases over the investigation of long-range strong correlations. This is particularly important for realistic investigations of 5f systems, which require the simultaneous inclusion of crystal-field effects, spin-orbit coupling interaction multiplets and lattice relaxation. Outstanding challenges in this area include the computation of phase diagrams and equations of state of elemental actinides and their alloys. These are problems of fundamental importance and of practical technological relevance, and that require simplified faster methods that still capture correlation effects accurately enough.

Several such methods have been developed in recent years, with a commonality with DMFT: the mapping of the lattice problem onto a simpler, yet nontrivial embedded quantum problem. Prominent examples include cluster perturbation theory (CPT, [8, 9]), derivable from the self-energy functional theory, SFT [10, 11]), self-energy embedding theory (SEET, [12, 13]), two-site DMFT [14, 15], and site-occupation embedding theory (SOET, [16, 17]).

Two particularly successful methods are the (mean-field) rotationally invariant slave-boson method (RISB, [18, 19]) and the density-matrix embedding theory (DMET, [20, 21]). RISB yields kinetic energy renormalizations, double occupancies and valence histograms very close to DMFT [22–24] and has been applied to numerous multiband models [19, 25–27] and realistic compounds [27–29]. These slave-boson methods have a close connection to the Gutzwiller approximation as shown in Ref. [30] for the single-site case and in Ref. [31] for the multiorbital case. DMET has been shown to yield very accurate ground-state energies for the Hubbard model [20, 21, 32–34] and quantum chemical systems [35, 36]. Both allow to reach ground-state (including superconducting [32, 37, 38]) properties and spectral properties [39], and have also been extended to tackle out-of-equilibrium problems [40–47].

However, the precise relation between these two methods has not been established to date and it is unclear whether they yield a complementary picture of correlations, or if on the contrary one corresponds to the simplification of the other. This work intends to fill this gap by showing that DMET is a simplification of RISB. We also illustrate the relation of RISB with DMFT, thereby giving a comprehensive picture of the interrelation and hierarchy between the three methods.

This paper is organized as follows: we first give an overview of the results presented in this paper (section I), then review the RISB formalism and its relation with DMFT (section II), and finally derive the DMET approximation and show that it is a simplified RISB with a quasiparticle weight equal to one (section III).

I. OVERVIEW

In this section, we highlight the common structure of RISB and DMET without providing detailed derivations. Our purpose is to provide the reader with the key ideas that these methods share and thus reveal their close connection.

Both RISB and DMET start with an interacting lattice model of the form

$$\hat{H} = \sum_{ij,\alpha\beta} \hat{t}_{i\alpha,j\beta} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\beta} + \sum_i \hat{H}_\text{loc}[\{\epsilon_{i\alpha}, \hat{c}_{i\alpha}^\dagger\}], \quad (1)$$

and depicted in Fig. 1, top panel. Greek indices $\alpha, \beta, \cdots = 1 \ldots N_c$ denote local or orbital indices (within
where the effect of correlations is described by a one-body potential \( \lambda \) related unit cell, called the effective medium Hamiltonian (without local hoppings).

Instead, they are contained in an environment is mapped to a “bath” of the same dimension. The hopping processes between different unit cells. The hopping \( t \) does not contain local hopping terms \( (t_{\alpha,\beta} = 0) \); instead, they are contained in \( \hat{H}_{\text{loc}} \). Later, we will denote by \( t \) the full hopping matrix, and by \( \hat{H}_{\text{int}} \) the interaction Hamiltonian (without local hoppings).

The key idea of RISB and DMET is to replace the lattice model by a reference model or effective medium that depicts correlations in an approximate fashion.

In DMET, this effective medium consists of one correlated unit cell, called the fragment, and an environment where the effect of correlations is described by a one-body potential \( \lambda \), as illustrated in Fig. 1, middle panel. (In the DMET literature, this potential is usually called \( u \) and is equal to \( \lambda \) up to a local hopping term: \( \lambda_{\alpha,\beta} = u_{\alpha,\beta} + [\varepsilon_{\text{loc}}]_{\alpha,\beta} \).) The Hamiltonian of this effective medium is:

\[
\hat{H}_{\text{eff}} \equiv \sum_{ij,\alpha,\beta} t_{i\alpha,j\beta} c_{i\alpha}^\dagger c_{j\beta} + \hat{H}_{\text{loc}}[\{c_{0\alpha}, c_{0\beta}^\dagger\}] + \sum_{i,\alpha,\beta \neq 0} \lambda_{\alpha,\beta} c_{i\alpha}^\dagger c_{i\beta}.
\]

RISB also has an effective medium, but it comes with an additional parameter (called \( R \) in the following) that allows to describe the mass of quasiparticles and cannot be described by a one-body potential only.

As a last step, both methods introduce an impurity or embedded problem illustrated in Fig. 1, bottom panel. It is obtained by the contraction of the environment (of size \( N - N_c \)) to \( N_c \) bath orbitals using a Schmidt decomposition. The embedded problem thus consists of \( N_c \) correlated or impurity orbitals hybridized (via a hybridization term \( D \)) to \( N_c \) uncorrelated bath orbitals (described by the one-body potential \( \lambda^c \)). It is given by a Hamiltonian of the form

\[
\hat{H}_{\text{embed}} = \sum_{\alpha,\beta} (D_{\alpha,\beta} c_{\alpha}^\dagger a_{\beta} + \text{h.c.}) + \hat{H}_{\text{loc}}[\{c_{\alpha}^\dagger, c_{\alpha}\}] + \sum_{\alpha,\beta} \lambda_{\alpha,\beta} a_{\alpha}^\dagger a_{\alpha},
\]

Here, \( c^\dagger / c \) (resp. \( a^\dagger / a \)) are creation/annihilation operators for the impurity (resp. bath) orbitals.

The goal of both methods is to determine the effective medium, i.e, to find the value of \( \lambda \) (and optionally \( R \)), such that the following self-consistency condition is satisfied: the one-particle density matrix of the impurity model (Eq. (3)) must match the projection of the reference medium’s density matrix onto the embedded subspace. \( \lambda \) (and optionally \( R \)) can then be used as approximations of the self-energy of the lattice model.

This is also the logic of DMFT, except that DMFT adjusts the local self-energy \( \Sigma_{\text{loc}}(i\omega) \) (instead of \( \lambda \) and \( R \) above) so that the (one-particle) Green’s function,

\[
[G_{\text{imp}}]_{\alpha\beta}(i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n\tau} \langle T(c_\alpha(\tau)c_{\beta}^\dagger(0))_{\text{imp}} \rangle.
\]

of the impurity model matches the projection of the reference medium’s Green’s function,

\[
G(k, i\omega) = [i\omega - \varepsilon_k - \Sigma_{\text{loc}}(i\omega)]^{-1},
\]

onto the impurity (where \( \varepsilon_k \) is the Fourier transform of the hopping matrix \( t_{ij} \) or LDA Hamiltonian in a LDA+DMFT context, see Eq. (7) below). Besides, because of this modified self-consistency condition, the impurity model of DMFT contains an infinite number of bath sites, contrary to Eq. (3).

While connections between RISB, DMET and DMFT were mentioned in passing (see e.g. [28]) and DMET was inspired by DMFT, a precise direct connection was not available in the literature to this date. This connection points to many possible generalizations of these methods.

II. OVERVIEW OF ROTATIONALLY INVARIANT SLAVE BOSONS

In this section, we briefly review the RISB formalism introduced by [19]. Our starting point is the lattice Hamiltonian Eq. (1). We note that \( \hat{H}_{\text{loc}} \) contains both
kinetic and interaction terms. Denoting by \( t_{ia,i\beta} \) hoppings internal to a unit cell, we can decompose:

\[
\hat{H}_{\text{loc}} = \hat{H}_{\text{int}} + \sum_i \sum_{\alpha\beta} t_{ia,i\beta} c_{i\alpha}^{\dagger} c_{i\beta},
\]

In the following, we will denote the \( i, j \) Fourier transform of \( t_{ia,j\beta} \) (resp. \( \tilde{t}_{ia,j\beta} \)) as

\[
\varepsilon_{k,\alpha\beta} = \frac{N_c}{N} \sum_{ij} e^{-i\mathbf{k} \cdot (r_i - r_j)} t_{ia,j\beta}
\]

(7)

(resp. \( \tilde{\varepsilon}_{k,\alpha\beta} \)). Correspondingly,

\[
[\varepsilon_{\text{loc}}]_{\alpha\beta} = \sum_k \varepsilon_{k,\alpha\beta} = t_{0\alpha,0\beta}.
\]

(8)

1. Slave bosons: Constraints and physical subspace

The second-quantized operators \( c_{i\alpha}^{\dagger}, c_{i\alpha} \) generate a Hilbert space \( \mathcal{H}_{\text{phys}} \) with local many body states \( |A_i\rangle \). RISB consists in introducing fermionic operators \( f_{i\alpha}^{\dagger}, f_{i\alpha} \) and bosonic operators \( \hat{\phi}_{A_{i,n_i}}^{\dagger}, \hat{\phi}_{A_{i,n_i}} \) (one for each pair of local many-body states, with \( n_i \) labelling local Fock states, which like \( A_i \) form a basis of the local Hilbert space) to replace \( c \) and \( c^{\dagger} \). Yet, these new operators generate a Hilbert space \( \mathcal{H} \) which is much larger than the original Hilbert space, so that one needs to define a “physical” subspace. This is done by defining physical states and the corresponding constraints. The physical states are defined as follows:

\[
|\mathcal{A}\rangle = \frac{1}{\sqrt{D_A}} \sum_{n_i}^{} \hat{\phi}_{A_{i,n_i}}^{\dagger} |0\rangle |n_i\rangle_f,
\]

(9)

with \( D_A = \left( \frac{N_c}{N} \right)^{N_A} \) (\( N_A \) is the number of electrons in state \( A \)) and the \( \{ |n_i\rangle_f \} \) are the local Fock states formed with \( f^{\dagger} \) operators:

\[
|n_i\rangle_f = \prod_{\alpha=1}^{N_c} \left( f_{i\alpha}^{\dagger} \right)^{n_{i\alpha}} |0\rangle.
\]

(10)

One can check the physical states \( |\mathcal{A}\rangle \) are normalized. One can prove [19] that these states (and only these states) satisfy the following constraints:

\[
\forall i \sum_{A_{i,n_i}} \hat{\phi}_{A_{i,n_i}}^{\dagger} \hat{\phi}_{A_{i,n_i}} = 1,
\]

(11a)

\[
\forall i \ f_{i\alpha}^{\dagger} f_{i\beta} = \sum_{A_{i,n_{i\alpha}}} f_{i\alpha}^{\dagger} f_{i\beta} |n_{i\alpha}\rangle_f \hat{\phi}_{A_{i,n_{i\alpha}}}^{\dagger} \hat{\phi}_{A_{i,n_{i\alpha}}}.
\]

(11b)

In the following, we drop the site index \( i \) for conciseness.

One then writes a faithful representation of the original Hamiltonian \( H \) in the physical subspace, where “faithful” is defined as follows: for any (local) operator \( O \), \( \mathcal{O} \) is said to be a faithful representation of \( O \) in the physical subspace if and only if:

\[
\forall A, B, \quad \langle O | \mathcal{O} | B \rangle = \langle O | B \rangle.
\]

(12)

One can show [19] that the faithful representation of the creation operator is given by the expression:

\[
\mathcal{C}_{\alpha} = \sum_{\beta} R_{\beta\alpha} f_{\beta}^{\dagger},
\]

(13)

with the \( \hat{\phi} \)-dependent matrix \( R \) defined by:

\[
R_{\beta\alpha} = \sum_{ABmn} \frac{\langle A | \mathcal{C}_{\alpha}^{\dagger} | B \rangle \langle n \rangle f_{\beta}^{\dagger} | m \rangle_f}{\sqrt{N_A (N_c - N_B)}} \hat{\phi}_{A_{n}}^{\dagger} \hat{\phi}_{B_{n}}.
\]

(14)

Eq. (13) is used to write down the faithful representation of the kinetic term of the Hamiltonian. For the local Hamiltonian term (which contains interactions and local hoppings, see above), one can show [19] that

\[
H_{\text{loc}} = \sum_{iABn} \langle A_i | H_{\text{loc}} | B_i \rangle \hat{\phi}_{A_{i,n}}^{\dagger} \hat{\phi}_{B_{i,n}}.
\]

(15)

One can thus write the faithful representation of \( H \) in terms of the \( f \) and \( \hat{\phi} \) fields:

\[
H = \sum_{ij\gamma\delta} \left\{ \sum_{\alpha\beta} R_{\gamma\alpha} \tilde{t}_{ia,j\beta} R_{\beta\delta}^{\dagger} \right\} f_{ij\gamma}^{\dagger} f_{ij\delta} + \sum_{iABn} \langle A_i | H_{\text{loc}} | B_i \rangle \hat{\phi}_{A_{i,n}}^{\dagger} \hat{\phi}_{B_{i,n}}.
\]

(16)

This Hamiltonian is nontrivial in the \( \hat{\phi} \) operators (through the \( \hat{\phi} \)-dependence of \( R \)), but quadratic in the \( f \) operators. In the following, we will thus carry out a mean-field approximation for the bosons, and integrate out the \( f \) fields.

2. Mean-field approximation and matrix notation

We now condense the bosons, i.e \( \hat{\phi}_{B_{i,n}} \) is chosen to be a c-number (and \( \hat{\phi}_{B_{i,n}}^{\dagger} \) becomes \( \phi_{B_{i,n}}^{\dagger} \)). For notational convenience, we define the \( 2^{N_c} \times 2^{N_c} \) matrices \( \Phi \) and \( F \):

\[
[\Phi]_{Am} = \phi_{Am},
\]

(17)

\[
[F]_{nm} = f_{n\alpha} m_f.
\]

(18)
In particular, \([\Phi^\dagger]_{nA} = [\Phi]_{nA}^* = \phi_{nA}^*\). We can always order the \(|A\rangle\) states in such a way that \(\langle A|c_\alpha B\rangle = [F_{\alpha}]_{AB}\). In particular, \([F_{\alpha}]_{AB} = [F_{\alpha}]_{BA} = (\langle B|c_\alpha A\rangle)^* = \langle A|c_\alpha^\dagger B\rangle\). If the coefficients of the \(F\) matrix are real (which is the case if one is dealing with Fock states, which is always possible), then

\[
[F^\dagger_{\alpha}]_{AB} = [F_{\alpha}]_{BA}. \tag{19}
\]

Thus, the expressions for the constraints become:

\[
\begin{align*}
\text{Tr}[\Phi^\dagger] &= 1, \tag{20a} \\
F_{\alpha}^\dagger \delta &\equiv \Delta_{\alpha,\beta}^p \forall \alpha, \beta., \tag{20b}
\end{align*}
\]

with

\[
\Delta_{\alpha,\beta}^p \equiv \sum_{Anmp} f(\langle m|f_{\alpha}^\dagger |p\rangle f_{\beta} \langle p|f_{\beta}^\dagger |n\rangle f_{\Phi}^\dagger)_{nA}^* [F_{\alpha}]_{Am} = \text{Tr} [F_{\alpha}^\dagger F_{\beta}^\dagger \Phi^\dagger \Phi]. \tag{21}
\]

Furthermore,

\[
R_{\alpha\beta} = \sum_{\gamma} \sum_{\Delta Bnm} F_{\alpha A, B}^\dagger F_{\gamma n m}^\dagger [\Phi^\dagger]_{nA} [\Phi]_{Bm} \times \left[ (\Delta^p(1 - \Delta^p))^{-1/2} \right]_{\gamma\beta}^\gamma = \sum_{\gamma} \text{Tr} \left[ \Phi^\dagger F_{\alpha}^\dagger \Phi F_{\gamma} \right] \left[ (\Delta^p(1 - \Delta^p))^{-1/2} \right]_{\gamma\beta}^\gamma,
\]

where, to obtain the second line, we have assumed \(F\) to be real valued (Eq. (19)). Equivalently, we have:

\[
R_{\gamma\alpha} \left[ (\Delta^p(1 - \Delta^p))^{1/2} \right]_{\gamma\beta} = \text{Tr} \left[ \Phi^\dagger F_{\alpha}^\dagger \Phi F_{\beta} \right]. \tag{22}
\]

The local part of the Hamiltonian reads:

\[
H_{\text{loc}} = \sum_i \sum_{A_i B_i n_i} \langle A_i | H_{\text{loc}} | B_i \rangle \langle [\Phi^\dagger]_{n_i A_i} | \Phi_{B_i n_i} \rangle = \sum_i \text{Tr}[\Phi^\dagger H_{\text{loc}} \Phi]. \tag{23}
\]

3. Mean field free-energy and Lagrange equations

The problem at hand now boils down to minimizing the free energy, a function of the slave-boson mean fields \(\Phi_{A_n}\), under the constraints (20a-20b). In the original formulation [19], inspired by previous slave-boson approaches [30], the fulfillment of the constraints was enforced by introducing two Lagrange multipliers \(E^c\) and \(\lambda\). It was then proposed [25, 28, 29], in order to overcome the remaining strong nonlinearity of the free energy as a function of \(\Phi\), to turn Eqs (21-22) into constraints, thereby making the free energy quadratic in \(\Phi\) at the price of adding two more Lagrange multipliers \(\lambda^c\) and \(D\) and turning \(\Delta^p\) and \(R\) into independent variables. Following this strategy, the free energy of the system is given by:

\[
\Omega[\Phi, R, \Delta^p; E^c, \lambda, D, \lambda^c] = -\beta \log \int D[f^*, f] e^{-S[\Phi, R, \Delta^p; E^c, \lambda, D, \lambda^c]}, \tag{24}
\]

with

\[
S[\Phi, R, \Delta^p; E^c, \lambda, D, \lambda^c] = -\sum_{k\omega} \text{Tr} \left\{ \text{log} \left( i\omega - R_{\alpha\gamma} \delta_{\delta\beta}^k F_{\alpha\beta}^\dagger - \lambda_{\alpha\beta} + \mu \delta_{\alpha\beta} \right) \right\} e^{i\omega 0^+} + \sum_i \text{Tr} \left[ E^c (\Phi^\dagger \Phi - 1) + \sum_{\alpha\beta} (D_{\alpha\beta} \Phi^\dagger F_{\alpha}^\dagger F_{\beta} + h.c) \right] + \sum_{\alpha\beta} \lambda^c_{\alpha\beta} (\Phi^\dagger F_{\alpha}^\dagger F_{\beta} + \Phi^\dagger H_{\text{loc}} \Phi) - \sum_{i;\alpha\beta} (\lambda_{\alpha\beta} + \lambda^c_{\alpha\beta}) \Delta_{\alpha\beta}^p - \sum_{i;\alpha\beta\gamma} (D_{\alpha\beta} R_{\gamma\alpha} + c.c.) \left( \Delta^p(1 - \Delta^p) \right)^{1/2}_{\gamma\beta}. \tag{25}
\]

Here, \(\sum_i\) is shorthand for \(\sum_{a,\alpha}\sum_{\gamma}\), and in principle, all the variables \(\Phi, R, \Delta^p, E^c, \lambda, D, \lambda^c\) depend on the site index \(i\) but we dropped it since we will be looking for uniform solutions.

The slave-boson amplitudes \(\Phi_{A_n}\) appear only in the second and third lines. Inspired by the fact that these amplitudes are defined on a local Hilbert space (spanned by \(A\)) and its copy (spanned by \(n\)), one can introduce [28] the corresponding tensor-product space, spanned by the basis \(\{|A\rangle \otimes |n\rangle\}_{A,n}\), where states \(|A\rangle\) are created by impurity operators \(c^\dagger, c\) and \(|n\rangle\) by “bath” operators \(a^\dagger, a\). In this construction, one interprets the amplitudes \(\Phi_{A_n}\) as coefficients of the Schmidt decomposition of general states \(|\Phi\rangle\) of this product space:

\[
|\Phi\rangle = \sum_{A_n} e^{i\Phi A_n(N_A-1)} \Phi_{A_n} \hat{U}_{\text{ph}} |A\rangle |n\rangle_a, \tag{26}
\]

where \(\hat{U}_{\text{ph}}\) is a particle-hole transformation acting only on the \(a\) operators. With this definition and the phase factor, one has [28]:

\[
\begin{align*}
\text{Tr} \left[ F_{\alpha}^\dagger F_{\beta}^\dagger \Phi^\dagger \Phi \right] = \langle \Phi | a_{\alpha} a_{\beta}^\dagger | \Phi \rangle, \tag{27a} \\
\text{Tr} \left[ \Phi^\dagger F_{\alpha}^\dagger F_{\beta} \right] = \langle \Phi | c_{\alpha} a_{\beta} | \Phi \rangle. \tag{27b}
\end{align*}
\]
which allows to express the right-hand sides of Eqs (21) and (22) as correlators of the $c$ and $a$ operators. Besides, the second and third lines of the right-hand side of (25) become $E^c(\Phi) = 1 + (\Phi \hat{H}_{\text{embed}} | \Phi)$, with $\hat{H}_{\text{embed}}$ defined in Eq. (3). This Hamiltonian describes an Anderson impurity level, described by the fields $c$, $c^\dagger$ interacting through the local Hamiltonian $H_{\text{int}}$, hybridized with noninteracting bath levels $a$, $a^\dagger$ of energies $-\lambda^c$ via the hybridization strengths $D$.

Finally, one extremizes the free energy with respect to its variables to find the Lagrange equations of the problem:

$$\Delta^p_{\alpha\beta} = \frac{1}{\omega} \sum_{k \in \text{BZ}, \omega} \left[ i \omega - R \tilde{\varepsilon}_k R^\dagger - \lambda + \mu \right]^{-1}_{\beta \alpha} e^{i t \omega + \omega}, \quad (28a)$$

$$\sum_{\mu} \left( (\Delta^p(1 - \Delta^p))^{1/2} \right)_{\alpha \mu} D_{\beta \mu} = 0, \quad (28b)$$

$$\lambda^c_{\alpha \beta} = - \lambda_{\alpha \beta}, \quad (28c)$$

$$\hat{H}_{\text{embed}} | \Phi \rangle = E^c_1 | \Phi \rangle, \quad (28d)$$

$$\langle \Phi | a\beta a^\dagger_\alpha | \Phi \rangle = \Delta^p_{\alpha \beta}, \quad (28e)$$

$$\langle \Phi | c\beta a^\dagger_\alpha | \Phi \rangle = R_{\alpha \beta} \left( (\Delta^p(1 - \Delta^p))^{1/2} \right)_{\gamma \beta}. \quad (28f)$$

4. Solution of the Lagrange equations

Root-solving In previous works [25, 28, 29], the Lagrange equations were solved by formulating the problem as a root-solving procedure by defining the functions

$$F^{(1)}[R, \lambda] \equiv \langle \Phi | a\beta a^\dagger_\alpha | \Phi \rangle - \Delta^p_{\alpha \beta}, \quad (29a)$$

$$F^{(2)}[R, \lambda] \equiv \langle \Phi | c\beta a^\dagger_\alpha | \Phi \rangle - R_{\alpha \beta} \left( (\Delta^p(1 - \Delta^p))^{1/2} \right)_{\gamma \beta}. \quad (29b)$$

$F^{(1)}$ and $F^{(2)}$ are implicit functions of $R$ and $\lambda$: for a given $R$ and $\lambda$, one can successively compute $\Delta^p$, $\mathcal{D}$, $\lambda^c$ and $| \Phi \rangle$ by using Eqs (28a), (28b), (28c) and (28d), respectively. The fulfillment of the last two equations, Eqs (28c) and (28f), thus amounts to solving the root problem:

$$F^{(1)}[R, \lambda] = 0, \quad F^{(2)}[R, \lambda] = 0.$$

We note that the same Lagrange equations can be cast as different root problems (depending on the choice of free variable; for instance, one could have chosen $\mathcal{D}$ and $\lambda^c$ instead of $R$ and $\lambda$). In the next paragraph, we give an alternative route to solve the Lagrange equations to shed light on the relation of RISB with the DMFT method.

Forward recursion and comparison to DMFT One can alternatively solve the Lagrange equations in a forward recursive fashion, as is usually done in DMFT:

1. Start from a guess $R$ and $\lambda$.

2. Compute the local density matrix $\Delta^p$ using (28a) and the local “kinetic energy”:

$$[\mathcal{K}_{\text{loc}}]_{\alpha \beta} \equiv \sum_{k \in \text{BZ}, \omega} \left[ (\tilde{\varepsilon}_k R^\dagger) \right]_{\beta \alpha} e^{i t \omega + \omega}. \quad (30)$$

3. Compute $\mathcal{D}$ and $\lambda^c$ using Eq. (28b), i.e

$$\mathcal{D}_{\beta \alpha} = \left( (\Delta^p(1 - \Delta^p))^{1/2} \right)_{\alpha \mu} [\mathcal{K}_{\text{loc}}]_{\mu \beta}, \quad (31)$$

and Eq. (28c).

4. Solve the embedded problem Eq (28d) for its (normalized) ground state $| \Phi \rangle$.

5. Compute a new $R$ as

$$R_{\alpha \beta} = \sum_{\gamma \delta \eta} \left\{ \mathcal{D}_{\gamma \delta} R_{\delta \gamma} \frac{\partial \left( (\Delta^p(1 - \Delta^p))^{1/2} \right)_{\gamma \beta}}{\partial N^a_{\alpha \beta}} + c.c \right\}, \quad (32)$$

with

$$N^a_{\alpha \beta} \equiv \langle \Phi | a\beta a^\dagger_\alpha | \Phi \rangle, \quad (33a)$$

$$M_{\alpha \beta} \equiv \langle \Phi | c\beta a^\dagger_\alpha | \Phi \rangle, \quad (33b)$$

and a new $\lambda$ as

$$\lambda_{\alpha \beta} = - \lambda^c_{\alpha \beta}$$

$$- \sum_{\gamma \delta \eta} \left\{ \mathcal{D}_{\gamma \delta} R_{\delta \gamma} \frac{\partial \left( (N^a(1 - N^a))^{1/2} \right)_{\gamma \beta}}{\partial N^a_{\alpha \beta}} + c.c \right\}. \quad (34)$$

6. Go back to step 2 until convergence of $R$ and $\lambda$.

This cycle is illustrated in Fig. 2 (panel (b)): in RISB, the impurity model is solved for $N_{\alpha \beta}$ and $M_{\alpha \beta}$ to obtain the two matrices $R_{\alpha \beta}$ and $\lambda_{\alpha \beta}$, which are used as a parametrization of the lattice self-energy:

$$\Sigma(k, i \omega_n) \approx i \omega_n \left( 1 - (R^\dagger R)^{-1} \right) + R^{-1} \lambda \left( R^\dagger \right)^{-1} - \varepsilon_{\text{loc}}. \quad (35)$$
The impurity model is also parametrized by two matrices, the hybridization strengths $D_{\alpha\beta}$ and bath hopping parameters $\lambda_{\alpha\beta}$, which are adjusted in such a way that the local density matrix $\Delta^p$ coincides with $N$ and 
\[
\left[ (\Delta^p(1 - \Delta^p))^{1/2} \right]^T R \text{ coincides with } M \text{ (Eqs (28c-28f)).}
\]

In practice, this loop allows to obtain stable solutions in the Mott phase of the Hubbard model more easily than by solving the Lagrange equations as a root problem. By contrast, DMFT (whose self-consistent loop is illustrated in the top panel of Fig. 2) requires the frequency-dependent local Green’s function $G_{\text{loc}}(i \omega_n)$ (defined as the $k$-summation of the lattice Green’s function $G(k, i \omega)$ defined in Eq. (5)) to match the impurity Green’s function $G_{\text{imp}}(i \omega_n)$ (Eq. (4)) by adjusting the hybridization function $\Delta(i \omega_n)$, at the cost of approximating the lattice self-energy by the impurity self-energy $\Sigma_{\text{imp}}(i \omega_n)$: all these functions depend on an infinite number of Matsubara frequencies, and correspondingly DMFT’s impurity model has an infinite number of bath levels: $\Delta(i \omega_n)$ can in general only be represented by an infinity of bath sites:

\[
\Delta_{\alpha\beta}(i \omega_n) = \sum_{b=1}^{\infty} \sum_{\gamma\delta} D_{\alpha\gamma}^b \left[ i \omega_n - [\gamma\delta]^{-1} D_{\beta\delta}^b \right]^*, \quad (36)
\]

contrary to RISB in which $b = 1$. Note that in the DMFT literature, $D$ (resp. $\lambda^c$) is usually denoted as $V$ (resp. $-\epsilon$).

Thus, RISB can be viewed as a well-defined way of drastically truncating the number of bath levels in the impurity problem, and of parametrizing the low-energy behavior of the impurity self-energy by two observables, the matrices $R$ and $\lambda$. Beyond the reduced number of bath levels of the impurity model, RISB only necessitates the computation of static correlators, $\langle \Phi_\alpha \Phi_\beta \rangle$ and $\langle \Phi_\alpha \Phi_\beta \rangle$, whereas DMFT requires the full frequency dependence of the Green’s function $G_{\text{imp}}(i \omega_n)$.

Alternative approaches to truncate the number of bath levels exist: two-site DMFT [14] uses the low and high-frequency limit of the DMFT self-consistency condition $G_{\text{imp}}(i \omega) = G_{\text{loc}}(i \omega)$ to fix the position and hybridization of a single bath level (in the context of a single-band model; see also [48, 49] for another prescription in a multiorbital context).

In a different perspective, solving the DMFT impurity model with an exact diagonalization method [50] also relies on a truncation procedure. There, the number as well as position and hybridization of bath sites is dictated not by formal considerations (as in RISB or two-site DMFT) but by computational limitations attached to the former and a (somewhat arbitrary) fitting procedure (using the parametrization of Eq. (36)) for the latter.

5. Equivalence to the multiband Gutzwiller approximation

RISB has been shown to be equivalent [31] to the multiband formulation of the Gutzwiller approximation. In other words, the above derivation can be carried out, instead of introducing slave bosons $\phi$ and quasiparticle fields $f$, by minimizing the variational energy $\langle \Psi_G | H | \Psi_G \rangle$ over the Gutzwiller wavefunctions

\[
\langle \Psi_G | H | \Psi_G \rangle = \prod_i \mathcal{P}_i (R, \lambda) | \Psi_0(R, \lambda) \rangle,
\]

where $| \Psi_0 \rangle$ is a noninteracting wavefunction (a Slater determinant $| \Psi_0 \rangle = \prod_{p=1}^{n_{\text{ooc}}} c_p^\dagger |0\rangle$ with $p = 1 \ldots n_{\text{ooc}}$ denoting the occupied states) and $\mathcal{P}_i$ is a projector on the local many-body Hilbert space defined above:

\[
\mathcal{P}_i = \sum_{A, B} \Lambda_{A, B}(R, \lambda) | A_i \rangle \langle B_i |.
\]
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Density-matrix embedding theory (DMET) has been introduced as a simplified version of DMFT \[\text{approximated by the identity matrix.}\]

In the next section, we show that the recently introduced DMET is a simplified form of RISB where the self-energy (here a matrix, \(\Sigma\)) is obtained by a self-consistent mapping of the reference problem (Eq. (2)) to be equivalent to the aforementioned RISB constraints, Eqs (20a)-(20b).

In this subsection, we give a brief summary of the DMET self-consistency

A. Summary of the DMET self-consistency

In this subsection, we give a brief summary of the DMET workflow. Having mapped the lattice problem onto a reference problem consisting in an interacting fragment (of size \(N_c\)) and a noninteracting environment (as illustrated in Fig. 1), DMET defines an embedded subspace through a projection operator \(P\) which projects the \(\hat{H}_{\text{imp}}\) onto the \(\hat{H}_{\text{eff}}\) of the embedded (i.e impurity+bath) problem. Then, the DMET self-consistency consists in matching:

(i) \[\text{the density matrix of the embedded problem}\]

\[\rho_{\text{imp}} = \begin{bmatrix} \langle \Phi | c_i^\dagger c_j | \Phi \rangle & \langle \Phi | c_i^\dagger a_j | \Phi \rangle & \langle \Phi | a_i^\dagger a_j | \Phi \rangle \end{bmatrix},\]

where \(|\Phi\rangle\) is the ground-state of \(H_{\text{embed}}\) (Eq. (3)), itself related to \(H_{\text{eff}}\) (Eq. (2)) by “projection” by \(P\), namely

\[H_{\text{embed}} = \hat{H}_{\text{loc}}(\{c_\alpha, a_\alpha\}) + \sum_{\alpha \beta} \left[ \begin{array}{c} c_\alpha \\ a_\alpha \end{array} \right]^\dagger \left[ \begin{array}{c} c_\beta \\ a_\beta \end{array} \right],\]

with

\[h_{\text{embed}} = P^\dagger h P,\]

and \(h\) the one-body part of \(H_{\text{eff}}:\)

\[h = t + \begin{bmatrix} 0 & 0 \\ 0 & u \end{bmatrix},\]

\[\left(\begin{array}{c} 0 \\ u \end{array}\right)\]

(\(u\) block is of size \((N - N_c) \times (N - N_c)\)) with

(ii) \[\text{the projection of the density matrix \(\rho\) of the reference problem}\]

in the embedded subspace:

\[\rho_{\text{embed}} = P^\dagger \rho P,\]

with

\[\rho_{\alpha \beta} = \sum_{\alpha \beta} e^{i\omega \alpha} |i \omega - h_{\text{ref}} + \mu_{\alpha \beta}^{-1}|,\]

We recall that the Latin indices \(i, j\) label the unit cells, while the Greek indices \(\alpha, \beta = 1 \ldots N_c\) label the internal orbital/cluster degrees of freedom. In the above expression, \(h_{\text{ref}}\) is the translation-invariant version of \(h\), i.e it contains a potential \(u\) on the upper-left \((i=0, j=0)\) block: \([h_{\text{ref}}]_{i\alpha, j\beta} = h_{i\alpha, j\beta} + u_{i\alpha, j\beta} \delta_{i,0} \delta_{j,0}.\) In practice, we will see that exactly matching those two density matrices is in general impossible, so that a minimization of a distance between both matrices is carried out.

In the following subsection, we show how the projector \(P\) is constructed.
B. Construction of the impurity and bath operators

In this section, we define the mapping from the effective medium (with \( N \) orbitals) to the embedded problem (with \( 2N_c \) orbitals), or in other words we construct the projector \( P \).

We start by explaining how to transform from the fragment (size \( N_c \)) to the impurity (size \( N_c \)) orbitals. First off, diagonalizing the lattice density matrix \( \rho \) (given in Eq. (47)) yields a transformation \( D_{\text{occ}} \) from the single-site levels of the fragment (denoted by Greek indices) to the occupied levels of \( H_{\text{eff}} \) (see Appendix A for details).

Second, we need to find a transformation from the occupied levels to the impurity orbitals. The central object for doing so is the overlap matrix between the fragment and the occupied states of the lattice, defined as:

\[
S_{pq}^{\text{occ}} = \langle \phi_p | P F | \phi_q \rangle, \tag{48}
\]

with \( p \) and \( q \) labelling two occupied states of \( H_{\text{eff}} \) (1 \( \leq p, q \leq n_{\text{occ}} \)), and \( \phi_p \) the corresponding single-particle state: \( | \phi_p \rangle \equiv c_p^\dagger | 0 \rangle \), and \( P F \) is the projector on the fragment (\( P F = \sum_{\alpha=1}^{N_c} | \phi_{\alpha} \rangle \langle \phi_{\alpha} | \)). We show in Appendix A that this matrix can be transformed to a diagonal form:

\[
S^{\text{occ}} = V_F n^0 F^\dagger, \tag{49}
\]

where \( n^0 \) is a \( N_c \times N_c \) diagonal matrix, and \( V_F \) is an \( n_{\text{occ}} \times N_c \) rectangular matrix such that \( V_F^\dagger V_F \equiv 1 \). \([V_F]_{\alpha \alpha'} \) defines a transformation from the occupied states (\( p, \ldots \)) to new states (denoted by primed Greek indices \( \alpha', \ldots \)) that correspond to the “natural orbitals” used e.g. in [25].

With these two transformations, one defines the transformation from the fragment to the impurity as:

\[
\tilde{C}_F = D_{\text{occ}}^{\text{occ}} V_F, \nonumber
\]

or rather, with orthonormal columns:

\[
[C_F]_{\alpha \alpha'} = \frac{D_{\text{occ}}^{\text{occ}} [V_F]_{\alpha \alpha'}}{\sqrt{n_{\alpha}'}}. \tag{50}
\]

(to determine the normalization, we have used: \( \tilde{C}_F^\dagger \tilde{C}_F = V_F D_{\text{occ}}^{\text{occ}} D_{\text{occ}}^{\text{occ}} \tilde{C}_F = V_F^\dagger V_F n^0 V_F^\dagger V_F = n^0 \)).

Likewise, the matrix which projects from the environment to the bath is defined as the product of the transformation from the environment levels to the occupied states (a matrix called \( D_{\text{env}}^{\text{occ}} \)) with the transformation from the occupied levels to the natural orbitals (\( V_F \)). After orthonormalization of the columns, we obtain:

\[
C_B = \frac{D_{\text{occ}}^{\text{occ}} V_F}{\sqrt{1 - n^0}}. \tag{51}
\]

We thus define the projector:

\[
\begin{bmatrix}
P \equiv \begin{bmatrix} C_F & C_B \end{bmatrix}, \tag{52}
\end{bmatrix}
\]

which projects the lattice problem (fragment \( \{ c_{\alpha \alpha}^i \}_{1 \leq \alpha \leq N_c} \) + environment \( \{ c_{\alpha \alpha}^i \}_{1 \leq \alpha \leq N_c} \)) onto the embedded problem (impurity \( \{ n_{\alpha'} \}_{1 \leq \alpha' \leq N_c} \) + bath \( \{ n_{\alpha} \}_{1 \leq \alpha \leq N_c} ):

\[
\begin{align}
\hat{c}_{\alpha}^\dagger &= \sum_{\alpha=1}^{N_c} C_{\alpha \alpha'} c_{\alpha' \alpha}^i, \tag{53} \\
\hat{n}_{\alpha} &= \sum_{i=2}^{N_c} \sum_{\alpha=1}^{N_c} C_{\alpha \alpha'} c_{\alpha' \alpha}^i. \tag{54}
\end{align}
\]

Instead of the natural-orbital basis, one can choose instead to use the original basis (denoted by unprimed Greek indices) as a single-site basis to express the creation operators \( c^\dagger \) and \( a^\dagger \) of the embedded problem. This is done by defining the alternative projector:

\[
P = \tilde{\mathcal{P}} \begin{bmatrix} C_F^\dagger \\ C_B^\dagger \end{bmatrix}, \tag{55}
\]

which is related to \( \mathcal{P} \) by a unitary transform,

\[
P = \tilde{\mathcal{P}} \begin{bmatrix} C_F^\dagger \\ C_B^\dagger \end{bmatrix}, \tag{56}
\]

where \( \tilde{\mathcal{P}} \) projects into the natural orbitals, while \( P \) projects into the original orbitals.

We note that the above construction corresponds to carrying out the Schmidt decomposition of \( | \Psi_0(u) \rangle \) [20].

In the next subsection, we use \( P \) to project lattice observables onto the embedded subspace.

C. Projections in the embedded subspace

After constructing the impurity and bath levels, one can now map the density matrix and lattice Hamiltonian onto the embedded subspace.
1. Embedded density matrix

The projection of the density matrix onto the embedded subspace is defined in Eq. (46), and similarly for $\rho_{\text{embed}}$. After a few algebraic steps detailed in Appendix B1, we obtain

$$
\rho_{\text{embed}} \equiv P^\dagger \rho P = \left[ \frac{\Delta^p}{\sqrt{\Delta^p(1 - \Delta^p)}} \frac{\Delta^p(1 - \Delta^p)}{1 - n^0} \right],
$$

(56)
i.e. $\rho_{\text{embed}}$ is entirely determined by the occupations of the natural orbitals $n^0$. Similarly, its expression in the original basis is

$$
\rho_{\text{embed}} \equiv \left[ \frac{\Delta^p}{\sqrt{\Delta^p(1 - \Delta^p)}} \right],
$$

(57)

with

$$
\Delta^p \equiv C_F n^0 c^\dagger_F = D_F^{\text{occ}} D_F^{\text{occ},\dagger} = \rho_F,
$$

and $\rho_F$ the top-left $N_c \times N_c$ block of $\rho$. Thus, $\Delta^p$ is the one-particle density matrix of the fragment, $\rho_F$. Using (47), we thus have:

$$
\Delta^p_{\alpha\beta} = \sum_{k,\omega} e^{i\omega\tau^+} [i\omega 1 - t - u + \mu]^{-1}_{\alpha\beta}
= \sum_{k,\omega} e^{i\omega\tau^+} [i\omega 1 - \varepsilon_k - u + \mu]^{-1}_{\alpha\beta}.
$$

We define

$$
\bar{u}_{\alpha\beta} \equiv u_{\alpha\beta} + [\varepsilon_{\text{loc}}]_{\alpha\beta}
$$

(58)
to obtain the analog of Eq. (28a) in the RISB formalism:

$$
\Delta^p_{\alpha\beta} = \sum_{k,\omega} e^{i\omega\tau^+} [i\omega 1 - \varepsilon_k - \bar{u} + \mu]^{-1}_{\alpha\beta}.
$$

(59)

Eqs (28a) and (59) can be identified provided:

$$
R = 1,
$$

(60a)

$$
\lambda = \bar{u}.
$$

(60b)

In the next subsection, we show that this identification holds for all other DMET observables.

2. Parameters of the embedded problem

Based on the two definitions of $H_{\text{embed}}$, Eqs. (3) and (43), we can write:

$$
h_{\text{embed}} = \left[ \frac{t_F}{D^\dagger} \frac{D}{-\lambda^c} \right].
$$

(61)

Identifying the right-hand sides of Eqs (44) and (61), and thanks to the definition [Eq. (55)] of $P$, one can show, after a few algebraic steps detailed in Appendix B2, that:

$$
D = \sum_{k,\omega} \bar{\xi}_k [i\omega - \bar{\xi}_k - \bar{u}]^{-1} \left[ \sqrt{\Delta^p(1 - \Delta^p)} \right]^{-1},
$$

(62a)

and

$$
\lambda^c = -\bar{u} - \left[ \frac{\sqrt{(1 - \Delta^p)\Delta^p}}{2} \right],
$$

(62b)

which respectively correspond to Eqs. (28b) and (28c) with the identification (60a-60b).

D. Self-consistency conditions

As mentioned in a previous section, the DMET self-consistency conditions consist in matching the embedded density matrix $\rho_{\text{embed}}$ obtained by projection of the lattice-density matrix onto the embedded subspace with the density matrix of the embedded or impurity problem, whose block structure reads:

$$
\rho_{\text{imp}} = \left[ \begin{array}{cc} N^c & M \\ M^\dagger & N^a \end{array} \right].
$$

(63)

with $N^a$ and $M$ defined in Eqs (33a-33b) and

$$
N^c_{\alpha\beta} \equiv \langle \Phi | c_{\alpha}^\dagger c_{\beta} | \Phi \rangle,
$$

(64)

where $| \Phi \rangle$ is the ground state of the impurity Hamiltonian, i.e the solution of Eq. (28d). Thus, the self-consistency conditions explicitly read

$$
\langle \Phi | a_{\alpha} a_{\beta}^\dagger | \Phi \rangle = \Delta^p_{\alpha\beta},
$$

(65a)

$$
\langle \Phi | c_{\alpha}^\dagger c_{\beta} | \Phi \rangle = \left[ \sqrt{\Delta^p(1 - \Delta^p)} \right]_{\alpha\beta},
$$

(65b)

$$
\langle \Phi | c_{\alpha}^\dagger c_{\beta} | \Phi \rangle = \Delta^p_{\alpha\beta}.
$$

(65c)

The first two lines, with the identification (60a), correspond to the RISB conditions (28c-28f).

E. Solution of the DMET equations: overdetermination, idempotency and alternative self-consistency conditions

The DMET equations presented in the previous sections have so far been solved in a forward recursive way:
1. Start from a guess for $u$.

2. Compute $\mathcal{D}$ and $\lambda^c$ from $\Delta^p$ and $K_{\text{loc}}$.

3. Solve the impurity model for $\rho_{\text{imp}}$, i.e. for $N^a$, $N^c$ and $M$.

4. From $u$, compute $\rho_{\text{embed}}(u')$ as given by Eq. (57). If $\rho_{\text{embed}}(u') = \rho_{\text{imp}}(u)$, self-consistency is reached and the solution is $u$. Otherwise, find $u'$ such that $\rho_{\text{embed}}(u') = \rho_{\text{imp}}(u)$ and go back to step 2 with the new $u'$ until self-consistency is reached. This loop is different from the loop presented in section II 4. The potential advantage of this alternative forward recursion is that it in principle requires fewer computations of the impurity solution: the root problem, 

$$ \mathcal{F}(u') \equiv \rho_{\text{embed}}(u') - \rho_{\text{imp}}(u) = 0, \quad (66) $$

requires only one impurity computation (to compute $\rho_{\text{imp}}(u)$). However, this root problem must be solved several times, so that the numerical gain is \textit{a priori} unclear.

On the other hand, the DMET self-consistency condition leads to an overdetermined root problem: there is only one unknown $u$ to satisfy three self-consistency conditions Eqs (65a-65b-65c). In comparison, the root problem to be solved in RISB has as many unknowns ($R$ and $\lambda$) as equations ($\mathcal{F}^{(1)} = 0$ and $\mathcal{F}^{(2)} = 0$). Another independent issue is that $\rho_{\text{embed}}$ as given in Eq. (56) or (57) is idempotent (one can check that $\rho_{\text{embed}}^2 = \rho_{\text{embed}}$), with the consequence that its eigenvalues must be zero or one. That $\rho_{\text{imp}}$ generically shares this property is improbable; in fact, converged RISB results in the literature (with $R \neq 1$) prove that $\rho_{\text{imp}}$ is in general not idempotent.

This has led to the exploration of several (arbitrary) procedures in the literature: the original papers proposed to minimize the sum of the squared differences between the matrix elements of $\rho_{\text{embed}}$ and $\rho_{\text{imp}}$ (instead of trying to find the root of Eq. (66)); other authors suggest to fulfill only the condition on the density (e.g. Eq (65a)), a scheme dubbed “density embedding theory”, DET [34].

In Fig. 2 (bottom panel), we illustrate another possible recursive scheme to solve the DMET equations inspired from DMFT (this scheme corresponds to the forward recursion presented in section II 4, only with $R = 1$). This figure, while emphasizing the similarities between the three methods, also hints at the overtermination problem we just discussed: while in RISB, two observables are needed to compute ($N^a$ and $M$) and parametrize ($\lambda$ and $R$) the self-energy and to characterize the embedded problem ($\lambda^c$ and $\mathcal{D}$), in DMET, two observables ($N^a$ and $M$) are computed at the level of the embedded problem (and needed to describe it, $\lambda^c$ and $\mathcal{D}$), but the self-energy is described by only one parameter ($\lambda$ or $u$), possibly pointing to an underexploitation of the physical information contained in the solution of the impurity model.

**IV. CONCLUSION**

In this work, we have derived the relation between two methods, RISB and DMET, which can both be regarded as simplified versions of DMFT. As such, they can access regimes of parameters and systems for which the exact solution, via quantum Monte-Carlo, of the DMFT impurity problem, is prohibitively costly if not out of reach due to the negative sign problem or very large computing times.

We have shown that the DMET equations can be obtained from the RISB equations by setting the quasiparticle weight factor to 1 in RISB. This allows to establish a clear connection between these two methods, which are both based on the mapping of a strongly correlated problem onto a simplified problem describing correlated orbitals embedded in a noninteracting host.

An additional comparison among the methods is possible if one uses the interpretation of the RISB method as a linear expansion of a self-energy [28]. Therefore, if one focusses on the low-energy behavior of the self-energy, DMFT has real and imaginary parts with a general frequency dependence, RISB keeps the constant and linear term in a real self-energy, and DMET is purely static. In this context, it is worth mentioning other approximate methods which use a very different parametrization of the self energy in terms of a continuous fraction expansion (see for instance Refs. 52 and 53).

This common perspective on the three methods naturally suggests transposing extensions of one method to the others. For instance, a simple generalization of the RISB/Gutzwiller ground-state energy to a temperature-dependent free energy, briefly exposed in Appendix C, can be used to derive a temperature-dependent DMET free energy.

This work opens additional questions for cluster extensions. For instance, DMET yields good spectra for the Hubbard model [39]. Given that RISB and DMET have the same computational cost (that of solving an impurity model with the same number of bath and impurity levels), similar calculations should be carried out with the RISB method to explore how that embedding accelerates the convergence to the thermodynamic limit for spectral properties.

Applications of DMFT to molecular systems already exist [54, 55], but it has been difficult to extend it to complex molecules. On the other hand, DMET has been
very successful in its applications to quantum chemistry [35]. It would be interesting to explore potential applications of RISB in that field as well.

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Appendix A: Transformation of the overlap matrix to diagonal form

We start by diagonalizing the noninteracting Hamiltonian $h$; we obtain:

$$ h = D \epsilon D^\dagger, $$

with $D$ a $N \times N$ unitary matrix and $\epsilon = \text{diag}(\{\epsilon_k\}_{k=1})$ a diagonal matrix. Thanks to the expression (47), $D$ also diagonalizes the density matrix, i.e.

$$ \rho = D_n D^\dagger, \quad (A1) $$

with $n$ a diagonal matrix with entries $n(\epsilon_k)$. The first $n_{\text{occ}}$ eigenvalues of $\rho$ (i.e. the first $n_{\text{occ}}$ entries of $n$) are unity (they correspond to the occupied states), while the other eigenvalues vanish (they correspond to the empty states).

We now split $D$ into its fragment and its environment blocks:

$$ D = \begin{bmatrix} D_F & \vdots \\ \vdots & D_E \end{bmatrix}, \quad (A2) $$

where $D_F$ is of size $N_c \times N$. Since $D$ is unitary, the following properties hold:

$$ D_F^\dagger D_F + D_E^\dagger D_E = 1, \quad (A3) $$

$$ D_F D_F^\dagger = 1, $$

$$ D_E D_E^\dagger = 1. $$

We further decompose $D_F$ into two blocks

$$ D_F = \begin{bmatrix} D_F^{\text{occ}} & D_F^{\text{unocc}} \end{bmatrix}, \quad (A4) $$

with $D_F^{\text{occ}}$ a $N_c \times n_{\text{occ}}$ matrix. Note that (A3) implies:

$$ D_F^{\text{occ}}\dagger D_F^{\text{occ}} + D_E^{\text{occ}}\dagger D_E^{\text{occ}} = 1. \quad (A5) $$

We now perform a singular value decomposition of $D_F^{\text{occ}}$. We obtain:

$$ D_F^{\text{occ}} = U \left\{ \text{diag} \{\sqrt{n^0}\}, 0 \right\} V^\dagger, \quad (A6) $$

with $U$ a $N_c \times N_c$ unitary matrix, $\left\{ \text{diag} \{\sqrt{n^0}\}, 0 \right\}$ a $N_c \times n_{\text{occ}}$ matrix (with $\text{diag} \{\sqrt{n^0}\}$ a $N_c \times N_c$ diagonal matrix, simply denoted as $\sqrt{n^0}$ in the following), and $V$ a $n_{\text{occ}} \times n_{\text{occ}}$ unitary matrix. We decompose $V$ into two blocks:

$$ V = \begin{bmatrix} V_F & V_E \end{bmatrix}, \quad (A7) $$

with $V_F$ a $n_{\text{occ}} \times N_c$ matrix. The unitarity of $V$ implies the properties

$$ V_F V_F^\dagger + V_E V_E^\dagger = 1, $$

$$ V_F^\dagger V_F = 1, $$

$$ V_E^\dagger V_E = 1. \quad (A8) $$

Plugging (A7) into (A6), we obtain:

$$ D_F^{\text{occ}} = U \sqrt{n^0} V_F^\dagger \quad (A9) $$

The last step is to notice that the overlap matrix $S^{\text{occ}}$, defined in Eq. (48), is also given by the expression

$$ S^{\text{occ}} = D_F^{\text{occ},\dagger} D_F^{\text{occ}}. \quad (A10) $$

Thus, using (A9), we obtain Eq. (49).

Appendix B: Projections into the embedded subspace

We start by noting that the transformation between site indices and natural orbital indices is given by $C_F$ (defined in Eq. (50)), itself equal to $U$:

$$ C_F = \frac{U \sqrt{n^0} V_F^\dagger V_F}{\sqrt{n^0}} = U, \quad (B1) $$

where we have used Eqs. (A9) and (A8).

1. Density matrix

Using the block decomposition of the lattice density matrix:

$$ \rho = \begin{bmatrix} \rho_F & \rho_c \\ \rho_c & \rho_E \end{bmatrix}, \quad (B2) $$

(with $\rho_F$ a $N_c \times N_c$ matrix, and so on) and the expressions (A1-A2-A4), we obtain:

$$ \rho = \begin{bmatrix} D_F^{\text{occ},\dagger} D_F^{\text{occ}} & D_F^{\text{occ}} D_E^{\text{occ},\dagger} \\ D_E^{\text{occ},\dagger} D_F^{\text{occ}} & D_E^{\text{occ}} D_E^{\text{occ},\dagger} \end{bmatrix}. $$
Thus, using Eq. (46):

\[ \mathcal{D} = h_c C_F^\dagger C_F = D_E \varepsilon D_E^\dagger V_F U \left[ \sqrt{1 - \Delta P^0} \right]^{-1} \left[ \left( 1 - \Delta P \right) \Delta P \right]^{-1} \left( 1 - \Delta P \right) \left( 1 - \Delta P \right)^{-1} \]

\[ = -h_c \rho_c^0 \left[ \sqrt{\Delta P(1 - \Delta P)} \right]^{-1}. \]

Comparing with Eq. (30), we note that:

\[ h_c \rho_c^0 = \mathcal{K}_{\text{loc}}[R = 1, \lambda = \hat{u}]. \]

Let us now simplify \( \chi^c \):

\[ \chi^c = -U \sqrt{n^0} V_F U \left[ \sqrt{\Delta P(1 - \Delta P)} \Delta P \right]^{-1} U V_F^\dagger D_E^\dagger \](B7)

To simplify \( \rho_c h_E \rho_c^0 \), let us first notice:

\[ \mathcal{K}_{\text{loc}} = h_c \rho_c^0 = D_F \varepsilon D_E^\dagger D_F \varepsilon D_E \]

\[ = D_F n_D^0 = h_F \Delta P^0. \]

Hence:

\[ \rho_c h_E \rho_c^0 = D_F n_D^0 D_E^\dagger D_E D_F \varepsilon D_E \varepsilon D_E^\dagger \] (B6)

This yields Eq. (62b) of the main text.

\[ \text{Appendix C: Ground-State energy and finite-temperature extension} \]

At \( T = 0 \), the total energy in RISB is given by

\[ E = \sum_k \text{Tr} \left[ n_F \left( R \tilde{\varepsilon}_k R^\dagger + \lambda - \mu \right) \right] \]

\[ + \sum_i \text{Tr} \left[ H_{\text{loc}} \Phi_i \Phi_i^\dagger \right], \]

where \( n_F \) is the Fermi function, and \( H_{\text{loc}} \) contains the chemical potential \( \mu \).
Note that it is straightforward to show that, using Eqs. (28b), (28f) and (27b), and with $R = 1$, Eq. (C1) is equivalent to the DMET ground-state energy given in [20, 33]:

$$
E = \sum_i \left\{ \text{Tr} \sum_{\alpha\beta} \left[ D_{\alpha\beta} \Phi_i^\dagger F_{\alpha\beta} F_i^\dagger + \text{h.c.} \right] + \text{Tr} \left[ H_{\text{loc}} \Phi_i^\dagger \Phi_i \right] \right\}.
$$

(C2)

In RISB, Eqs. (C1) and (C2) produce the same total energies because the Lagrange equations, Eqs. (28a)-(28f), are exactly satisfied. However, in DMET, since the Lagrange equation, Eq. (66), can merely be minimized, Eqs. (C1) and (C2) no longer yield the same energy. One has to evaluate the total energy using Eq. (C2) as done in the DMET literature.

The RISB formalism can be readily extended to finite temperatures, as will be explored in a separate publication. We give the final expression for the resulting free energy:

$$
\Omega = -T \sum_k \log \left( 1 + e^{-\beta (R \tilde{H} + \lambda - \mu) \delta_{k\tilde{I}}} \right)
+ T \sum_i \text{Tr} \log \left[ 1 - e^{-\beta (E_{\text{embed}} - E^{\text{loc}})} \right] + E^{\text{loc}}
$$

$$
- \sum_{i,\alpha\beta} \left( \lambda_{\alpha\beta} + \chi_{\alpha\beta} \right) \Delta^p_{\alpha\beta}
- \sum_{i,\alpha\beta\gamma} \left( D_{\alpha\beta} R_{\gamma\alpha} + \text{c.c.} \right) \left( \Delta^p (1 - \Delta^p) \right)^{1/2},
$$

(C3)

where $\tilde{I}$ is an identity matrix with the size of the Hilbert space of $H_{\text{embed}}$.

The fact that DMET is a simplification of RISB with $R = 1$ gives an easy way to generalize DMET to finite temperatures. The implications of this finite-temperature extension of RISB and DMET will be explored in a separate publication.

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