

15 Slave-Boson Theories of Multi-Orbital Correlated Systems

Nicola Lanatà

School of Physics and Astronomy

Rochester Institute of Technology

84 Lomb Memorial Drive, Rochester, NY 14623, USA

Contents

1	Introduction	2
2	The multi-orbital Hubbard Hamiltonian	3
3	Multi-orbital ghost Gutzwiller approximation (variational formulation)	4
4	Reformulation using local reduced density-matrix	12
5	Reformulation in terms of slave-boson amplitudes (connection with RISB)	13
6	Reformulation in terms of embedding states (connection with DMET)	15
7	Lagrange formulation of gGA (QE algorithmic structure)	19
8	Generalizations, research directions and open problems	23
9	Code availability	25
A	Useful mathematical definitions	26
B	Preliminaries on fermionic algebra and Fock states	27
C	One-body Hamiltonians and the Fermi-function matrix	31
D	Wick's theorem for one-body thermal states	34
E	Reduced density-matrix of a fermionic subsystem	36
F	Promoting of functions to independent variables	37
G	A useful matrix derivative	38

1 Introduction

Strongly correlated electron systems, where electron-electron interactions are non-negligible, have captivated the condensed matter physics community due to the rich and often exotic physical phenomena they exhibit, including high-temperature superconductivity and magnetism. The theoretical study of such systems is indispensable in uncovering the underlying physics and holds tremendous promise for technological advancements. However, this is no small feat, as strongly correlated systems are notoriously difficult to describe accurately due to the complexity arising from these interactions. Advanced graduate students, Ph.D. students, and postdoctoral researchers venturing into the electronic structure of materials must be adept with an array of theoretical tools to effectively address these challenges.

Within the broad spectrum of techniques available for tackling strongly correlated systems, “slave-boson methods” have emerged as a versatile and powerful class of approaches [1–20]. These methods employ auxiliary particles, including both fermions and bosons, as subsidiary degrees of freedom to model strong electron-electron interactions, a concept shared across various theoretical frameworks such as tensor networks [21, 22] and neural-network quantum states [23]. In the context of slave-boson methods, the Gutzwiller Approximation (GA) theory and its extension, the ghost Gutzwiller Approximation (gGA), employ auxiliary fermionic degrees of freedom [10–12], while the Rotationally Invariant Slave Boson (RISB) theory and its extension, the ghost RISB (gRISB), utilize auxiliary bosonic degrees of freedom [19, 20].

Historically, slave-boson methods such as the GA were developed as computationally efficient alternatives to more demanding techniques, but this efficiency was achieved with a compromise on accuracy. However, recent advancements have shown that extensions like gGA [10–12], which incorporates auxiliary fermionic degrees of freedom to enrich the variational space, offer both computational efficiency and the potential for high accuracy. Notably, gGA has demonstrated an accuracy that is comparable to the more computationally demanding Dynamical Mean-Field Theory (DMFT) [24, 25], indicating that it might serve as an advantageous alternative, especially when aiming for a combination of accuracy and computational manageability.

This set of lecture notes is designed to provide a comprehensive overview of “slave-boson methods” with a particular focus on the gGA variational perspective. Through detailed technical expositions and unified, consistent notation, these notes aim to serve as a pedagogical resource for readers looking to delve into this field. While scientific literature often prioritizes conciseness over extensive derivations, this can sometimes leave out pedagogical explanations that are instrumental for learners and non-specialists. Our objective is to bridge this gap, furnishing the reader with a self-contained and in-depth comprehension of the subject matter. Furthermore, in the light of the active and burgeoning nature of this research area, we also elucidate the reformulations in terms of RISB/gRISB and explore connections with Quantum Embedding (QE) methods such as Density-Matrix Embedding Theory (DMET), while discussing their potential for catalyzing further theoretical and algorithmic advancements.

We suggest the reader begin with the Appendix, where we recapitulate some useful general notions of many-body theory. While the reader may already be familiar with these concepts, the

Appendix employs a consistent notation with the main text, making it a valuable starting point. Following this, in Sec. 3, we introduce the formalism from the variational perspective underlying the GA/gGA frameworks. In Sec. 5, we delve into the concept of slave-boson amplitudes; while keeping the focus on the GA/gGA formulation and the role of slave-boson amplitudes in formulating an efficient framework from this perspective, this is the juncture where the connection with RISB emerges, and we will guide the reader to the relevant literature exploring this connection. Sections 6 and 7 present the concept of embedding states; again, while maintaining a focus on the GA/gGA formulation, we highlight the role of embedding states in developing an efficient framework, and this is where the connection with Quantum Embedding theories such as DMET becomes apparent. Finally, Sec. 8 discusses further generalizations, new research directions, and open problems that aspiring researchers might find intriguing and rewarding to explore in their careers.

2 The multi-orbital Hubbard Hamiltonian

In this section, we describe the multi-orbital Hubbard Hamiltonian, which plays a fundamental role in the context of strongly correlated electron systems. We will elaborate on the terms and the notation involved. For readers not familiar with the mathematical structure of fermionic Fock spaces, a brief introduction is provided in Appendix B.

The multi-orbital Hubbard Hamiltonian encompasses local interactions as well as hopping terms. We contemplate a lattice system comprised of \mathcal{N} fragments, each with multiple orbitals. The total Hamiltonian \hat{H} can be formulated as:

$$\hat{H} = \sum_{i=1}^{\mathcal{N}} \hat{H}_{loc}^i [c_{i\alpha}^\dagger, c_{i\alpha}] + \sum_{i \neq j} \hat{T}_{ij}, \quad (1)$$

$$\hat{T}_{ij} = \sum_{\alpha=1}^{\nu_i} \sum_{\beta=1}^{\nu_j} [t_{ij}]_{\alpha\beta} c_{i\alpha}^\dagger c_{j\beta}, \quad (2)$$

where:

- i and j represent the indices of the fragments of the lattice.
- \hat{H}_{loc}^i denotes an arbitrary local operator on fragment i , encompassing one-body and two-body terms.
- α and β index the fermionic modes (orbitals) within each fragment.
- \hat{T}_{ij} symbolizes the hopping term between *different* fragments i and j .
- $[t_{ij}]_{\alpha\beta}$ are the matrix elements of the hopping term.

This Hamiltonian serves as the basis for our discussions on the ghost Gutzwiller approximation for multi-orbital systems in the subsequent sections.

3 Multi-orbital ghost Gutzwiller approximation (variational formulation)

In this section, we delve into the multi-orbital ghost Gutzwiller approximation (gGA) [10, 11], which is rooted in the variational principle and the limit of infinite dimensionality [1,2], building upon the multi-orbital Gutzwiller Approximation (GA) [1–9]. The gGA enriches the variational space by introducing auxiliary “ghost” fermionic degrees of freedom. This concept resonates with various theoretical frameworks such as extensions to DMET [26], matrix-product states and projected entangled pair states [27], ancilla qubit techniques [28], and extensions of neural network states [29], as well as the physical notions of “hidden Fermion” [30] and “hidden Fermi liquid” [31]. Given the close resemblance in derivation and algorithmic structure between gGA and multi-orbital GA, and the fact that the gGA framework includes the GA itself as a special case, we focus on the gGA framework for clarity and conciseness.

3.1 The gGA variational ansatz

Let us begin by introducing the structure of the variational ansatz used in gGA. We define a wavefunction $|\Psi_G\rangle$, which is obtained by applying an operator, indicated as $\hat{\mathcal{P}}_G$, to a reference single-particle wavefunction (Slater determinant) $|\Psi_0\rangle$

$$|\Psi_G\rangle = \hat{\mathcal{P}}_G |\Psi_0\rangle, \quad \text{with} \quad \hat{\mathcal{P}}_G = \prod_{i=1}^{\mathcal{N}} \hat{\mathcal{P}}_i, \quad (3)$$

Here, $|\Psi_0\rangle$ is the single-particle reference state, and $\hat{\mathcal{P}}_G$ is an operator composed of “local” operators $\hat{\mathcal{P}}_i$, whose precise mathematical structure will be described below.

Within our framework, the single-particle wavefunction $|\Psi_0\rangle$ is conceived in an auxiliary Hilbert space, while the operator $\hat{\mathcal{P}}_G$ maps states from the auxiliary space to the physical space. This is illustrated schematically in Fig. 1. Both $|\Psi_0\rangle$ and $\hat{\mathcal{P}}_i$ have to be optimized variationally, in order to minimize the variational energy

$$\mathcal{E}(\Psi_0, \hat{\mathcal{P}}_G) = \langle \Psi_G | \hat{H} | \Psi_G \rangle. \quad (4)$$

Specifically, we assume that the local operators $\hat{\mathcal{P}}_i$ (traditionally called “projectors” for historical reasons, but here not assumed to be projectors) have the following mathematical structure

$$\hat{\mathcal{P}}_i = \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} [\Lambda_i]_{\Gamma n} |\Gamma, i\rangle \langle n, i|, \quad (5)$$

$$|\Gamma, i\rangle = [c_{i1}^\dagger]^{q_1(\Gamma)} \dots [c_{iq_{\nu_i}}^\dagger]^{q_{\nu_i}(\Gamma)} |0\rangle, \quad (6)$$

$$|n, i\rangle = [f_{i1}^\dagger]^{q_1(n)} \dots [f_{iq_{B\nu_i}}^\dagger]^{q_{B\nu_i}(n)} |0\rangle. \quad (7)$$

In these equations we utilize the notation introduced in Sec. B.2, where $q_a(n)$ denotes the a -th occupation number of a Fock state $|n, i\rangle$, which is the a -th digit of the integer n in binary form. Additionally, the entries of the matrix Λ_i are variational parameters parametrizing $\hat{\mathcal{P}}_i$.

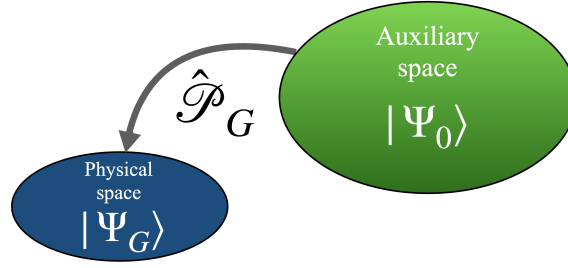


Fig. 1: Diagrammatic representation of the gGA variational ansatz. The wavefunction $|\Psi_G\rangle$ is obtained by mapping a generic single-particle wavefunction $|\Psi_0\rangle$ through an operator $\hat{\mathcal{P}}_G$. Both $|\Psi_0\rangle$ and $\hat{\mathcal{P}}_G$ are optimized variationally.

Remark. We point out that, in the traditional Gutzwiller Approximation (GA), the reference wavefunction $|\Psi_0\rangle$ is constructed directly within the physical Hilbert space, and the “Gutzwiller projector” $\hat{\mathcal{P}}_G$ in GA only operates within the physical space.

In contrast, in the gGA, the operator $\hat{\mathcal{P}}_G$ plays also the critical role of mapping the reference wavefunction $|\Psi_0\rangle$, which resides in the auxiliary space, onto a variational state $|\Psi_G\rangle$ residing in the physical space. Thus, the operator $\hat{\mathcal{P}}_G$ is inherently operating across both the auxiliary and physical spaces. It implements this mapping, while modulating the weights of the local electronic configurations, for optimizing the variational energy.

Remark. It is important to note that if the auxiliary space is configured as a mere replica of the physical space by setting $B = 1$ in Eqs. (5) and (7), gGA becomes mathematically equivalent to the traditional GA. In this specific case the resulting variational function $|\Psi_G\rangle$ would be as if $\hat{\mathcal{P}}_G$ and $|\Psi_0\rangle$ resided exclusively within the physical space. However, by setting B as an integer higher than 1 (generally an odd number for reasons that will be clarified later), the auxiliary space is enlarged, and gGA introduces additional degrees of freedom, thereby systematically enriching the variational ansatz. This gives the gGA the flexibility to explore the space of variational wavefunctions more comprehensively, establishing its primary distinction and advantage over the traditional GA.

While the remarks above are conceptually important, the gGA and the classic multi-orbital GA share essentially the same derivation and algorithmic structure. Consequently, for the sake of brevity and clarity, we will present the formalism directly in the context of the gGA framework.

3.2 Restriction to the “normal” variational states

We will focus on the normal phase, i.e., we will consider variational states $|\Psi_G\rangle$ that are eigenvectors of the physical number operator $\sum_{i\alpha} c_{i\alpha}^\dagger c_{i\alpha}$. It is important to note that, for $|\Psi_G\rangle$ to be an eigenstate of the number operator, it is not necessary that $\hat{\mathcal{P}}_i$ commutes with the number operator, as is the case in classic GA. Instead, it is sufficient that

- the auxiliary state $|\Psi_0\rangle$ is an eigenstate of the auxiliary-space number operator $\sum_{ia} f_{ia}^\dagger f_{ia}$,
- the coefficients $[A_i]_{\Gamma n}$ of $\hat{\mathcal{P}}_i$ satisfy the condition

$$\sum_{j=1}^{B\nu_i} q_j(n) - \sum_{j=1}^{\nu_i} q_j(\Gamma) = N(n) - N(\Gamma) = m_i \quad \forall \Gamma, n \mid [A_i]_{\Gamma n} \neq 0, \quad (8)$$

where m_i is an integer.

This condition ensures that the $\hat{\mathcal{P}}_i$ operators, defined in Eqs. (5) and (7), map the auxiliary states $|n, i\rangle$ into physical states $|l, i\rangle$, with the number of physical fermions being reduced by an integer amount in each subsystem i . Consequently, the total number of physical fermions in $|\Psi_G\rangle$ is well defined and differs from the number of auxiliary fermions in $|\Psi_0\rangle$ by $\sum_{i=1}^N m_i$.

In principle, m_i could be regarded as an additional variational parameters, to be optimized for minimizing the variational energy. However, previous work such as Ref. [11] showed that we can generally make the assumption that B is odd and

$$m_i = (B-1)\nu_i/2. \quad (9)$$

This particular choice for m_i , which reduces to $m_i = 0$ for $B = 1$ (consistent with the standard GA ansatz), has been empirically found to be the best variational choice. Therefore, in these notes we are going to make this assumption from now on.

3.3 Approximations for evaluating the variational energy

Our primary goal is to find the ground state of the Hamiltonian \hat{H} by minimizing the variational energy. The variational energy \mathcal{E} is a function of the wavefunction $|\Psi_0\rangle$ and the operator $\hat{\mathcal{P}}_G$, and is given by

$$\mathcal{E}(\Psi_0, \hat{\mathcal{P}}_G) = \langle \Psi_0 | \hat{\mathcal{P}}_G^\dagger \hat{H} \hat{\mathcal{P}}_G | \Psi_0 \rangle. \quad (10)$$

However, evaluating the variational energy in Eq. (10) is a highly non-trivial task due to the complexity associated with many-body interactions and the vastness of the Hilbert space. Without making approximations, numerical approaches such as Variational Monte Carlo could be used, but are computationally demanding.

To simplify the problem, let us first recognize that since $|\Psi_0\rangle$ is a single-particle wavefunction, Wick's theorem can be applied. According to Wick's theorem, the expectation value of a product of creation and annihilation operators can be decomposed into a sum of products of expectation values of pairs of operators (see appendix D for details). However, even with Wick's theorem, the number of possible contractions contributing to the expectation value of \hat{H} in $\langle \Psi_0 | \hat{\mathcal{P}}_G^\dagger \hat{H} \hat{\mathcal{P}}_G | \Psi_0 \rangle$ is prohibitively large.

3.3.1 The Gutzwiller approximation and the Gutzwiller constraints

In light of the above, we must employ approximations that simplify the problem while still capturing the essential physics. Here, we introduce two main approximations:

1. **The Gutzwiller Constraints:** These constraints are limitations imposed on the variational wave function $|\Psi_G\rangle$, linking the variational parameters of $\hat{\mathcal{P}}_i$ and $|\Psi_0\rangle$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1 \quad (11)$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \quad \forall a, b = 1, \dots, B\nu_i. \quad (12)$$

These constraints slightly reduce the variational freedom, but, as we are going to see, they make the evaluation of the variational energy more manageable.

2. **The Gutzwiller Approximation:** The approximation consists in neglecting some of the Wick contractions arising when evaluating Eq. (10), based on the key observation that such terms would vanish in the particular limit of infinite coordination number. This approximation, that we are going to specify in detail below, constitutes a key connection with Dynamical Mean-Field Theory (DMFT), which is exact in this limit.

Let us now proceed to analyze how these approximations combined help in evaluating the variational energy efficiently.

3.3.2 Key consequence of the Gutzwiller constraints

For this purpose, it is essential to consider the left-hand side of Eq. (12)

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle, \quad (13)$$

using Theorem D.2 discussed in Sec. D.1 of the Appendix.

- In this context, we can treat the operator $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$, which resides entirely in the auxiliary space and is therefore some algebraic combination of the f modes, as the operator X of Theorem D.2. Following this theorem, we can write

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle + \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle. \quad (14)$$

This identity separates the expression into a disconnected term, where f_{ia}^\dagger is contracted with f_{ib} and $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$ is contracted with itself, and a connected term, where f_{ia}^\dagger and f_{ib} are both contracted with $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$.

- We can further simplify the first term on the right side of Eq. (14). Using the first Gutzwiller constraint [Eq. (11)], where it is specified that $\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle = 1$, the first term can be simplified as

$$\begin{aligned} \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle &= \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \\ &= 1 \cdot \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle. \end{aligned} \quad (15)$$

By substituting it in Eq. (14) we obtain

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle + \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \quad (16)$$

- Comparing Eq. (16) with the second Gutzwiller constraint in Eq. (12)

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle, \quad (17)$$

it follows that

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = 0. \quad (18)$$

- Applying the second part of Theorem D.2 to the left side of Eq. (18), we can express the sum of all connected terms in our expression as

$$\langle \Psi_0 | \overbrace{\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i}^{\text{connected}} f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \sum_{a'b'} \xi_i^{a'b'} \langle \Psi_0 | f_{ia'} f_{ia}^\dagger | \Psi_0 \rangle \langle \Psi_0 | f_{ib'}^\dagger f_{ib} | \Psi_0 \rangle = 0, \quad (19)$$

where the coefficients $\xi_i^{a'b'}$ depend only on $|\Psi_0\rangle$ and the operator $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$, but not on the indices a and b .

- Let us analyze the implications of Eq. (19). Defining the matrix Δ_i as

$$[\Delta_i]_{ab} = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle, \quad (20)$$

we can rewrite Eq (19) as

$$(\mathbf{1} - \Delta_i) \xi_i \Delta_i = 0, \quad (21)$$

from which it follows that, as long as neither Δ_i nor $\mathbf{1} - \Delta_i$ are degenerate, i.e., as long as none of the eigenvalues of Δ_i is equal to 0 or 1, we have

$$\xi_i = 0. \quad (22)$$

The significance of Eq. (22), which arises from the Gutzwiller constraints in Eqs. (11) and (12), is pivotal for streamlining the computation of the variational energy. This is due to its bearing on terms involving two contraction lines connecting $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$ with an arbitrary operator \hat{X} built from algebraic combinations of the f and f^\dagger modes.

Theorem 3.1. *Consider evaluating the expectation value $\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i \hat{X} | \Psi_0 \rangle$. In this scenario, all terms comprising two contraction lines connecting $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$ with \hat{X} do not contribute. More formally, if we depict the two contraction lines emerging from $\hat{\mathcal{P}}_i^\dagger$ and $\hat{\mathcal{P}}_i$, and linking them to \hat{X} , we can establish that*

$$\langle \Psi_0 | \overbrace{\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i}^{\text{connected}} \hat{X} | \Psi_0 \rangle = \sum_{a'b'} \xi_i^{a'b'} \langle \Psi_0 | f_{ia'} f_{ia}^\dagger | \Psi_0 \rangle \langle \Psi_0 | f_{ib'}^\dagger f_{ib} | \Psi_0 \rangle x^{ab} = 0. \quad (23)$$

Proof. The proof hinges on an observation we made in Sec. D.1. There, we noted that the coefficients $\xi_i^{a'b'}$ in Eq. (22) represent the sum of all terms stemming from self-contractions among the operators in $\hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i$ after excluding a' and b' , which are contracted with a and b respectively. Meanwhile, the coefficients x^{ab} signify the sum of all terms that originate from self-contractions among the operators in \hat{X} , excluding a and b which are contracted with a' and b' respectively.

Importantly, the coefficients $\xi_i^{a'b'}$ are only dependent on $|\Psi_0\rangle$, a' and b' , and are unaffected by \hat{X} . As such, they are equivalent to the ones in Eq. (19), which we have proven to be zero due to the Gutzwiller constraints (see Eq. (22)). This completes the proof. \square

3.3.3 The Gutzwiller approximation: Explicit definition

The Gutzwiller approximation is a key simplification used in conjunction with the Gutzwiller constraints, and it plays an essential role in streamlining the computation of the expectation value of the Hamiltonian with respect to the gGA variational states.

Specifically, the approximation involves neglecting terms in the expectation values with respect to $|\Psi_0\rangle$ that contain more than two non-local contractions. In this context, a non-local contraction refers to one that involves operators acting on different sites, such as $\langle\Psi_0|f_{ia}^\dagger f_{jb}|\Psi_0\rangle$, where $i \neq j$. The rationale behind this approximation is rooted in the behavior of these terms in the limit of infinite coordination number, where each site is infinitely connected. In this limit, all terms with more than two non-local contractions vanish. This aspect is particularly significant as dynamical mean-field theory (DMFT) becomes exact in this limit, establishing a meaningful link between the Gutzwiller approximation and DMFT.

In subsequent sections, we will delve into how the synergistic application of the Gutzwiller approximation and the Gutzwiller constraints considerably simplifies the evaluation of expectation values in our gGA variational framework.

3.4 Evaluation of the local expectation values

In this section, we will focus on one of the essential steps in the ghost Gutzwiller approximation (gGA) — the computation of the expectation value of local Hamiltonian terms with respect to the gGA wavefunction, $|\Psi_G\rangle$. To this end, let us consider a local Hamiltonian term, \hat{H}_{loc}^i , acting on fragment i as defined in Eq. (1). The expectation value of this term with respect to $|\Psi_G\rangle$ can be expressed as

$$\langle\Psi_G|\hat{H}_{\text{loc}}^i|\Psi_G\rangle = \langle\Psi_0|\left(\prod_{k=1}^{\mathcal{N}}\hat{\mathcal{P}}_k^\dagger\right)\hat{H}_{\text{loc}}^i\left(\prod_{k=1}^{\mathcal{N}}\hat{\mathcal{P}}_k\right)|\Psi_0\rangle = \langle\Psi_0|\prod_{k\neq i}\left(\hat{\mathcal{P}}_k^\dagger\hat{\mathcal{P}}_k\right)\left(\hat{\mathcal{P}}_i^\dagger\hat{H}_{\text{loc}}^i\hat{\mathcal{P}}_i\right)|\Psi_0\rangle. \quad (24)$$

At first glance, this expression appears challenging to evaluate without approximations due to the enormous number of possible Wick contractions.

Fortunately, the Gutzwiller constraints, as outlined in Eqs. (11) and (12), and the Gutzwiller approximation discussed previously, offer significant simplifications.

Consider a block $\hat{\mathcal{P}}_k^\dagger\hat{\mathcal{P}}_k$ within the product in Eq. (24). Wick's theorem allows us to categorize all possible terms contributing to this expectation value as follows:

- **Disconnected terms:** These are terms where there are no contraction lines between $\hat{\mathcal{P}}_k^\dagger\hat{\mathcal{P}}_k$ and the other operators. Utilizing the first Gutzwiller constraint, Eq. (11), the contribution of these terms is

$$\langle\Psi_0|\hat{\mathcal{P}}_k^\dagger\hat{\mathcal{P}}_k|\Psi_0\rangle\langle\Psi_0|\prod_{k'\neq i,k}\left(\hat{\mathcal{P}}_{k'}^\dagger\hat{\mathcal{P}}_{k'}\right)\left(\hat{\mathcal{P}}_i^\dagger\hat{H}_{\text{loc}}^i\hat{\mathcal{P}}_i\right)|\Psi_0\rangle = \langle\Psi_0|\prod_{k'\neq i,k}\left(\hat{\mathcal{P}}_{k'}^\dagger\hat{\mathcal{P}}_{k'}\right)\left(\hat{\mathcal{P}}_i^\dagger\hat{H}_{\text{loc}}^i\hat{\mathcal{P}}_i\right)|\Psi_0\rangle. \quad (25)$$

- **Terms with two contraction lines:** These terms have two contraction lines between $\hat{\mathcal{P}}_k^\dagger \hat{\mathcal{P}}_k$ and the other operators. As demonstrated in previous sections, the contribution of these terms is zero due to the Gutzwiller constraints.
- **Terms with four contraction lines:** These terms have four contraction lines between $\hat{\mathcal{P}}_k^\dagger \hat{\mathcal{P}}_k$ and the other operators. Due to the Gutzwiller approximation, these non-local contractions are effectively zero.

We can now understand that the logic discussed in the itemized list above applies to each block $\hat{\mathcal{P}}_k^\dagger \hat{\mathcal{P}}_k$ independently. We can iteratively apply it to each block, effectively eliminating all of them one by one. This iterative process simplifies the expression until we are only left with the block corresponding to fragment i .

Combining these observations, we arrive at a significant simplification of Eq. (24)

$$\langle \Psi_G | \hat{H}_{\text{loc}}^i | \Psi_G \rangle \approx \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{H}_{\text{loc}}^i \hat{\mathcal{P}}_i | \Psi_0 \rangle. \quad (26)$$

This expression vastly reduces the complexity involved in computing the expectation values of local Hamiltonian terms, making it feasible for practical implementations.

3.5 Evaluation of the one-body non-local expectation values

In this section, we will extend the methodology discussed in the previous section for local operators to calculate the expectation values of one-body non-local operators within the ghost Gutzwiller approximation (gGA). Specifically, we will consider operators of the form $c_{i\alpha}^\dagger c_{j\beta}$, where i and j are fragment labels and α and β are additional quantum numbers, such as spin. We are interested in computing the expectation value of this operator with respect to the gGA wavefunction $|\Psi_G\rangle$.

The expectation value of this one-body non-local operator can be written as

$$\begin{aligned} \langle \Psi_G | c_{i\alpha}^\dagger c_{j\beta} | \Psi_G \rangle &= \langle \Psi_0 | \left(\prod_{k=1}^{\mathcal{N}} \hat{\mathcal{P}}_k^\dagger \right) c_{i\alpha}^\dagger c_{j\beta} \left(\prod_{k=1}^{\mathcal{N}} \hat{\mathcal{P}}_k \right) | \Psi_0 \rangle \\ &= \langle \Psi_0 | \left(\prod_{k \neq i, j} \hat{\mathcal{P}}_k^\dagger \hat{\mathcal{P}}_k \right) \left(\hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i \right) \left(\hat{\mathcal{P}}_j^\dagger c_{j\beta} \hat{\mathcal{P}}_j \right) | \Psi_0 \rangle. \end{aligned} \quad (27)$$

Similar to the treatment in the previous section, we have grouped the terms with $k \neq i, j$ together. The additional complexity here arises from the fact that the non-local operator involves two different fragments, i and j .

We can employ the same considerations as in the previous section to simplify the expression in Eq. (27). Just as before, the Gutzwiller constraints and approximations allow us to iteratively eliminate all the $\hat{\mathcal{P}}_k^\dagger \hat{\mathcal{P}}_k$ blocks for $k \neq i, j$. In a manner analogous to the local terms, disconnected terms, terms with two contraction lines, and terms with four contraction lines can be handled exactly as was done for the local Hamiltonian terms, resulting in

$$\langle \Psi_G | c_{i\alpha}^\dagger c_{j\beta} | \Psi_G \rangle \approx \langle \Psi_0 | \left(\hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i \right) \left(\hat{\mathcal{P}}_j^\dagger c_{j\beta} \hat{\mathcal{P}}_j \right) | \Psi_0 \rangle. \quad (28)$$

The expression in Eq. (28) can be further simplified by making several key observations:

- **Grouping terms by the number of Wick contractions:** We can organize the terms in Eq. (28) by grouping them according to the number of Wick contractions between the blocks i and j . Specifically, we classify terms by collecting together all terms with only one Wick contraction between the blocks i and j , then those with three, five, and so on.
- **Neglecting terms with more than one Wick contraction:** Due to the Gutzwiller approximation, terms with three or more Wick contraction between blocks i and j are neglected. Therefore, only the terms with a single Wick contraction need to be considered.
- **Auxiliary space representation:** It is important to recognize that $\hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i$ operates entirely within the auxiliary space, so it can be represented as an algebraic combination of f_{ia} and f_{ia}^\dagger modes. This applies analogously to the j block with f_{jb} and f_{ja}^\dagger modes.
- **Matrix representation for self-contractions:** We can factor the contribution of all self-contractions within $\hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i$ that are left after having contracted f_{ia}^\dagger with an annihilation operator belonging to the j subsystem, and encode it into a $B\nu_i \times \nu_i$ matrix $[\mathcal{R}_i]_{a\alpha}$ as

$$\langle \Psi_0 | \left(\hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i \right) \left(\hat{\mathcal{P}}_j^\dagger c_{j\beta} \hat{\mathcal{P}}_j \right) | \Psi_0 \rangle = \sum_{a=1}^{B\nu_i} \sum_{b=1}^{B\nu_j} \langle \Psi_0 | \left([\mathcal{R}_i]_{a\alpha} f_{ia}^\dagger \right) \left([\mathcal{R}_j]_{\beta b}^\dagger f_{jb} \right) | \Psi_0 \rangle, \quad (29)$$

for all $i \neq j$.

- **Computing local expectation values using coefficient matrices:** The same coefficient matrices \mathcal{R}_i would arise from self-contractions also in the following expression

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i f_{ia} | \Psi_0 \rangle = \sum_{b=1}^{B\nu_i} [\mathcal{R}_i]_{b\alpha} \langle \Psi_0 | f_{ib}^\dagger f_{ia} | \Psi_0 \rangle. \quad (30)$$

As we are going to see, the steps above can be used for calculating \mathcal{R}_i , therefore facilitating the computation of Eq. (29).

3.6 Recap: Evaluation of the variational energy

Let us take a moment to recapitulate the key developments in our evaluation of the variational energy within the ghost Gutzwiller approximation (gGA), employing the Gutzwiller constraints and the Gutzwiller approximation.

1. **Expectation value of local operators:** In Sec. 3.4 we derived the equation

$$\langle \Psi_G | \hat{H}_{\text{loc}}^i | \Psi_G \rangle \approx \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{H}_{\text{loc}}^i \hat{\mathcal{P}}_i | \Psi_0 \rangle. \quad (31)$$

2. **Expectation value of non-local one-body operators:** In Sec. 3.5 we derived

$$\langle \Psi_G | c_{i\alpha}^\dagger c_{j\beta} | \Psi_G \rangle \approx \sum_{a=1}^{B\nu_i} \sum_{b=1}^{B\nu_j} \langle \Psi_0 | \left([\mathcal{R}_i]_{a\alpha} f_{ia}^\dagger \right) \left([\mathcal{R}_j]_{\beta b}^\dagger f_{jb} \right) | \Psi_0 \rangle, \quad (32)$$

where we introduced the \mathcal{R}_i , characterized by

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i f_{ia} | \Psi_0 \rangle = \sum_{b=1}^{B\nu_i} [\mathcal{R}_i]_{b\alpha} \langle \Psi_0 | f_{ib}^\dagger f_{ia} | \Psi_0 \rangle. \quad (33)$$

Summing up the above contributions, the variational energy \mathcal{E} can be expressed as

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}_j^\dagger \right]_{ab} \langle \Psi_0 | f_{ia}^\dagger f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{H}_{loc}^i [c_{i\alpha}^\dagger, c_{i\alpha}] \hat{\mathcal{P}}_i | \Psi_0 \rangle,$$

where the matrices \mathcal{R}_i are determined by Eq. (33).

This energy must be minimized subject to the fulfillment of the Gutzwiller constraints

$$\begin{aligned} \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle &= \langle \Psi_0 | \Psi_0 \rangle = 1, \\ \langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle &= \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle \quad \forall a, b = 1, \dots, B\nu_i. \end{aligned}$$

In essence, we have reduced the problem to computing expectation values with respect to $|\Psi_0\rangle$ of local operators: those appearing in the Gutzwiller constraints, the terms of the local interactions, and the terms entering in the characterization of the system for computing the \mathcal{R}_i matrices. We will learn how to calculate these terms systematically and efficiently in the following sections.

4 Reformulation using local reduced density-matrix

In order to compute all the expectation values of local observables with respect to $|\Psi_0\rangle$, which appear in our variational problem as summarized above in Sec. 3.6, we need to introduce the local reduced density-matrix of the i -th auxiliary-space subsystem i . According to Theorem E.1 from the appendix (following Refs. [6, 20, 11]), the local reduced density-matrix is given by

$$\hat{P}_i^0 \propto \exp \left(- \sum_{a,b=1}^{B\nu_i} \left[\ln \left(\frac{\mathbf{1} - \Delta_i^T}{\Delta_i^T} \right) \right]_{ab} f_{ia}^\dagger f_{ib} \right), \quad (34)$$

where Δ_i is the $B\nu_i \times B\nu_i$ matrix with elements:

$$[\Delta_i]_{ab} = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle. \quad (35)$$

Utilizing these definitions and the matrix representation of the Gutzwiller projector in Eq. (5), it is straightforward to derive the relations

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i | \Psi_0 \rangle = \text{Tr} \left[P_i^0 \Lambda_i^\dagger \Lambda_i \right], \quad (36)$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{\mathcal{P}}_i f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = \text{Tr} \left[P_i^0 \Lambda_i^\dagger \Lambda_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib} \right], \quad (37)$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger \hat{H}_{loc}^i [c_{i\alpha}^\dagger, c_{i\alpha}] \hat{\mathcal{P}}_i | \Psi_0 \rangle = \text{Tr} \left[P_i^0 \Lambda_i^\dagger \hat{H}_{loc}^i [F_{i\alpha}^\dagger, F_{i\alpha}] \Lambda_i \right], \quad (38)$$

$$\langle \Psi_0 | \hat{\mathcal{P}}_i^\dagger c_{i\alpha}^\dagger \hat{\mathcal{P}}_i f_{ia} | \Psi_0 \rangle = \text{Tr} \left[P_i^0 \Lambda_i^\dagger F_{i\alpha}^\dagger \Lambda_i \tilde{F}_{ia} \right], \quad (39)$$

where Tr denotes the trace operator restricted within the $2^{B\nu_i}$ -dimensional many-body Fock space of the i -th auxiliary-space subsystem. The matrices $F_{i\alpha}$, and \tilde{F}_{ia} are representations of the local reduced density-matrix, the physical annihilation operators and the auxiliary annihilation operators in their own Fock basis, respectively, which are defined as

$$[F_{i\alpha}]_{\Gamma\Gamma'} = \langle \Gamma, i | c_{i\alpha} | \Gamma', i \rangle \quad (\Gamma, \Gamma' \in \{0, \dots, 2^{\nu_i} - 1\}), \quad (40)$$

$$[\tilde{F}_{ia}]_{nn'} = \langle n, i | f_{ia} | n', i \rangle \quad (n, n' \in \{0, \dots, 2^{B\nu_i} - 1\}), \quad (41)$$

while the matrix representation of \hat{P}_i^0 with entries $[P_i^0]_{nn'} = \langle n, i | \hat{P}_i^0 | n', i \rangle$ is given by

$$P_i^0 \propto \exp \left(- \sum_{a,b=1}^{B\nu_i} \left[\ln \left(\frac{\mathbf{1} - \Delta_i^T}{\Delta_i^T} \right) \right]_{ab} \tilde{F}_{ia}^\dagger \tilde{F}_{ib} \right). \quad (42)$$

Summing up the above contributions, with the local terms expressed in terms of the reduced density-matrix, the variational energy \mathcal{E} can be expressed as

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}_j^\dagger \right]_{ab} \langle \Psi_0 | f_{ia}^\dagger f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \text{Tr} \left[P_i^0 \Lambda_i^\dagger \hat{H}_{\text{loc}}^i [F_{i\alpha}^\dagger, F_{i\alpha}] \Lambda_i \right], \quad (43)$$

where the matrices \mathcal{R}_i are determined by the relation

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger F_{i\alpha}^\dagger \Lambda_i \tilde{F}_{ia} \right] = \sum_{b=1}^{B\nu_i} [\mathcal{R}_i]_{b\alpha} \langle \Psi_0 | f_{ib}^\dagger f_{ia} | \Psi_0 \rangle = \sum_{b=1}^{B\nu_i} [\mathcal{R}_i]_{b\alpha} [\Delta_i]_{ba}. \quad (44)$$

This energy must be minimized subject to the fulfillment of the Gutzwiller constraints, which in terms of the reduced density-matrix are

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger \Lambda_i \right] = \langle \Psi_0 | \Psi_0 \rangle = 1, \quad (45)$$

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger \Lambda_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib} \right] = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = [\Delta_i]_{ab} \quad \forall a, b = 1, \dots, B\nu_i. \quad (46)$$

5 Reformulation in terms of slave-boson amplitudes (connection with RISB)

In this section, we delve into the concept of ‘‘slave-boson amplitudes’’ through the lens of the gGA. Within the Rotationally-Invariant Slave-Boson (RISB) approach [15, 19, 20], slave-boson amplitudes emerge from a distinct perspective, where auxiliary bosons are introduced to represent local modes within each system fragment. A remarkable aspect about this alternative perspective is that the gGA can be viewed as the mean-field approximation of the ghost RISB (gRISB) [32], and analogously, the Gutzwiller approximation (GA) bears a similar relationship to RISB [33, 6, 20]. As such, the RISB/gRISB formulation opens avenues for devising practical implementations that systematically incorporate quantum-fluctuation corrections toward obtaining the exact solution. Although we will not embark on a detailed derivation of RISB or gRISB within this section, we encourage readers to peruse the referenced literature for a more comprehensive understanding of this connection and the exciting possibilities it harbors for theoretical and algorithmic advancements in the many-body problem.

5.1 The slave-boson amplitudes

We can rewrite all the key local quantities in an alternative way in terms of the so-called matrices of slave-boson amplitudes. This is not only useful for technical purposes but also for establishing a formal connection with the rotationally-invariant slave-boson theory (RISB).

Let us introduce the matrix of slave-boson amplitudes, ϕ_i , as defined in Refs. [6, 33, 7, 11]

$$\phi_i = \Lambda_i \sqrt{P_i^0} = \Lambda_i [P_i^0]^{\frac{1}{2}}. \quad (47)$$

Substituting this into Eqs. (36)-(39) yields the following equations

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger \Lambda_i \right] = \text{Tr} \left[\phi_i^\dagger \phi_i \right], \quad (48)$$

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger \Lambda_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib} \right] = \text{Tr} \left[\phi_i^\dagger \phi_i [P_i^0]^{-\frac{1}{2}} \tilde{F}_{ia}^\dagger \tilde{F}_{ib} [P_i^0]^{\frac{1}{2}} \right], \quad (49)$$

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger \hat{H}_{\text{loc}}^i [F_{i\alpha}^\dagger, F_{i\alpha}] \Lambda_i \right] = \text{Tr} \left[\phi_i \phi_i^\dagger \hat{H}_{\text{loc}}^i [F_{i\alpha}^\dagger, F_{i\alpha}] \right], \quad (50)$$

$$\text{Tr} \left[P_i^0 \Lambda_i^\dagger F_{i\alpha}^\dagger \Lambda_i \tilde{F}_{ia} \right] = \text{Tr} \left[\phi_i^\dagger F_{i\alpha}^\dagger \phi_i [P_i^0]^{-\frac{1}{2}} \tilde{F}_{ia} [P_i^0]^{\frac{1}{2}} \right]. \quad (51)$$

We note that Eqs. (49) and (51) involve a similarity transformations of the matrix representations of the auxiliary-mode operators, such as those described in the Appendix, see Sec. B.4.2.

By applying theorems B.2 and B.3, we obtain

$$\begin{aligned} [P_i^0]^{-\frac{1}{2}} \tilde{F}_{ia}^\dagger [P_i^0]^{\frac{1}{2}} &= e^{\frac{1}{2} \sum_{a,b=1}^{B\nu_i} \left[\ln \left(\frac{1-\Delta_i^T}{\Delta_i^T} \right) \right]} \tilde{F}_{ia'}^\dagger \tilde{F}_{ib'} \tilde{F}_{ia}^\dagger e^{-\frac{1}{2} \sum_{a'',b''=1}^{B\nu_i} \left[\ln \left(\frac{1-\Delta_i^T}{\Delta_i^T} \right) \right]} \tilde{F}_{ia''}^\dagger \tilde{F}_{ib''} \\ &= \sum_{a'=1}^{B\nu_i} \left[e^{\frac{1}{2} \ln \left(\frac{1-\Delta_i^T}{\Delta_i^T} \right)} \right]_{a'a} \tilde{F}_{ia'}^\dagger = \sum_{a'=1}^{B\nu_i} \left[\frac{1-\Delta_i^T}{\Delta_i^T} \right]^{\frac{1}{2}}_{a'a} \tilde{F}_{ia'}^\dagger = \sum_{a'=1}^{B\nu_i} \left[\frac{1-\Delta_i}{\Delta_i} \right]^{\frac{1}{2}}_{aa'} \tilde{F}_{ia'}^\dagger, \end{aligned} \quad (52)$$

$$[P_i^0]^{-\frac{1}{2}} \tilde{F}_{ia} [P_i^0]^{\frac{1}{2}} = \sum_{a'=1}^{B\nu_i} \left[e^{-\frac{1}{2} \ln \left(\frac{1-\Delta_i^T}{\Delta_i^T} \right)} \right]_{aa'} \tilde{F}_{ia'} = \sum_{a'=1}^{B\nu_i} \left[\frac{\Delta_i^T}{1-\Delta_i^T} \right]^{\frac{1}{2}}_{aa'} \tilde{F}_{ia'} = \sum_{a'=1}^{B\nu_i} \left[\frac{\Delta_i}{1-\Delta_i} \right]^{\frac{1}{2}}_{a'a} \tilde{F}_{ia'}. \quad (53)$$

- By substituting Eq. (48) in Eq. (45) and Eq. (52) in Eq. (46) we obtain

$$\text{Tr} \left[\phi_i^\dagger \phi_i \right] = \langle \Psi_0 | \Psi_0 \rangle = 1 \quad (54)$$

$$\text{Tr} \left[\phi_i^\dagger \phi_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib} \right] = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = [\Delta_i]_{ab} \quad \forall a, b = 1, \dots, B\nu_i. \quad (55)$$

- By substituting Eq. (53) into Eq. (44) we obtain the following equation for \mathcal{R}_i

$$\text{Tr} \left[\phi_i^\dagger F_{i\alpha}^\dagger \phi_i \tilde{F}_{ia} \right] = \sum_{c=1}^{B\nu_i} [\mathcal{R}_i]_{c\alpha} [\Delta_i (1-\Delta_i)]_{ca}^{\frac{1}{2}}, \quad (56)$$

which can always be inverted, as long as neither Δ_i nor $1-\Delta_i$ are degenerate, which we already assumed after Eq. (21), to prove Eq. (22).

5.2 Recap: the variational problem in terms of slave-boson amplitudes

Summing up the above contributions, with the local terms expressed in terms of the slave-boson amplitudes, the variational energy \mathcal{E} can be expressed as

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i t_{ij} \mathcal{R}_j^\dagger \right]_{ab} \langle \Psi_0 | f_{ia}^\dagger f_{jb} | \Psi_0 \rangle + \sum_{i=1}^{\mathcal{N}} \text{Tr} \left[\phi_i \phi_i^\dagger \hat{H}_{\text{loc}}^i [F_{i\alpha}^\dagger, F_{i\alpha}] \right], \quad (57)$$

where the matrices \mathcal{R}_i are determined by Eq. (56). It must be minimized subject to the Gutzwiller constraints, which in terms of the slave-boson amplitudes are given by Eqs. (54) and (55).

6 Reformulation in terms of embedding states (connection with DMET)

In this section, building on the foundation laid in the preceding section, we take a further step by expressing key local quantities in terms of “embedding states”. This concept was first introduced in Ref. [7] within the context of the multi-orbital GA and later extended and further developed for the gGA in Refs. [10, 11]. The mapping presented in this section is computationally advantageous, as it makes it possible to reformulate the energy-optimization problem into a recursive computation of the ground state of an auxiliary “impurity model” with a finite bath. Furthermore, this perspective plays a critical role in bridging the gGA with quantum embedding theories such as DMET [34, 26], enabling a more unified understanding of these frameworks [35].

6.1 The embedding states

The embedding states are vectors belonging to an auxiliary Fock space and serve to map the slave-boson amplitudes ϕ_i to a fermionic impurity Hamiltonian.

Definition 6.1 (Embedding States). The embedding states, denoted as $|\Phi_i\rangle$, are defined as

$$|\Phi_i\rangle = \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2}N(n)(N(n)-1)} [\phi_i]_{\Gamma n} |\Gamma; i\rangle \otimes U_{\text{PH}} |n; i\rangle, \quad (58)$$

where:

- $|\Gamma; i\rangle$ and $|n; i\rangle$ are Fock states generated by auxiliary fermionic modes

$$|\Gamma; i\rangle = [c_{i1}^\dagger]^{q_1(\Gamma)} \dots [c_{iB\nu_i}^\dagger]^{q_{\nu_i}(\Gamma)} |0\rangle, \quad (59)$$

$$|n; i\rangle = [b_{i1}^\dagger]^{q_1(n)} \dots [b_{iB\nu_i}^\dagger]^{q_{B\nu_i}(n)} |0\rangle. \quad (60)$$

- Consistently with the notation introduced in Sec. B.2 (also used above in Sec. 3), $q_a(n)$ denotes the a -th occupation number of a Fock state $|n, i\rangle$, which is the i -th digit of the integer n in binary form, and

$$N(n) = \sum_{a=1}^{B\nu_i} q_a(n) \quad (61)$$

represents the total number of Fermions in each state $|n; i\rangle$.

- Additionally, U_{PH} represent a particle-hole transformation acting on the $|n; i\rangle$ states, defined by the following conditions

$$U_{\text{PH}}^\dagger b_{ia}^\dagger U_{\text{PH}} = b_{ia}, \quad (62)$$

$$U_{\text{PH}}^\dagger b_{ia} U_{\text{PH}} = b_{ia}^\dagger, \quad (63)$$

$$U_{\text{PH}}^\dagger c_{ia}^\dagger U_{\text{PH}} = c_{ia}^\dagger, \quad (64)$$

$$U_{\text{PH}}^\dagger c_{ia} U_{\text{PH}} = c_{ia}, \quad (65)$$

$$U_{\text{PH}}|0\rangle = \prod_{a=1}^{B\nu_i} b_{ia}^\dagger |0\rangle = |2^{B\nu_i} - 1; i\rangle. \quad (66)$$

Remark. The basis vectors $|\Gamma; i\rangle \otimes U_{\text{PH}}|n; i\rangle$ in the expansion of Eq. (58) are orthogonal and thus linearly independent. This orthogonality implies that the slave-boson amplitudes $[\phi_i]_{\Gamma n}$ uniquely represent the expansion coefficients in this auxiliary Fock space. Consequently, we have established a one-to-one correspondence between the states $|\Phi_i\rangle$ in the Fock space and the variational parameters encoded in the slave-boson amplitudes.

Remark. The set of all embedding states forms a Fock space, which can be interpreted as a composite system consisting of a subsystem generated by the fermionic degrees of freedom $c_{i\alpha}^\dagger$ with $\alpha \in \{1, \dots, \nu_i\}$ and a subsystem (larger than the previous for $B > 1$) generated by the fermionic degrees of freedom b_{ia}^\dagger with $a \in \{1, \dots, B\nu_i\}$.

Theorem 6.1 (Half-filled Embedding States). *Under the variational assumption made in Sec. 3.2*

$$N(n) - N(\Gamma) = m_i = (B-1)\nu_i/2 \quad (67)$$

(see Eq. (8)), the embedding states $|\Phi_i\rangle$ as defined in Eq. (58) have a total of $(B+1)\nu_i/2$ Fermions, signifying that they are half-filled, i.e., they contain half of the maximum possible number of Fermions, which is the total number of modes.

Proof. Consider the action of the total number operator \hat{N}_{tot} on the embedding state $|\Phi_i\rangle$

$$\hat{N}_{\text{tot}}|\Phi_i\rangle = \left(\sum_{a=1}^{B\nu_i} (b_{ia}^\dagger b_{ia} + c_{ia}^\dagger c_{ia}) \right) |\Phi_i\rangle \quad (68)$$

$$= \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2}N(n)(N(n)-1)} [\phi_i]_{\Gamma n} (N(\Gamma) + B\nu_i - N(n)) |\Gamma; i\rangle \otimes U_{\text{PH}}|n; i\rangle \quad (69)$$

$$= \underbrace{(-m_i + B\nu_i)}_{=(B+1)\nu_i/2} \underbrace{\sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2}N(n)(N(n)-1)} [\phi_i]_{\Gamma n} |\Gamma; i\rangle \otimes U_{\text{PH}}|n; i\rangle}_{|\Phi_i\rangle} = \left(\frac{B+1}{2} \nu_i \right) |\Phi_i\rangle. \quad (70)$$

This demonstrates that the embedding state $|\Phi_i\rangle$ has a total of $(B+1)\nu_i/2$ electrons, and is therefore half-filled. \square

Remark. As a recap, it is worth highlighting that the significance of Theorem 6.1 is that we can reformulate the variational assumption made initially for ensuring that the gGA variational state has a well-defined number of fermions (see Eq. (8)) into the condition that the embedding states are “half-filled”.

As we are going to show in the next sections, the mapping introduced above is not only computationally advantageous, but also plays a critical role in positioning the gGA within the context of quantum embedding frameworks such as Density-Matrix Embedding Theory and Dynamical Mean Field Theory, thereby fostering a unified perspective.

6.2 Expectation values of local operators in terms of embedding states

Here, we aim to study the expectation values of local operators, which were initially represented using slave-boson amplitudes, and establish equivalent representations using the embedding states.

- **Expression for $\text{Tr}[\phi_i^\dagger \phi_i]$ in terms of embedding states:**

$$\begin{aligned} \langle \Phi_i | \Phi_i \rangle &= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i}-1} \sum_{n, n'=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2}(N(n)(N(n)-1) - N(n')(N(n')-1))} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \\ &\quad \times \langle \Gamma; i | \Gamma'; i \rangle \langle n; i | U_{\text{PH}}^\dagger U_{\text{PH}} | n'; i \rangle \\ &= \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma n} = \text{Tr}[\phi_i^\dagger \phi_i]. \end{aligned} \quad (71)$$

We expanded the expression $\langle \Phi_i | \Phi_i \rangle$ according to the definition of embedding states, involving a summation over all Γ and n . Utilizing the orthonormality properties of the states $\langle \Gamma; i | \Gamma'; i \rangle$ and $\langle n; i | n'; i \rangle$, we retained terms for which $\Gamma = \Gamma'$ and $n = n'$. The summation over these terms involved the product of coefficients $[\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma n}$. The expression was then concisely written as the trace of $\phi_i^\dagger \phi_i$.

- **Expression for $\text{Tr}[\phi_i \phi_i^\dagger \hat{H}_{\text{loc}}^i [F_{i\alpha}^\dagger, F_{i\alpha}]]$ in terms of embedding states:**

$$\begin{aligned} \langle \Phi_i | \hat{H}_{\text{loc}}^i [c_{i\alpha}^\dagger, c_{i\alpha}] | \Phi_i \rangle &= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i}-1} \sum_{n, n'=0}^{2^{B\nu_i}-1} e^{\frac{i\pi}{2}(N(n)(N(n)-1) - N(n')(N(n')-1))} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \\ &\quad \times \langle \Gamma; i | \hat{H}_{\text{loc}}^i [c_{i\alpha}^\dagger, c_{i\alpha}] | \Gamma'; i \rangle \langle n; i | U_{\text{PH}}^\dagger U_{\text{PH}} | n'; i \rangle \\ &= \sum_{\Gamma=0}^{2^{\nu_i}-1} \sum_{n=0}^{2^{B\nu_i}-1} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma n} \langle \Gamma; i | \hat{H}_{\text{loc}}^i [c_{i\alpha}^\dagger, c_{i\alpha}] | \Gamma; i \rangle \\ &= \text{Tr}[\phi_i \phi_i^\dagger \hat{H}_{\text{loc}}^i [F_{i\alpha}^\dagger, F_{i\alpha}]]. \end{aligned} \quad (72)$$

The expectation value of the local Hamiltonian was expanded using embedding states, analogously to the initial equation. The orthonormality of the states helped to simplify the expression into a trace of the product of $\phi_i \phi_i^\dagger$ with the matrix representation of the local Hamiltonian in the $|\Gamma; i\rangle$ basis. (Eq. (72))

- **Expression for $\text{Tr}[\phi_i^\dagger \phi_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib}]$ in terms of embedding states:**

$$\begin{aligned}
\langle \Phi_i | b_{ib} b_{ia}^\dagger | \Phi_i \rangle &= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} e^{\frac{i\pi}{2}(N(n)(N(n)-1) - N(n')(N(n')-1))} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \\
&\quad \times \langle \Gamma; i | \Gamma'; i \rangle \langle n; i | U_{\text{PH}}^\dagger b_{ib} b_{ia}^\dagger U_{\text{PH}} | n'; i \rangle \\
&= \sum_{\Gamma=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma n'} \langle n; i | b_{ib}^\dagger b_{ia} | n'; i \rangle \\
&= \sum_{\Gamma=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma n'} [\tilde{F}_{ib}^\dagger \tilde{F}_{ia}]_{nn'} \\
&= \sum_{\Gamma=0}^{2^{\nu_i-1}} \sum_{n=0}^{2^{B\nu_i-1}} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma n'} [\tilde{F}_{ia}^\dagger \tilde{F}_{ib}]_{n'n} = \text{Tr}[\phi_i^\dagger \phi_i \tilde{F}_{ia}^\dagger \tilde{F}_{ib}]. \tag{73}
\end{aligned}$$

Initially, the terms were expanded and the particle-hole transformation was incorporated. The orthonormality of $\langle \Gamma; i | \Gamma'; i \rangle$ allowed us to combine the summations over Γ and Γ' . The operators b_{ib}^\dagger and b_{ia} were then expressed using their matrix representations. Furthermore, the real nature of the matrix elements of \tilde{F}_{ib} and \tilde{F}_{ia}^\dagger (as established in Sec. B.3) was employed to simplify the expression. Finally, a compact representation was obtained by writing it as the trace of a product of matrices.

- **Expression for $\text{Tr}[\phi_i^\dagger F_{i\alpha}^\dagger \phi_i \tilde{F}_{ia}]$ in terms of embedding states:**

$$\begin{aligned}
\langle \Phi_i | c_{i\alpha}^\dagger b_{ia} | \Phi_i \rangle &= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} e^{\frac{i\pi}{2}(N(n)(N(n)-1) - N(n')(N(n')-1))} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \\
&\quad \times \langle \Gamma; i | \langle n; i | U_{\text{PH}}^\dagger c_{i\alpha}^\dagger b_{ia} U_{\text{PH}} | \Gamma'; i \rangle | n'; i \rangle \\
&= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} e^{\frac{i\pi}{2}(N(n)(N(n)-1) - N(n')(N(n')-1))} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \\
&\quad \times \langle \Gamma; i | \langle n; i | c_{i\alpha}^\dagger b_{ia}^\dagger | \Gamma'; i \rangle | n'; i \rangle \\
&= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} (-1)^{n'} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \langle \Gamma; i | \langle n; i | c_{i\alpha}^\dagger b_{ia}^\dagger | \Gamma'; i \rangle | n'; i \rangle \\
&= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} \langle \Gamma; i | c_{i\alpha}^\dagger | \Gamma; i \rangle \langle n; i | b_{ia}^\dagger | n'; i \rangle \\
&= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} [F_{i\alpha}^\dagger]_{\Gamma \Gamma'} [\tilde{F}_{ia}^\dagger]_{nn'} \\
&= \sum_{\Gamma, \Gamma'=0}^{2^{\nu_i-1}} \sum_{n, n'=0}^{2^{B\nu_i-1}} [\phi_i]_{\Gamma n}^* [\phi_i]_{\Gamma' n'} [F_{i\alpha}^\dagger]_{\Gamma \Gamma'} [\tilde{F}_{ia}]_{n'n} = \text{Tr}[\phi_i^\dagger F_{i\alpha}^\dagger \phi_i \tilde{F}_{ia}]. \tag{74}
\end{aligned}$$

The particle-hole transformation was applied first in this derivation. The relationship $N(n') = N(n)+1$ was then used to simplify the phase factor, yielding $(-1)^{n'}$. We then rewrote $\langle \Gamma; i | \langle n; i | c_{i\alpha}^\dagger b_{ia}^\dagger | \Gamma'; i \rangle | n'; i \rangle$ in terms of matrix representations of $c_{i\alpha}^\dagger$ and b_{ia}^\dagger . Interestingly, the phase factor that emerged from permutations nullified the $(-1)^{n'}$ from the earlier step. As in previous derivations, the realness of the entries of \tilde{F}_{ia} allowed us to transpose it and take its Hermitian conjugate. Lastly, the summations were collected into a single trace expression.

6.3 Recap: the variational problem in terms of embedding states

Recalling the expressions obtained above, we can now rewrite the Gutzwiller constraints [Eqs. (54) and (55)] in terms of the embedding states $|\Phi_i\rangle$ as

$$\langle \Phi_i | \Phi_i \rangle = \langle \Psi_0 | \Psi_0 \rangle = 1, \quad (76)$$

$$\langle \Phi_i | b_{ib}^\dagger b_{ia} | \Phi_i \rangle = \langle \Psi_0 | f_{ia}^\dagger f_{ib} | \Psi_0 \rangle = [\Delta_i]_{ab}, \quad \forall a, b = 1, \dots, B\nu_i. \quad (77)$$

We can also express the matrix \mathcal{R}_i , see Eq. (56), as the solution of the equation

$$\langle \Phi_i | c_{i\alpha}^\dagger b_{ia} | \Phi_i \rangle = \sum_{a=1}^{B\nu_i} [\mathcal{R}_i]_{a\alpha} [\Delta_i (\mathbf{1} - \Delta_i)]_{ab}^{\frac{1}{2}}. \quad (78)$$

With these expressions in terms of embedding states, the variational energy \mathcal{E} takes the form

$$\mathcal{E} = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i^\dagger t_{ij} \mathcal{R}_j \right]_{ab} f_{ia}^\dagger f_{jb} + \sum_{i=1}^{\mathcal{N}} \langle \Phi_i | \hat{H}_{\text{loc}}^i [c_{i\alpha}^\dagger, c_{i\alpha}] | \Phi_i \rangle, \quad (79)$$

where \mathcal{R}_i is given by Eq. (78). This variational energy must be minimized with respect to the variational parameters, subject to the Gutzwiller constraints expressed in terms of the embedding states $|\Phi_i\rangle$, formulated with Eqs. (76) and (77).

7 Lagrange formulation of gGA (QE algorithmic structure)

In the previous section (Sec. 6.3), we discussed how the Gutzwiller approximation is formulated in terms of embedding states. However, this poses a complex optimization problem since the dimension of $|\Phi_i\rangle$, which is exponential in ν_i and B , is non-linear. To tackle this, we make use of a mathematical trick, as elaborated in Refs. [7, 20, 10], which reformulates the problem into a linear eigenvalue problem for $|\Phi_i\rangle$, with parameters to be computed recursively. This trick is facilitated by the theorem based on Lagrange multipliers, derived in Appendix F.

7.1 The gGA Lagrange function

We first define the Lagrange function, which encodes the gGA variational-energy function in Eq. (79) and the Gutzwiller constraints [Eqs. (76) and (77)] into a single function, and reduces to the variational energy when evaluated at the saddle point:

$$\begin{aligned}
\mathcal{L}[\Phi, E^c; \mathcal{R}, \Lambda; \mathcal{D}, \Lambda^c; \Delta, \Psi_0, E] = & \\
& \langle \Psi_0 | \hat{H}_{\text{qp}}[\mathcal{R}, \Lambda] | \Psi_0 \rangle + E (1 - \langle \Psi_0 | \Psi_0 \rangle) \\
& + \sum_{i=1}^{\mathcal{N}} \left[\langle \Phi_i | \hat{H}_i^{\text{emb}}[\mathcal{D}_i, \Lambda_i^c] | \Phi_i \rangle + E_i^c (1 - \langle \Phi_i | \Phi_i \rangle) \right] \\
& - \sum_{i=1}^{\mathcal{N}} \left[\sum_{a,b=1}^{B\nu_i} ([\Lambda_i]_{ab} + [\Lambda_i^c]_{ab}) [\Delta_i]_{ab} + \sum_{c,a=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \left([\mathcal{D}_i]_{a\alpha} [\mathcal{R}_i]_{c\alpha} [\Delta_i (1 - \Delta_i)]_{ca}^{\frac{1}{2}} + \text{c.c.} \right) \right], \tag{80}
\end{aligned}$$

where \mathcal{N} is the total number of unit cells. The Lagrange function introduces several Lagrange multipliers and variables. Specifically:

- E is a Lagrange multiplier that enforces the normalization condition $\langle \Psi_0 | \Psi_0 \rangle = 1$, which is the right-hand side of Eq. (76).
- E_i^c is a Lagrange multiplier that enforces the normalization condition $\langle \Phi_i | \Phi_i \rangle = 1$ for each embedding state $|\Phi_i\rangle$, corresponding to the left-hand side of Eq. (76).
- Δ_i has been promoted to a matrix of independent variables using the Lagrange multipliers Λ_i . Both Δ_i and Λ_i are $B\nu_i \times B\nu_i$ Hermitian matrices.
- Λ_i^c is a $B\nu_i \times B\nu_i$ Hermitian matrix, serving as a Lagrange multiplier to enforce the second Gutzwiller constraints presented in Eq. (77).
- \mathcal{D}_i and \mathcal{R}_i are rectangular matrices with dimensions $B\nu_i \times \nu_i$. \mathcal{D}_i is introduced as a Lagrange multiplier for enforcing the definition of \mathcal{R}_i , which is given in Eq. (78).

Note that the Lagrange function has amalgamated all terms involving $|\Psi_0\rangle$ and $|\Phi_i\rangle$ into two auxiliary Hamiltonians, \hat{H}_{qp} and \hat{H}_{emb} , respectively

$$\hat{H}_{\text{qp}}[\mathcal{R}, \Lambda] = \sum_{i,j=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} \left[\mathcal{R}_i^\dagger t_{ij} \mathcal{R}_j^\dagger \right]_{ab} f_{ia}^\dagger f_{jb} + \sum_{i=1}^{\mathcal{N}} \sum_{a,b=1}^{B\nu_i} [\Lambda_i]_{ab} f_{ia}^\dagger f_{ib}, \tag{81}$$

$$\hat{H}_{\text{emb}}^i[\mathcal{D}_i, \Lambda_i^c] = \hat{H}_{\text{loc}}^i[c_{i\alpha}, c_{i\alpha}^\dagger] + \sum_{a=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \left([\mathcal{D}_i]_{a\alpha} c_{i\alpha}^\dagger b_{ia} + \text{H.c.} \right) + \sum_{a,b=1}^{B\nu_i} [\Lambda_i^c]_{ab} b_{ib} b_{ia}^\dagger, \tag{82}$$

where Eq. (81) is called ‘‘quasi-particle Hamiltonian’’ and Eq. (82), representing an impurity model consisting of the i -th fragment of the system coupled to a bath, is called embedding Hamiltonian (EH).

The introduction of the Lagrange function has converted the dependencies on $|\Psi_0\rangle$ and $|\Phi_i\rangle$ into linear ones. As we are going to see, this significantly simplifies the problem.

7.2 The gGA Lagrange equations

The saddle point conditions with respect to $|\Psi_0\rangle$ and E result in a Schrödinger equation for \hat{H}_{qp} . Similarly, the saddle point conditions with respect to $|\Phi_i\rangle$ and E_i^c result in a series of Schrödinger equations for \hat{H}_{emb}^i .

To write all Lagrange equations, including the remaining saddle point conditions with respect to the parameters Λ_i , Λ_i^c , Δ_i , \mathcal{D}_i , and \mathcal{R}_i , we rewrite Eq. (81) as

$$\hat{H}_*[\mathcal{R}, \Lambda] = \sum_{i,j=1}^{\mathcal{N}} [\Pi_i h_* \Pi_j]_{ab} f_{ia}^\dagger f_{jb}, \quad (83)$$

where we introduce the matrix

$$h_* = \begin{pmatrix} \Lambda_1 & \mathcal{R}_1 t_{12} \mathcal{R}_2^\dagger & \dots & \mathcal{R}_1 t_{1\mathcal{N}} \mathcal{R}_\mathcal{N}^\dagger \\ \mathcal{R}_2 t_{21} \mathcal{R}_1^\dagger & \Lambda_2 & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{R}_\mathcal{N} t_{\mathcal{N}1} \mathcal{R}_1^\dagger & \dots & \dots & \Lambda_\mathcal{N} \end{pmatrix} \quad (84)$$

and the projectors over the degrees of freedom corresponding to each fragment

$$\Pi_i = \begin{pmatrix} \delta_{i1} [\mathbf{1}]_{B\nu_1 \times B\nu_1} & \dots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \dots & \delta_{iM} [\mathbf{1}]_{B\nu_\mathcal{N} \times B\nu_\mathcal{N}} \end{pmatrix}, \quad (85)$$

where $[\mathbf{1}]_{n \times n}$ is the $n \times n$ identity matrix. We also represent the matrices Δ_i , Λ_i , and Λ_i^c as expansions in terms of an orthonormal basis of Hermitian matrices, denoted $[h_i]_s$ (with respect to the canonical scalar product $(A, B) = \text{Tr}[A^\dagger B]$)

$$\Delta_i = \sum_{s=1}^{(B\nu_i)^2} [d_i^0]_s [h_i^T]_s \quad (86)$$

$$\Lambda_i = \sum_{s=1}^{(B\nu_i)^2} [l_i]_s [h_i]_s \quad (87)$$

$$\Lambda_i^c = \sum_{s=1}^{(B\nu_i)^2} [l_i^c]_s [h_i]_s, \quad (88)$$

where $[d_i^0]_s$, $[l_i]_s$, and $[l_i^c]_s$ are real-valued coefficients.

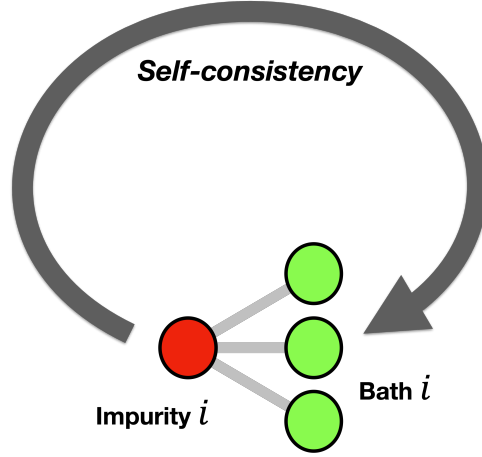


Fig. 2: Representation of algorithmic structure for solving the gGA Lagrange equations.

The saddle-point of the gGA Lagrange function \mathcal{L} defined in Eq. (80) is given by the equations

$$\hat{H}_*[\mathcal{R}, \Lambda]|\Psi_0\rangle = E_0|\Psi_0\rangle, \quad (89)$$

$$[\Delta_i]_{ab} = \langle\Psi_0|f_{ia}^\dagger f_{ib}|\Psi_0\rangle, \quad (90)$$

$$\sum_{c=1}^{B\nu_i} [\mathcal{D}_i]_{c\alpha} [\Delta_i(\mathbf{1}-\Delta_i)]_{ac}^{\frac{1}{2}} = \sum_j \left[t_{ij} \mathcal{R}_j^\dagger \Pi_j f(h_*) \Pi_j \right]_{\alpha a}, \quad (91)$$

$$[l_i^c]_s = -[l_i]_s - \sum_{c,b=1}^{B\nu_i} \sum_{\alpha=1}^{\nu_i} \frac{\partial}{\partial [d_i^0]_s} \left([\Delta_i(\mathbf{1}-\Delta_i)]_{cb}^{\frac{1}{2}} [\mathcal{D}_i]_{b\alpha} [\mathcal{R}_i]_{c\alpha} + \text{c.c.} \right), \quad (92)$$

$$\hat{H}_{\text{emb}}^i|\Phi_i\rangle = E_i^c|\Phi_i\rangle, \quad (93)$$

$$\langle\Phi_i|b_{ib} b_{ia}^\dagger|\Phi_i\rangle = [\Delta_i]_{ab}, \quad (94)$$

$$\langle\Phi_i|c_{i\alpha}^\dagger b_{ia}|\Phi_i\rangle = \sum_{c=1}^{B\nu_i} [\Delta_i(\mathbf{1}-\Delta_i)]_{c\alpha}^{\frac{1}{2}} [\mathcal{R}_i]_{c\alpha}, \quad (95)$$

where f is the zero-temperature Fermi function.

Numerous numerical implementations have been proposed in the literature to solve these equations [7, 36, 37]. However, they all fundamentally consist of iteratively computing the ground state of \hat{H}_{emb}^i (see Eq. (93)), which constitutes the computational bottleneck. This algorithmic structure is schematically represented in Fig. 2. We will list some examples of practical implementations in Sec. 9.

Remark. The matrix derivative in Eq. (92) is non-trivial, as $[h_i^T]_s$ and Δ_i do not commute. A method for computing it is outlined in Sec. G of the Appendix. It's important to note that the computational cost of evaluating this derivative is primarily determined by the diagonalization of Δ_i . However, this operation is computationally inexpensive, rendering the overall cost essentially negligible. Furthermore, a recent work exploring the connection between the gGA and DMET [35] provides an equivalent expression to Eq. (92), that avoids the need for matrix derivatives, potentially offering a more efficient approach for practical implementations.

7.3 Gauge invariance of the gGA equations

It can be readily shown that the gGA Lagrangian is invariant with respect to the following gauge transformation

$$|\Psi_0\rangle \rightarrow \mathcal{U}^\dagger(\theta) |\Psi_0\rangle \quad (96)$$

$$|\Phi_i\rangle \rightarrow U_i^\dagger(\theta_i) |\Phi_i\rangle \quad (97)$$

$$\mathcal{R}_i \rightarrow u_i^\dagger(\theta_i) \mathcal{R}_i \quad (98)$$

$$\mathcal{D}_i \rightarrow u_i^T(\theta_i) \mathcal{D}_i \quad (99)$$

$$\Delta_i \rightarrow u_i^T(\theta_i) \Delta_i u_i^*(\theta_i) \quad (100)$$

$$\lambda_i \rightarrow u_i^\dagger(\theta_i) \lambda_i u_i(\theta_i) \quad (101)$$

$$\lambda_i^c \rightarrow u_i^\dagger(\theta_i) \lambda_i^c u_i(\theta_i) , \quad (102)$$

with

$$u_i(\theta_i) = e^{i\theta_i} \quad (103)$$

$$U_i(\theta_i) = e^{i \sum_{a,b=1}^{B\nu_i} [\theta_i]_{ab} b_{ia}^\dagger b_{ib}} \quad (104)$$

$$\mathcal{U}(\theta) = e^{i \sum_i \sum_{a,b=1}^{B\nu_i} [\theta_i]_{ab} f_{Ria}^\dagger f_{Rib}} , \quad (105)$$

where $u_i(\theta_i) \in \mathbb{C}^{B\nu_i \times B\nu_i}$, $U_i(\theta_i) \in \mathbb{C}^{2^{B\nu_i} \times 2^{B\nu_i}}$ and $\mathcal{U}(\theta) \in \mathbb{C}^{2^{B\nu} \times 2^{B\nu}}$ (where $\nu = \sum_{i=1}^{\mathcal{N}} \nu_i$), and the θ_i are Hermitian matrices.

The name ‘‘gauge’’ here refers to the fact that modifications of the parameters generated by such a gauge transformation do not influence any physical observable. This property of the equations is relevant in relation to the connection with the RISB framework, which is based on an exact reformulation of the many-electron problem in terms of an actual gauge theory, that reduces to the Lagrange equations above at the mean-field level.

8 Generalizations, research directions and open problems

This section aims to explore further generalizations, new research directions, and open problems in the realm of the ghost Gutzwiller approximation (gGA). The evolution of gGA has led to several innovative adaptations and methodologies that harness its potential in various contexts. Here, we mention three of such avenues: the connection of gGA with dynamical mean-field theory (DMFT) through spectral functions, the extension of gGA for time-dependent dynamics, and the reformulation of gGA within quantum-embedding theories. These avenues represent exciting frontiers in the study of strongly correlated electron systems and may offer interesting opportunities for future research.

8.1 The spectral function (connection with DMFT)

Let us consider the gGA zero-temperature spectral function, defined as

$$\mathcal{A}_{i\alpha,j\beta}(\omega) = \langle \Psi_G | c_{i\alpha} \delta(\omega - \hat{H}) c_{j\beta}^\dagger | \Psi_G \rangle + \langle \Psi_G | c_{j\beta}^\dagger \delta(\omega + \hat{H}) c_{i\alpha} | \Psi_G \rangle. \quad (106)$$

Following Refs. [10, 11], in the limit for $\mathcal{N} \rightarrow \infty$, it is possible to write an approximate representation of excitations of \hat{H} in terms of the gGA variational parameters, from which it is possible to obtain the following approximation to the physical Green's function

$$\mathcal{G}_{i\alpha,j\beta}(\omega) = \int_{-\infty}^{\infty} d\epsilon \frac{\mathcal{A}_{i\alpha,j\beta}(\omega)}{\omega - \epsilon} \simeq \left[\mathcal{R}_i^\dagger \Pi_i \frac{1}{\omega - h_*} \Pi_j \mathcal{R}_j \right]_{\alpha\beta}, \quad (107)$$

capturing both the low-energy quasi-particle excitations and the Hubbard bands.

From such a formula, it is possible to obtain a pole-expansion expression for the self-energy [10, 11, 36] that closely resembles an expansion proposed in previous DMFT literature [38] and was numerically shown to approach the DMFT solution in the limit of $B \rightarrow \infty$ on several examples of single-band and multi-orbital systems [36].

These analytical and numerical results suggest a profound connection with DMFT, which is subject of ongoing research.

8.2 Time-dependent dynamics

The time-dependent ghost Gutzwiller approximation (td-gGA), as introduced in Ref. [39], extends the gGA to the domain of non-equilibrium physics. Specifically, td-gGA builds upon the standard time-dependent Gutzwiller approximation [40, 41], by systematically incorporating the auxiliary gGA degrees of freedom.

A key strength of td-gGA is its capability to capture the relaxation of local observables, which is something the standard time-dependent Gutzwiller method falls short of. Moreover, it offers comparable accuracy to the more computationally demanding time-dependent dynamical mean-field theory (td-DMFT), while requiring significantly fewer computational resources. Therefore, it can serve as a versatile tool for delving into the non-equilibrium properties of correlated electron systems, ranging from energy-related materials to quantum control, and other areas where the accurate treatment of strong correlations is required. As such, researchers and students venturing into the field of correlated electron systems may find this method to be a valuable addition to their toolkit.

8.3 Quantum-embedding reformulation (connection with DMET)

The formulation of gGA in terms of quantum embedding states, see Sec. 6.2, has led to the development of a conceptual connection between gGA and density-matrix embedding theory (DMET). In particular, within the ghost density-matrix embedding theory (gDMET) [35], the gGA equations are recast, based on quantum-embedding principles similar to those of DMET. Such alternative interpretation of the gGA equations may open up possibilities for new unexplored generalizations.

9 Code availability

In this section, we draw attention to the available codes for the Gutzwiller approximation (GA) and the ghost Gutzwiller approximation (gGA).

9.1 ComRISB for DFT+GA

The ComRISB package, developed by Yongxin Yao *et al.*, is an efficient tool for integrating density-functional theory (DFT) with the Gutzwiller approximation (GA) and the rotationally-invariant slave-boson (RISB) method. It specifically incorporates the gGA with a single bath site ($B = 1$), which is a particular case within the gGA framework. This package is valuable for studying correlated electron systems by effectively melding the electronic structure calculations of DFT with the Gutzwiller approximation's correlation treatment. ComRISB is available for download at ComRISB at BNL.

The URL is: <https://www.bnl.gov/comscope/software/downloads.php>

For further inquiries, you can contact Yongxin Yao at ykent@iastate.edu.

9.2 gGA code for the single band Hubbard Model

Marius Frank *et al.* have developed a simplified gGA code aimed at the single-band Hubbard model, which is a valuable resource especially for students seeking to comprehend the intricacies of the ghost Gutzwiller approximation (gGA) implementation. The code serves not only as an instructive material but also as a groundwork for researchers endeavoring to build more sophisticated multi-orbital implementations. This hands-on tool provides practical insights into the methodologies and techniques integral to gGA, consistent with the discussions in these lecture notes. The code is available for download at gGA Code at GitLab.

The URL is: <https://gitlab.com/collaborations3/g-ga-hubbard>

For further inquiries, you can contact Marius Frank at marius.frank@chem.au.dk.

Appendices

A Useful mathematical definitions

A.1 Function of an Hermitian matrix

In this section, we will introduce the notion of “function of an Hermitian matrix”, that will be used extensively in these lecture notes.

Let H be a Hermitian matrix. It can be diagonalized by a unitary matrix U such that

$$H = UEU^\dagger \quad (108)$$

where E is a diagonal matrix with entries E_n , the eigenvalues of H . The matrix U can be written as $U = [U_1|U_2|\dots|U_N]$, where each U_n is an eigenvector of H corresponding to the eigenvalue E_n .

Given a real-valued function $f: \mathbb{R} \rightarrow \mathbb{R}$, we define the function of the Hermitian matrix H , denoted as $f(H)$, by

$$f(H) = Uf(E)U^\dagger \quad (109)$$

where $f(E)$ is a diagonal matrix with entries $f(E_n)$.

This means that the action of $f(H)$ on the eigenvectors of H is the same as the action of H , but with eigenvalues $f(E_n)$ instead of E_n . Specifically, for any eigenvector U_n of H ,

$$f(H)U_n = f(E_n)U_n. \quad (110)$$

A.2 Exponential of a Hermitian matrix through Taylor expansion

Another important approach to defining the function of a matrix, especially for the exponential function, is through the Taylor expansion. For a general function $f(x)$, its Taylor series (around $x = 0$) is given by:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n, \quad (111)$$

where $f^{(n)}(0)$ is the n -th derivative of f evaluated at 0.

When we focus on the exponential function, particularly e^{iH} or e^H , where H is an Hermitian matrix, the Taylor expansion becomes:

$$e^{iH} = \sum_{n=0}^{\infty} \frac{(iH)^n}{n!} \quad (112)$$

$$e^H = \sum_{n=0}^{\infty} \frac{(H)^n}{n!}. \quad (113)$$

This can be seen as an infinite sum of powers of H . It should be noted that the Taylor expansion gives an equivalent expression to the one provided in the previous section, where the exponential of an Hermitian matrix is defined through its eigenvalues and eigenvectors.

B Preliminaries on fermionic algebra and Fock states

B.1 Recap about the fermionic algebra

As a preamble to the discussion on slave-boson theories and the Gutzwiller approximation, we review some necessary algebraic tools. In particular, we will focus on the fermionic algebra.

Definition B.1 (Fermionic algebra). Consider a set of operators c_1, \dots, c_ν , together with their adjoints $c_1^\dagger, \dots, c_\nu^\dagger$. The fermionic algebra is the algebra generated by these operators and the complex numbers, subject to the following canonical anticommutation relations:

$$\{c_\alpha, c_\beta\} = 0, \quad (114)$$

$$\{c_\alpha^\dagger, c_\beta^\dagger\} = 0, \quad (115)$$

$$\{c_\alpha, c_\beta^\dagger\} = \delta_{\alpha\beta}, \quad (116)$$

where $\{A, B\} = AB + BA$ denotes the anticommutator, and $\delta_{\alpha\beta}$ is the Kronecker delta.

The anticommutation relations are central in describing fermionic systems. The first two relations reflect the exclusion principle, ensuring that states remain orthogonal under the action of these operators. The last relation essentially states that the operators act as creation and annihilation operators for fermions in the respective modes.

B.2 Recap about the fermionic Fock space

The next step is to construct a representation of the fermionic algebra on a linear space, which we will refer to as the Fock space. This construction is fundamental for analyzing many-body fermionic systems.

Definition B.2 (Fock Space). Let us postulate the existence of a vacuum state $|0\rangle$, which is annihilated by all the annihilation operators c_α ,

$$c_\alpha|0\rangle = 0, \quad \text{for all } \alpha.$$

Additionally, let there be an inner product with respect to which the conjugation operation is represented as the Hermitian conjugate.

From these properties, it follows that the linear space realizing this representation has dimension 2^ν and is spanned by a basis which we refer to as the Fock basis. In this text, we choose to represent elements of the Fock basis as

$$|\Gamma\rangle = [c_1^\dagger]^{q_1(\Gamma)} \dots [c_\nu^\dagger]^{q_\nu(\Gamma)} |0\rangle,$$

where Γ is an integer ranging from 0 to $2^\nu - 1$, and its binary representation is $\Gamma = q_1(\Gamma) \dots q_\nu(\Gamma)$. Here, the digits $q_\alpha(\Gamma)$ represent the occupation numbers.

With the Fock basis defined, let us introduce the occupation number operators.

Definition B.3 (Occupation Number Operators). For each mode α , the occupation number operator \hat{n}_α is defined as

$$\hat{n}_\alpha = c_\alpha^\dagger c_\alpha.$$

The Fock states are eigenvectors of these operators with eigenvalues $q_\alpha(\Gamma)$. That is,

$$\hat{n}_\alpha |\Gamma\rangle = q_\alpha(\Gamma) |\Gamma\rangle.$$

We can also define a full occupation number operator by summing over all modes.

Definition B.4 (Full Occupation Number Operator). The full occupation number operator is given by

$$\hat{N} = \sum_{\alpha=1}^{\nu} c_\alpha^\dagger c_\alpha.$$

The Fock states are also eigenvectors of this operator. Specifically,

$$\hat{N} |\Gamma\rangle = \left(\sum_{\alpha=1}^{\nu} q_\alpha(\Gamma) \right) |\Gamma\rangle = N(\Gamma) |\Gamma\rangle,$$

where $N(\Gamma)$ is defined as the sum of all occupation numbers, representing the total number of fermions.

B.3 Matrix representation of creation and annihilation operators

In this section, we will focus on the matrix representation of the creation and annihilation operators in the Fock basis. These matrix representations are essential for practical calculations in many-body fermionic systems.

By using the anticommutation rules, it can be readily verified that the elements of the matrix representation of the creation operator c_α^\dagger are given by the following equations:

$$[F_\alpha^\dagger]_{\Gamma, \Gamma'} = \langle \Gamma | c_\alpha^\dagger | \Gamma' \rangle = \delta_{q_\alpha(\Gamma), q_\alpha(\Gamma') + 1} \prod_{s \neq \alpha} \delta_{q_s(\Gamma), q_s(\Gamma')} (-1)^{\sum_{s=1}^{\alpha-1} q_s(\Gamma)}. \quad (117)$$

The identity above means that the occupation numbers of Γ and Γ' are all equal except for $q_\alpha(\Gamma)$, which is raised by 1 unit with respect to $q_\alpha(\Gamma')$. Furthermore, an appropriate sign has to be taken into account, due to the anticommutation rules.

Example. Let us consider the case where $\nu = 2$, and so the Fock space has a dimension of 4. The matrices representing the creation and annihilation operators in this case are 4×4 matrices. Below are the matrix representations for both creation operators c_1^\dagger and c_2^\dagger and their Hermitian conjugates:

$$F_1^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad F_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad F_2^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad F_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

B.4 Useful single-particle transformations

B.4.1 Unitary canonical transformations

Let us first consider a unitary transformation of the creation and annihilation operators, which is a familiar useful transformation in the context of many-body quantum systems. We will define a unitary operator \hat{U} as

$$\hat{U} = \exp\left(i \sum_{\alpha,\beta=1}^{\nu} h_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}\right), \quad (118)$$

where h is a Hermitian matrix. We can now state the following theorem:

Theorem B.1. *The unitary operator \hat{U} leaves the vacuum state unchanged, i.e.,*

$$\hat{U}|0\rangle = |0\rangle. \quad (119)$$

Furthermore, the transformed creation operator $\hat{U}c_{\alpha}^{\dagger}\hat{U}^{\dagger}$ can be expressed in terms of the original creation operators c_{α}^{\dagger} as

$$\hat{U}c_{\alpha}^{\dagger}\hat{U}^{\dagger} = \sum_{\beta=1}^{\nu} [e^{ih}]_{\beta\alpha} c_{\beta}^{\dagger}, \quad (120)$$

where e^{ih} is the exponential of the Hermitian matrix h , understood as a function of an Hermitian matrix in the sense defined in Section A.1.

Proof. Let us begin with the first part of the proof. Since, by definition, the vacuum state $|0\rangle$ satisfies Eq. (B.2), the operator at the exponents $\hat{H} = \sum_{\alpha,\beta} h_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}$ annihilates the vacuum, i.e., $\hat{H}|0\rangle = 0$. In the Taylor expansion of the exponential, the zeroth-order term is the identity operator, and all other terms contain \hat{H} . Therefore, $\hat{U}|0\rangle = |0\rangle$.

Now, let us move on to the second part of the proof:

- a) Let V be the unitary matrix such that $V^{\dagger}hV = e$, where e is diagonal.
- b) Consider the transformed creation operators in the new basis:

$$f_a^{\dagger} = \sum_{\alpha} V_{\alpha a} c_{\alpha}^{\dagger}, \quad (121)$$

and write the reversed relation as

$$c_{\alpha}^{\dagger} = \sum_a V_{\alpha a}^{\dagger} f_a^{\dagger}. \quad (122)$$

- c) Let us now express $\hat{U}c_{\alpha}^{\dagger}\hat{U}^{\dagger}$ explicitly using the definition of \hat{U} :

$$\hat{U}c_{\alpha}^{\dagger}\hat{U}^{\dagger} = \exp\left(i \sum_{\alpha',\beta'=1}^{\nu} h_{\alpha'\beta'} c_{\alpha'}^{\dagger} c_{\beta'}\right) c_{\alpha}^{\dagger} \exp\left(-i \sum_{\alpha'',\beta''=1}^{\nu} h_{\alpha''\beta''} c_{\alpha''}^{\dagger} c_{\beta''}\right) \quad (123)$$

$$= \exp\left(i \sum_{b'=1}^{\nu} e_{b'b'} f_{b'}^{\dagger} f_{b'}\right) \sum_a V_{\alpha a}^{\dagger} f_a^{\dagger} \exp\left(-i \sum_{b''=1}^{\nu} e_{b''b''} f_{b''}^{\dagger} f_{b''}\right) \quad (124)$$

$$= \sum_a V_{\alpha a}^{\dagger} e^{ie_{aa}} f_a^{\dagger} = \sum_{\beta} (V e^{ie} V^{\dagger})_{\beta\alpha} c_{\beta}^{\dagger} = \sum_{\beta} [e^{ih}]_{\beta\alpha} c_{\beta}^{\dagger}. \quad (125)$$

Here, we replaced the number operators in the exponents with occupation numbers, and noticed that the left exponent has an extra mode, allowing the exponents to partially cancel out. We are then left with the phase factor $e^{ie_{aa}}$, and rewriting f_a^\dagger back in terms of c_β^\dagger , we observe the coefficients are of the form $V e^{ie} V^\dagger$, which is equal to e^{ih} based on the definition of a function of a matrix. \square

B.4.2 Similarity transformations with anti-Hermitian generators

In the derivation of the multi-orbital GA and gGA framework, presented in the main text, we employ a similarity transformation related to the one described in the theorem above. However, in contrast to the unitary transformation, the transformation we use is not unitary. Specifically, the theorem can be generalized to transformations where there is no imaginary unit in the exponent.

Theorem B.2. *Let \hat{U} be defined as*

$$\hat{U} = \exp\left(\sum_{\alpha,\beta=1}^{\nu} h_{\alpha\beta} c_\alpha^\dagger c_\beta\right), \quad \text{and} \quad \hat{U}^{-1} = \exp\left(-\sum_{\alpha,\beta=1}^{\nu} h_{\alpha\beta} c_\alpha^\dagger c_\beta\right).$$

Then, the transformed creation operator $\hat{U} c_\alpha^\dagger \hat{U}^{-1}$ can be expressed in terms of the original creation operators c_α^\dagger as

$$\hat{U} c_\alpha^\dagger \hat{U}^{-1} = \sum_{\beta=1}^{\nu} [e^h]_{\beta\alpha} c_\beta^\dagger, \quad (126)$$

where e^h is the exponential of the Hermitian matrix h .

The proof proceeds analogously to the proof of the previous theorem. The only distinction lies in the absence of the imaginary unit in the exponents. The steps that involve the Taylor expansion of the exponential, replacement of number operators in the exponents with occupation numbers, and manipulation of coefficients as functions of matrices still apply. The result is obtained by simply removing the imaginary units from the exponents throughout the steps of the proof.

Theorem B.3. *From Eq. (126) and the fact that h , \hat{U} and \hat{U}^{-1} are both Hermitian, it also follows that:*

$$\hat{U} c_\alpha \hat{U}^{-1} = \sum_{\beta=1}^{\nu} [e^{-h}]_{\alpha\beta} c_\beta. \quad (127)$$

C One-body Hamiltonians and the Fermi-function matrix

In the study of quantum systems, particularly fermionic systems, one often encounters one-body Hamiltonians. These Hamiltonians describe the energy of the system in terms of single-particle states. A special case, which we will focus on, is when the one-body Hamiltonian is diagonal in the second quantization formalism. This simplifies the description and allows us to connect the properties of the system to the Fermi function.

C.1 Partition function and thermal distribution

Before diving into one-body Hamiltonians, let us first define the partition function Z and the thermal distribution for a generic Hamiltonian \hat{H} . The partition function is given by

$$Z(T) = \text{Tr} \left[e^{-\frac{1}{T}\hat{H}} \right], \quad (128)$$

where T is the temperature of the system, and the trace is taken over the entire Fock space. The thermal distribution at temperature T is defined as the normalized density-matrix

$$\rho_T = \frac{e^{-\frac{1}{T}\hat{H}}}{Z(T)}, \quad (129)$$

which allows us to compute expectation values of operators in the system at finite temperature. Specifically, for the expectation value of the number operator $f_a^\dagger f_b$, we define

$$n_{ab}(T) = \text{Tr} \left[\rho_T f_a^\dagger f_b \right]. \quad (130)$$

C.2 One-body diagonal Hamiltonian

Now, let us consider a specific one-body Hamiltonian that is diagonal,

$$\hat{H} = \sum_{a=1}^{\nu} e_{aa} f_a^\dagger f_a. \quad (131)$$

We can state the following theorem regarding the calculation of Z and n_{ab} for this Hamiltonian:

Theorem C.1. *For the one-body diagonal Hamiltonian $\hat{H} = \sum_a e_{aa} f_a^\dagger f_a$, the partition function $Z(T)$ and the thermal expectation values $n_{ab}(T)$ are given by*

$$Z(T) = \prod_{a=1}^{\nu} \left(1 + e^{-\frac{e_{aa}}{T}} \right), \quad (132)$$

$$n_{ab}(T) = \delta_{ab} f_T(e_{aa}), \quad (133)$$

where $f_T(x)$ is the Fermi function at temperature T defined as

$$f_T(x) = \frac{1}{e^{x/T} + 1}. \quad (134)$$

Proof. We begin by expressing the partition function $Z(T)$ as a trace over the Fock space,

$$\begin{aligned} Z(T) &= \text{Tr} \left[e^{-\frac{1}{T} \sum_a e_{aa} f_a^\dagger f_a} \right] \\ &= \sum_{\Gamma=0}^{2^\nu-1} \langle \Gamma | e^{-\frac{1}{T} \sum_a e_{aa} f_a^\dagger f_a} | \Gamma \rangle = \sum_{\Gamma=0}^{2^\nu-1} \langle \Gamma | \exp \left(-\frac{1}{T} \sum_a e_{aa} q_a(\Gamma) \right) | \Gamma \rangle, \end{aligned} \quad (135)$$

where we have used the Fock basis representation $|\Gamma\rangle = [c_1^\dagger]^{q_1(\Gamma)} \dots [c_\nu^\dagger]^{q_\nu(\Gamma)} |0\rangle$, and the relation $f_a^\dagger f_a |\Gamma\rangle = q_a(\Gamma) |\Gamma\rangle$.

We can further break down the sum over Γ into a sum over the occupation numbers q_a for each a ,

$$\begin{aligned} Z(T) &= \sum_{q_1=0}^1 \dots \sum_{q_\nu=0}^1 \exp \left(-\frac{1}{T} \sum_a e_{aa} q_a \right) \\ &= \prod_{a=1}^\nu \left(\sum_{q_a=0}^1 \exp \left(-\frac{e_{aa} q_a}{T} \right) \right) = \prod_{a=1}^\nu \left(1 + \exp \left(-\frac{e_{aa}}{T} \right) \right). \end{aligned} \quad (136)$$

Here, in the second step, we have used that the exponential of the sum is the product of the exponentials and separated the terms corresponding to each a . The expression obtained is the desired result for the partition function $Z(T)$ in terms of the eigenvalues of the one-body Hamiltonian. \square

Proof. Let us first compute $Z(T) n_{ab}$, which can be written as a trace:

$$Z(T) n_{ab} = \text{Tr} \left[e^{-\frac{1}{T} \sum_c e_{cc} f_c^\dagger f_c} f_a^\dagger f_b \right] = \sum_{\Gamma=0}^{2^\nu-1} \langle \Gamma | e^{-\frac{1}{T} \sum_c e_{cc} f_c^\dagger f_c} f_a^\dagger f_b | \Gamma \rangle. \quad (137)$$

If $a \neq b$, this is zero since expanding in terms of the Fock states will always have different occupation numbers on the left and right sides.

Now, let us focus on the case $a = b$,

$$\begin{aligned} Z(T) n_{aa} &= \sum_{\Gamma=0}^{2^\nu-1} \langle \Gamma | e^{-\frac{1}{T} \sum_c e_{cc} q_c(\Gamma)} q_a(\Gamma) | \Gamma \rangle \\ &= \sum_{q_1=0}^1 \dots \sum_{q_\nu=0}^1 q_a \exp \left(-\frac{1}{T} \sum_c e_{cc} q_c \right) \\ &= \exp \left(-\frac{e_{aa}}{T} \right) \prod_{c \neq a} \left(1 + \exp \left(-\frac{e_{cc}}{T} \right) \right) = Z(T) \frac{\exp(-e_{aa}/T)}{1 + \exp(-e_{aa}/T)}. \end{aligned} \quad (138)$$

Dividing by $Z(T)$, we get

$$n_{aa} = \frac{\exp(-e_{aa}/T)}{1 + \exp(-e_{aa}/T)} = \frac{1}{e^{e_{aa}/T} + 1} = f_T(e_{aa}), \quad (139)$$

which is the Fermi function at temperature T . \square

C.3 Fermi-function matrix for non-diagonal one-body Hamiltonians

Now we consider a general one-body Hamiltonian, \hat{H} , given by

$$\hat{H} = \sum_{\alpha,\beta=1}^{\nu} h_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}. \quad (140)$$

We aim to generalize the results from the previous section for a diagonal Hamiltonian to this more general case.

Theorem C.2. *For an arbitrary one-body Hamiltonian \hat{H} , the thermal expectation value $\Delta_{\alpha\beta}(T) = \langle c_{\alpha}^{\dagger} c_{\beta} \rangle$ is given by*

$$\Delta_{\alpha\beta}(T) = [f_T(h)]_{\beta\alpha}, \quad (141)$$

where f_T is the Fermi function at temperature T .

Proof. We start by diagonalizing the matrix h . This can be done by writing $h = VeV^{\dagger}$, where V is a unitary matrix that diagonalizes h and e is the resulting diagonal matrix. The Hamiltonian can then be rewritten as $\hat{H} = \sum_a e_{aa} f_a^{\dagger} f_a$, where

$$f_a^{\dagger} = \sum_{\alpha} V_{\alpha a} c_{\alpha}^{\dagger}, \quad (142)$$

$$c_{\alpha}^{\dagger} = \sum_a V_{a\alpha}^{\dagger} f_a^{\dagger}. \quad (143)$$

Using this, we can write the thermal expectation value $\langle c_{\alpha}^{\dagger} c_{\beta} \rangle_T$ as

$$\Delta_{\alpha\beta}(T) = \langle c_{\alpha}^{\dagger} c_{\beta} \rangle_T \quad (144)$$

$$= \text{Tr} \left[\rho_T \left(\sum_a V_{a\alpha}^{\dagger} f_a^{\dagger} \right) \left(\sum_b V_{\beta b} f_b \right) \right] \quad (145)$$

$$= \sum_a V_{a\alpha}^{\dagger} \sum_b V_{\beta b} n_{ab} = \sum_a V_{a\alpha}^{\dagger} \sum_b V_{\beta b} \delta_{ab} f_T(e_{aa}) = [V f_T(e) V^{\dagger}]_{\beta\alpha}, \quad (146)$$

where $f_T(e)$ is the Fermi function at temperature T defined as

$$f_T(e) = \frac{1}{e^{e/T} + 1}. \quad (147)$$

Finally, using the definition of the function of a Hermitian matrix, as discussed in Section A.1, we can write

$$\Delta_{\alpha\beta}(T) = [f_T(h)]_{\beta\alpha}, \quad (148)$$

which concludes the proof. \square

D Wick's theorem for one-body thermal states

Wick's theorem provides a powerful tool for evaluating the expectation values of products of creation and annihilation operators with respect to thermal states of one-body Hamiltonians, including the ground state, which is going to be essential within the formalism of the GA and the gGA.

Theorem D.1 (Wick's Theorem). *Wick's Theorem provides a systematic method to decompose the expectation value of a product of creation and annihilation operators into a sum of products of expectation values of pairs of operators.*

Consider a system described by a generic one-body Hamiltonian of the form

$$\hat{H} = \sum_{\alpha, \beta=1}^{\nu} h_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}, \quad (149)$$

and a corresponding generic thermal density-matrix ρ_T , as defined in Eq. (129).

Let $O = o_1 o_2 \cdots o_n$ be a string of creation and annihilation operators, where each o_i is either c_{α}^{\dagger} or c_{β} .

Wick's theorem states that the thermal expectation value $\langle O \rangle_T$ can be expanded as a sum of products of contracted pairs:

$$\langle O \rangle_T = \sum_{\text{all contractions}} (-1)^{\text{crossings}} \prod_{\text{contractions}} \langle o_i o_j \rangle_T. \quad (150)$$

Here, each term in the sum corresponds to a distinct way of pairing the creation and annihilation operators into contractions. A contraction between o_i and o_j is represented as $\langle o_i o_j \rangle_T$. The number of crossings is the number of times the contraction lines cross each other, and the sign is determined by the parity (even or odd) of the number of crossings.

The thermal expectation values for pairs of creation and annihilation operators are given by

$$\langle c_{\alpha}^{\dagger} c_{\beta} \rangle_T = [f_T(h)]_{\beta\alpha}, \quad (151)$$

$$\langle c_{\beta} c_{\alpha}^{\dagger} \rangle_T = \delta_{\alpha\beta} - [f_T(h)]_{\beta\alpha}. \quad (152)$$

This theorem, which is presented here without proof, is best understood through examples. The examples below illustrate how Wick's Theorem works in practice.

Example. Consider calculating the expectation value of $c_1^{\dagger} c_1 c_1^{\dagger} c_1$. This can be written as a sum of two terms corresponding to different contractions:

$$\begin{aligned} \langle c_1^{\dagger} c_1 c_1^{\dagger} c_1 \rangle_T &= \langle c_1^{\dagger} c_1 c_1^{\dagger} c_1 \rangle_T + \langle c_1^{\dagger} c_1 c_1^{\dagger} c_1 \rangle_T \\ &= [f_T(h)]_{11}^2 + [f_T(h)]_{11} (1 - [f_T(h)]_{11}) = [f_T(h)]_{11}. \end{aligned}$$

The first contribution comes from the contraction lines between the pairs of creation and annihilation operators that are next to each other, while the second contribution is from the pairs that are more distant. The sum of these contributions gives $[f_T(h)]_{11}$. This is consistent with the fact that $c_1^{\dagger} c_1 c_1^{\dagger} c_1 = c_1^{\dagger} c_1$ at the operator level.

Example. Consider calculating the expectation value of $c_1^\dagger c_1^\dagger c_1 c_1$. This can be written as a sum of two terms corresponding to different contractions

$$\langle c_1^\dagger c_1^\dagger c_1 c_1 \rangle_T = \overbrace{\langle c_1^\dagger c_1^\dagger c_1 c_1 \rangle_T} + \overbrace{\langle c_1^\dagger c_1^\dagger c_1 c_1 \rangle_T} = -[f_T(h)]_{11}^2 + [f_T(h)]_{11}^2 = 0.$$

The first contribution comes with a negative sign due to one crossing, while the second contribution comes with a positive sign. The sum of these contributions gives 0, consistent with the fact that $c_1^\dagger c_1^\dagger c_1 c_1 = 0$ at the operator level.

Example. Consider calculating the expectation value of $c_1^\dagger c_2^\dagger c_2 c_1$. This can be written as a sum of two terms corresponding to different contractions

$$\langle c_1^\dagger c_2^\dagger c_2 c_1 \rangle_T = \overbrace{\langle c_1^\dagger c_2^\dagger c_2 c_1 \rangle_T} + \overbrace{\langle c_1^\dagger c_2^\dagger c_2 c_1 \rangle_T} = [f_T(h)]_{11} [f_T(h)]_{22} - [f_T(h)]_{12} [f_T(h)]_{21}.$$

The first contribution comes with no crossings, while the second contribution has one crossing and comes with a negative sign.

D.1 A useful observation involving Wick contractions

In this subsection, we present a useful observation based on Wick's theorem, which plays an important role in the formal derivation of the multi-orbital GA and gGA equations. We consider a thermal state of a one-body Hamiltonian (refer to Eq. (129)) and focus on the calculation of $\langle X c_\alpha^\dagger c_\beta \rangle_T$, where X represents a product of creation and annihilation operators.

Theorem D.2 (Classification of Contractions with Additional Operators). *Let us consider a thermal state of a one-body Hamiltonian as defined in Wick's Theorem (see Theorem D.1), and let X be a generic fermionic operator, which can be represented as a linear combination of strings of creation and annihilation operators. Consider the expectation value $\langle X c_\alpha^\dagger c_\beta \rangle_T$. By applying Wick's theorem, we can classify the terms obtained into two types:*

1. **Type 1:** Terms where $c_\alpha^\dagger c_\beta$ are contracted with each other. The sum of all such "disconnected" terms yields

$$\overbrace{\langle X c_\alpha^\dagger c_\beta \rangle_T} = \langle X \rangle_T \langle c_\alpha^\dagger c_\beta \rangle_T. \quad (153)$$

2. **Type 2:** The sum of all remaining "connected" terms, which can be written in the form

$$\overbrace{\langle X c_\alpha^\dagger c_\beta \rangle_T} = \sum_{\alpha' \beta'} \xi_T^{\alpha' \beta'} \langle c_{\alpha'} c_\alpha^\dagger \rangle_T \langle c_{\beta'}^\dagger c_\beta \rangle_T. \quad (154)$$

Here the coefficients $\xi_T^{\alpha' \beta'}$ depend only on T and X , but not on α and β . In fact, these coefficients correspond to the sum of all terms that arise from self-contractions among the operators remaining in X once we exclude α' and β' (which are contracted with α and β , respectively).

This observation is particularly helpful in simplifying calculations involving thermal expectation values with additional operators, and it is extensively employed in the derivation of equations within the multi-orbital GA and gGA formalisms.

E Reduced density-matrix of a fermionic subsystem

In this section, we discuss the reduced many-body density-matrix of a subsystem in a one-body fermionic system, as described in Wick's theorem (see Theorem D.1). This concept plays an important role in the formal derivation of the multi-orbital GA and gGA equations.

Let us recall that the Hamiltonian is given by

$$\hat{H} = \sum_{\alpha, \beta=1}^{\nu} h_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}, \quad (155)$$

as stated in Theorem D.1, and the corresponding thermal states are represented by Eq. (129).

We denote the modes in the full system as c_1, \dots, c_{ν} and the modes in a subsystem S as c_1, \dots, c_{η} , where $\eta < \nu$.

Let us consider the so-called single-particle reduced density-matrix for the subsystem S , which is the following $\eta \times \eta$ matrix

$$\Delta_{\alpha\beta} = \langle c_{\alpha}^{\dagger} c_{\beta} \rangle_T = [f_T(h)]_{\beta\alpha} \quad \forall \alpha, \beta = 1, \dots, \eta, \quad (156)$$

where f_T is the Fermi function at temperature T , as shown in Sec. C.3.

Theorem E.1 (Reduced Many-Body Density-Matrix for a Subsystem). *Let S be a subsystem with η modes, and let Δ be the single-particle reduced density-matrix for the subsystem. The reduced many-body density-matrix of S with respect to a thermal state of the Hamiltonian \hat{H} is given by*

$$\rho_T^S = \frac{\exp\left(-\sum_{\alpha, \beta=1}^{\eta} F_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}\right)}{\text{Tr}_S \left[\exp\left(-\sum_{\alpha, \beta=1}^{\eta} F_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}\right) \right]}, \quad (157)$$

where Tr_S denotes the trace over the many-body Fock space of the subsystem S , and F is an $\eta \times \eta$ matrix that can be expressed in terms of Δ as

$$F = \ln \left(\frac{1 - \Delta^T}{\Delta^T} \right), \quad (158)$$

where the superscript T denotes the transpose.

In other words, given any operator \hat{O} acting on the subsystem S (i.e., any operator constructed as algebraic combinations of fermionic modes from 1 to η), its expectation value can be calculated as

$$\langle \hat{O} \rangle_T = \text{Tr}_S \left[\rho_T^S \hat{O} \right]. \quad (159)$$

Proof. We will split the proof into two parts.

Part 1: First, we prove that Eq. (159) holds for operators of the form $\hat{O} = c_{\alpha}^{\dagger} c_{\beta}$ with $\alpha, \beta = 1, \dots, \eta$. Notice that ρ_T^S has the form of a thermal density-matrix with $T = 1$ and a Hamiltonian parameterized by F . Therefore, we can apply the theorem proved before Sec. C.3 to express $\text{Tr}_S[\rho_T^S c_{\alpha}^{\dagger} c_{\beta}]$ in terms of the corresponding Fermi function as

$$\text{Tr}_S[\rho_T^S c_{\alpha}^{\dagger} c_{\beta}] = [f_{T=1}(F)]_{\beta\alpha}. \quad (160)$$

However, by the definition of F ,

$$f_{T=1}(F) = \frac{1}{1 + e^F} = \Delta^T. \quad (161)$$

This establishes the desired result for operators of the form $\hat{O} = c_\alpha^\dagger c_\beta$.

Part 2: Now, we extend the result to arbitrary operators \hat{O} in the subsystem S . Since both sides of Eq. (159) resemble thermal expectation values, Wick's theorem (Theorem D.1) applies. Wick's theorem reduces the calculation of expectation values to algebraic combinations of Wick contractions. Since we have already proven that Eq. (159) holds for Wick contractions, it follows that Eq. (159) holds for arbitrary operators \hat{O} acting on the subsystem S . \square

Remark. It is important to note that we have implicitly assumed that the eigenvalues of Δ^T (equivalently, the eigenvalues of Δ) lie strictly between 0 and 1, that is, in the interval $(0, 1)$. This assumption is crucial for the well-definedness of F , as the logarithm in the expression for F would be ill-defined if the eigenvalues were 0 or 1.

F Promoting of functions to independent variables

In the context of formulating the ghost Gutzwiller approximation (gGA) equations, it proves beneficial to adopt a certain mathematical trick involving Lagrange multipliers. This trick is particularly useful for extremizing functions that have a specific structure, and it facilitates obtaining a QE algorithmic structure. Specifically, let us consider a real multivariable function $f(\mathbf{X})$ of the form $f(\mathbf{X}) = g(a_1(\mathbf{X}), \dots, a_n(\mathbf{X}))$, where $\mathbf{X} = (X_1, \dots, X_m)$ is a set of variables. We are interested in extremizing f with respect to \mathbf{X} .

Theorem F.1. *Let $L(\boldsymbol{\lambda}, \mathbf{a}, \mathbf{X})$ be a function constructed as*

$$L(\boldsymbol{\lambda}, \mathbf{a}, \mathbf{X}) = g(a_1, \dots, a_n) - \sum_{k=1}^n \lambda_k (a_k - a_k(\mathbf{X})), \quad (162)$$

where $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_n)$ and $\mathbf{a} = (a_1, \dots, a_n)$. If $\bar{\mathbf{X}}$ is an extremum of $f(\mathbf{X})$, then there exist values $\bar{\boldsymbol{\lambda}}$ and $\bar{\mathbf{a}}$ such that $(\bar{\boldsymbol{\lambda}}, \bar{\mathbf{a}}, \bar{\mathbf{X}})$ is an extremum of $L(\boldsymbol{\lambda}, \mathbf{a}, \mathbf{X})$.

Proof. Let us examine the saddle point conditions for L . These conditions imply:

1. Differentiating with respect to λ_i yields

$$a_i = a_i(\bar{\mathbf{X}}). \quad (163)$$

2. Differentiating with respect to a_i yields

$$\frac{\partial g}{\partial a_i} = \lambda_i. \quad (164)$$

3. Differentiating with respect to X_l yields

$$\sum_{k=1}^n \lambda_k \frac{\partial a_k}{\partial X_l} = 0. \quad (165)$$

Substituting Eqs. (163) and (164) into Eq. (165), we obtain

$$\sum_{k=1}^n \frac{\partial g}{\partial a_k} (a_1(\bar{\mathbf{X}}), \dots, a_n(\bar{\mathbf{X}})) \frac{\partial a_k}{\partial X_l} = \frac{\partial f}{\partial X_l}(\bar{\mathbf{X}}) = 0, \quad (166)$$

which is a necessary condition for an extremum of f . Hence, if $\bar{\mathbf{X}}$ is an extremum of f , it follows that $(\bar{\lambda}, \bar{a}, \bar{\mathbf{X}})$ is an extremum of L . \square

This technique is particularly useful because it provides us with different options for how to implement the saddle-point search in practice. For example, we can first calculate the saddle-point conditions with respect to \mathbf{X} for L , and this may be easier than deriving f with respect to \mathbf{X} , especially if the functions $a_i(\mathbf{X})$ are relatively simple compared to g . This is the kind of scenario that we will encounter in the main text.

G A useful matrix derivative

One of the gGA/GA equations requires to compute a matrix derivative of the form:

$$X = \left. \frac{d}{d\lambda} [K + \lambda H]^{-\frac{1}{2}} \right|_{\lambda=0}, \quad (167)$$

where K and H are Hermitian matrices that do not commute. A simple way to compute this derivative is by reducing the calculation to a Sylvester equation [19], as follows.

Define

$$Y = \left. \frac{d}{d\lambda} [K + \lambda H]^{-1} \right|_{\lambda=0} = -K^{-1} \left. \frac{d}{d\lambda} [K + \lambda H] \right|_{\lambda=0} K^{-1}. \quad (168)$$

Deriving both sides of the equation $[K + \lambda H]^{-1} = ([K + \lambda H]^{-\frac{1}{2}})^2$, it follows that

$$XK^{-1} + K^{-1}X = Y, \quad (169)$$

which is a Sylvester equation that can be solved using standard methods.

Let us call U the unitary matrix that diagonalizes K , i.e., $U^\dagger K U = k$, where k is a diagonal matrix. By applying this unitary transformation to Eq. (169), we get:

$$U^\dagger X U k^{-1} + k^{-1} U^\dagger X U = U^\dagger Y U, \quad (170)$$

which can be easily inverted since k is diagonal:

$$[U^\dagger X U]_{ab} = \frac{[U^\dagger Y U]_{ab}}{k_{aa}^{-1} + k_{bb}^{-1}}. \quad (171)$$

The desired matrix X can be obtained by applying the inverse unitary transformation to both sides of Eq. (171).

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