We develop an extension of the Gutzwiller Approximation (GA) formalism that includes the effects of Coulomb interactions of arbitrary range (including density density, exchange, pair hopping and Coulomb assisted hopping terms). This formalism reduces to the ordinary GA formalism for the multi-band Hubbard models in the presence of only local interactions. This is accomplished by combining the $1/z$ expansion —where $z$ is the coordination number and only the leading order terms contribute in the limit of infinite dimensions — with a $P^R_1 P^R - I$ expansion, where $P^R$ is the Gutzwiller projector on the site $R$. The method is conveniently formulated in terms of a Gutzwiller Lagrange function. We apply our theory to the extended single band Hubbard model. Similarly to the usual Brinkman-Rice mechanism we find a Mott transition. A valence skipping transition is observed, where the occupation of the empty and doubly occupied states for the Gutzwiller wavefunction is enhanced with respect to the uncorrelated Slater determinant wavefunction.

I. INTRODUCTION

Over the last three decades there has been renewed interest and substantial progress in the development of methods for treating strongly correlated electron systems. Various approximations to the Density Functional Theory (DFT) such as the Local Density Approximation (LDA) proved to be a good starting point for combinations with more advanced methodologies [1] to study strongly correlated systems. In this regard, of particular interest are quantum embedding methods, such as the Dynamical Mean Field Theory (DMFT) [2], Density Matrix Embedding Theory (DMET) [3], the GA [4–6], and the slave particles methods [7, 8, 25, 27], which share many common elements [8, 9, 15, 19, 26, 28]. In this work we focus on the GA, which has been actively developed in recent years. Combining these embedding methods with density functional theory gives rise to (LDA+DMFT) [39–41] and LDA in combination with the GA (LDA+GA) [15, 31, 33]. Furthermore these methods can be cast in a framework of functionals of multiple observables, making them convenient for ab-initio numerical simulations [15, 34].

In many currently available theoretical frameworks to study strongly correlated systems, the non-local components of the Coulomb interaction have been treated at the mean field level. On the other hand, this may not be sufficient in many cases. For example, the non-local Coulomb interactions can be as important as the local contributions in organic materials, where even the electrons of $s$ and $p$ orbitals can induce strong-correlation effects [35]. More generally, in many materials the bare nearest neighbor Coulomb matrix elements are the same order of magnitude as the hopping matrix elements [36, 37], suggesting that it is necessary to take them into account more accurately.

Many techniques to treat short-ranged non-local interactions have been developed in the context of model Hamiltonians. For extensions of DMFT to treat this problem see [37–39]. In this work we will focus on extensions of the GA, that is computationally significantly less expensive than DMFT. A pioneering extension of the GA to treat the t-J model was introduced by Zhang et al. [41]. Ogata et al. made calculations of higher order corrections for the t-J model within the GA [42]. The effects of different intersite interactions for the extended t-J model were studied by Sensarma et al. within the GA [43]. An operatorial approach to the GA, where expectation values of Gutzwiller projected operators were calculated in a $1/z$ expansion, was proposed in [60]. Benchmark calculations for hydrogen like systems, including the effects of intersite interactions within the framework of the extended Hubbard model, were performed within the GA in Refs. [51, 52]. The so called “statistically consistent GA” for non-local interactions was studied in [43, 50] and the so called “diagrammatic expansion of the Gutzwiller wavefunction” with intersite interactions was developed in [57, 59] for many models. However, GA methodologies able to account systematically for the effects of non-local interactions in realistic first-principle calculations, without empirical adjustments, are still not available. Here we propose a new generalization of the GA, that constitutes a step towards this ambitious goal. In fact we show that, combining the ideas underlying the $1/z$ expansion [61] with the $P^R_1 P^R - I$ expansion [53, 54, 57, 58, 52], it is possible to tackle systematically non-local two site interactions for general multi-orbital Hubbard models. Our work is an extension of the GA to intersite interactions, in the same spirit as the extended DMFT [89, 14, 45] and the dual boson method [63, 64] extend Dynamical Mean Field Theory [2]. To illustrate our method we present calculations for the extended single band Hubbard model, including nearest-neighbor hopping, density density, correlated hopping, pair hopping and exchange interactions. In particular, our calculations of the single band extended Hubbard model indicate that the nearest-neighbor Coulomb interactions can induce a phase transition where charge fluctuations are enhanced.
rather than suppressed.

The setup of the paper is as follows: in Sec. II we present the main Hamiltonian studied throughout the text. In Sec. III we discuss the simplifications of GA formalism arising from retaining only the leading order in the $P_R^+P_R - I$ expansion. In Sec. IV we show that by combining the $P_R^+P_R - I$ formalism with the $1/z$ expansion it is possible to express semi-analytically the variational energy (including the contribution of the non-local interaction terms) as function of the GA variational parameters. In Sec. V we conveniently reformulate our theory in terms of a GA Lagrange function, which reduces to the result of Ref. [65] for the special case of only-local interactions. In Sec. VI we explicitly show how the general GA Lagrange function reduces for the extended single-band Hubbard model, we then present our benchmark calculations of the extended single-band Hubbard model. In Sec. VII we conclude. The more technical derivations are relegated to the appendices.

II. EXTENDED MULTI-ORBITAL HUBBARD HAMILTONIAN

We consider a generic electronic Hamiltonian, which can be represented in second quantization notation as follows:

$$H = \sum_{R}^{N} \sum_{\alpha,\beta=1} E_R^{\alpha\beta} [c_R^{\dagger \alpha} c_R^{\beta}] + \sum_{R_{1} \neq R_{2}}^{N} \sum_{\alpha,\beta=1}^{N} t_{R_{1};R_{2}}^{\alpha\beta} [c_{R_{1}}^{\dagger \alpha} c_{R_{2}}^{\beta}] + \sum_{R}^{N} \sum_{\alpha,\beta,\gamma,\delta=1}^{N} U_{R}^{\alpha\beta\gamma\delta} [c_{R_{1}}^{\dagger \alpha} c_{R_{2}}^{\beta} c_{R_{3}}^{\gamma} c_{R_{4}}^{\delta}]$$

$$+ \sum_{R_{1} \neq R_{2} \neq R_{3}}^{N} \sum_{\alpha,\beta,\gamma,\delta=1}^{N} V_{R_{1};R_{2}}^{\alpha\beta\gamma\delta} [c_{R_{1}}^{\dagger \alpha} c_{R_{2}}^{\beta} c_{R_{3}}^{\gamma} c_{R_{4}}^{\delta}] + \sum_{R_{1} \neq R_{2} \neq R_{3}}^{N} \sum_{\alpha,\beta,\gamma,\delta=1}^{N} V_{R_{1};R_{2};R_{3}}^{\alpha\beta\gamma\delta} [c_{R_{1}}^{\dagger \alpha} c_{R_{2}}^{\beta} c_{R_{3}}^{\gamma} c_{R_{4}}^{\delta}]$$

$$+ \sum_{R_{1} \neq R_{2} \neq R_{3} \neq R_{4}}^{N} \sum_{\alpha,\beta,\gamma,\delta=1}^{N} S_{R_{1};R_{2};R_{3};R_{4}}^{\alpha\beta\gamma\delta} [c_{R_{1}}^{\dagger \alpha} c_{R_{2}}^{\beta} c_{R_{3}}^{\gamma} c_{R_{4}}^{\delta}] + h.c.) + \sum_{R_{1} \neq R_{2} \neq R_{3} \neq R_{4}}^{N} \sum_{\alpha,\beta,\gamma,\delta=1}^{N} V_{R_{1};R_{2};R_{3}}^{\alpha\beta\gamma\delta} [c_{R_{1}}^{\dagger \alpha} c_{R_{2}}^{\beta} c_{R_{3}}^{\gamma} c_{R_{4}}^{\delta}]$$

Here $\alpha, \beta, \gamma, \delta$ represent both spin and orbital degrees of freedom per site, of which there are $N$ in total. We note that this Hamiltonian represents all possible one and two particle terms that come from the kinetic energy and Coulomb interaction of a first principles Hamiltonian. In particular it includes the regular Hubbard Hamiltonian (the first three terms of the first line). The square brackets are used to mark explicitly the operators acting over the same site.

For later convenience, we formally express the Hamiltonian also in [Eq. (1)] as follows:

$$H = \sum_{R}^{N} H_{R}^{loc} + \sum_{R_{1} \neq R_{2}}^{2N} \sum_{\mu,\nu=1}^{J_{R_{1};R_{2}}^{\mu\nu} O_{R_{1}\mu} O_{R_{2}\nu}} + \sum_{R_{1} \neq R_{2}}^{2N} \sum_{\mu,\nu,\eta=1}^{J_{R_{1};R_{2};R_{3}}^{\mu\nu\eta} O_{R_{1}\mu} O_{R_{2}\nu} O_{R_{3}\eta}}$$

where $O_{R_{1}}^{\dagger} = \{ c_{R_{1}}^{\dagger}, c_{R_{2}} \}$ is a basis of the linear space of local operators (which can be written in terms of the local creation and annihilation operators $\{ c_{R_{1}}^{\dagger}, c_{R_{2}} \}$) and the $J$ are complex coefficients.

III. GA + $P_R^+P_R - I$ EXPANSION

As in the classic GA theory, we consider the following variational wave function:

$$|\Psi\rangle = \prod_{R} P_{R} |\Psi_{0}\rangle , \quad (3)$$

where $P_{R_{1}}$ is the most general operator acting on a single site $R$ and $|\Psi_{0}\rangle$ is any generic multi-band Slater determinant wave-function. For simplicity, here we consider the case of no superconductivity, so in particular the projector $P_{R}$ satisfies $[P_{R}, \hat{N}] = 0$, where $\hat{N}$ is the number operator. We introduce the following subsidiary conditions,
known as the Gutzwiller constraints [15, 60, 65, 69]:

\[
\langle \Psi_0 | P_R^\dagger P_R | \Psi_0 \rangle = 1
\]

\[
\langle \Psi_0 | P_R^\dagger P_R c_{R\alpha} c_{R\beta} | \Psi_0 \rangle = \langle \Psi_0 | c_{R\alpha}^\dagger c_{R\beta} | \Psi_0 \rangle .
\]

(4)

Our goal is to evaluate the expectation value of the Hamiltonian in Eq. (1) with respect to the Gutzwiller wavefunction in Eq. (3) subject to the Gutzwiller constraints.

The treatment of the terms of Eq. (1) involving three and four sites will be discussed in Appendix C.

For simplicity, in the main text of this work we will explicitly account only for the two-site contributions to the Hamiltonian, corresponding to the following terms of Eq. (1) and the first line of Eq. (6):

\[
\langle \Psi H | \Psi \rangle \equiv \langle \Psi_0 | H_F | \Psi_0 \rangle ,
\]

(5)

where:

\[
H_F = \sum_R P_R^\dagger H^{loc}_R P_R + \sum_{R_1 \neq R_2} \sum_{\mu \nu} J_{R_1;R_2}^{\mu,\nu} P_{R_1}^\dagger O_{R_1,\mu} P_{R_1} P_{R_2}^\dagger O_{R_2,\nu} P_{R_2} + \\
+ \sum_{R_1 \neq R_2 \neq R_3} \sum_{\mu \nu} J_{R_1;R_2;R_3}^{\mu,\nu,\eta} P_{R_1}^\dagger O_{R_1,\mu} P_{R_1} P_{R_2}^\dagger O_{R_2,\nu} P_{R_2} P_{R_3}^\dagger O_{R_3,\eta} P_{R_3} + \\
+ \sum_{R_1 \neq R_2 \neq R_3 \neq R_4} \sum_{\mu \nu} J_{R_1;R_2;R_3;R_4}^{\mu,\nu,\rho} P_{R_1}^\dagger O_{R_1,\mu} P_{R_1} P_{R_2}^\dagger O_{R_2,\nu} P_{R_2} P_{R_3}^\dagger O_{R_3,\eta} P_{R_3} P_{R_4}^\dagger O_{R_4,\rho} P_{R_4} .
\]

(6)

Note that this is a key simplification, as in all terms of Eq (6) only the operators \( P_R \) acting over sites with operators \( O_R \) appear.

**IV. EQUIVALENCES**

For simplicity, in the main text of this work we will explicitly account only for the two-site contributions to the Hamiltonian, corresponding to the following terms of Eq. (1) and the first line of Eq. (6):

\[
H = \sum_{R} \sum_{\alpha,\beta = 1}^N E_R^{ab} \left[ c_{Ra}^\dagger c_{Rb} \right] + \sum_{R_1 \neq R_2} \sum_{\alpha,\beta = 1}^N \tilde{J}_{R_1;R_2}^{ab} \left[ c_{Ra}^\dagger c_{Rb} \right] + \sum_{R} \sum_{\alpha,\beta,\gamma,\delta = 1}^N U_R^{ab,\gamma\delta} \left[ c_{Ra} c_{Rb} c_{R\gamma} c_{R\delta} \right] \\
+ \sum_{R_1 \neq R_2} \sum_{\alpha,\beta,\gamma,\delta = 1}^N V_{R_1;R_2}^{ab,\gamma\delta} \left[ c_{Ra} c_{Rb} c_{R\gamma} c_{R\delta} \right] + \sum_{R_1 \neq R_2} \sum_{\alpha,\beta,\gamma,\delta = 1}^N Y_{R_1;R_2}^{ab,\gamma\delta} \left[ c_{R\alpha} c_{R\beta} c_{R\gamma} c_{R\delta} \right] \\
+ \left( \sum_{R_1 \neq R_2} \sum_{\alpha,\beta,\gamma,\delta = 1}^N X_{R_1;R_2}^{ab,\gamma\delta} \left[ c_{Ra} c_{Rb} c_{R\gamma} c_{R\delta} \right] + \text{h.c.} \right) .
\]

(7)

Therefore, the effective Hamiltonian \( \hat{H}_F \) of Eq. (6) reduces to:

\[
\hat{H}_F = \sum_R P_R^\dagger H^{loc}_R P_R + \sum_{R_1 \neq R_2} \sum_{\mu \nu} J_{R_1;R_2}^{\mu,\nu} \left[ P_{R_1}^\dagger O_{R_1,\mu} P_{R_1} P_{R_2}^\dagger O_{R_2,\nu} P_{R_2} \right] .
\]

(8)

The treatment of the terms of Eq. (1) involving three and four sites will be discussed in Appendix C.

As we are going to demonstrate, at the leading order of the 1/z expansion the expression for the total energy simplifies as follows:

\[
\langle \Psi_0 | \hat{H}_F | \Psi_0 \rangle \equiv \langle \Psi_0 | \hat{H}_{eff} | \Psi_0 \rangle ,
\]

(9)

where

\[
\hat{H}_{eff} = \sum_R P_R^\dagger H^{loc}_R P_R + \sum_{R_1 \neq R_2} \sum_{\mu \nu} J_{R_1;R_2}^{\mu,\nu} \left[ \sum_i Z_{R_1,\mu i} O_{R_1 i} \right] \left[ \sum_j Z_{R_2,vj} O_{R_2 j} \right] .
\]

(10)
and the $Z_{R\alpha i}$ are complex numbers that can be expressed as a function of the Gutzwiller variational parameters.

We note that, analogously to previous work [15 60 65 68], this simplification amounts to formally replace the operators $P_R^\dagger O_{R\alpha} P_R$ of Eq. (8) with $\sum R \alpha i \sum Z_{R\alpha i} O_{Ri}$. From now on we are going to refer to these formal substitutions as “Gutzwiller equivalences”. As shown in Appendix E, $H_{Eff}$ is Hermitian (consistently with the fact that the total energy for the Hamiltonians in Eq. (9) is real).

### A. Definitions

For completeness, here we summarize the definitions of the variational parameters previously introduced in Refs. [15 60 65], in terms of which it will be possible to express conveniently the total energy also for the non-local interactions at the core of the present theory.

We express the Gutzwiller operators in the so-called “mixed-basis representation” [15 65 68] defined as follows:

$$P_R = \sum_{\Gamma,n} [\Lambda_R |\Gamma_n \rangle \langle n_R| , \quad (11)$$

where

$$|\Gamma_R \rangle = (\hat{c}_{R1} \rangle \ n_1(\Gamma_R) \ldots (\hat{c}_{RN} \rangle \ n_N(\Gamma_R) |0,R\rangle ,$$

$$|n_R\rangle = (\hat{f}_{R1} \rangle n_{1(\Gamma_R)} \ldots (\hat{f}_{RN} \rangle n_{N(\Gamma_R)} |0,R\rangle . \quad (12)$$

Here $n_{\alpha}(\Gamma, R), n_{\alpha}(n, R) \in \{0,1\}$ represent the occupation numbers of the states $|n_R\rangle$, $|\Gamma_R\rangle$ respectively and the operators $f_{R\alpha}$ are the so-called “quasi-particle” fermionic operators, which are related to the operators $c_{R\alpha}$ through an arbitrary unitary transformation.

We conveniently express the local reduced density matrix of $|\Psi_0\rangle$ as follows:

$$\rho_R^0 = TR\neq R |\Psi_0\rangle \langle \Psi_0|$$

$$= \exp \left( - \sum_{ab} \left[ \ln \left( \frac{1 - \Delta_{RR}}{\Delta_{RR}} \right) \right]_{ab} f_{Ra}^\dagger f_{Rb} \right) , \quad (13)$$

where

$$[\Delta_{RR})_{ab} = \langle \Psi_0 | f_{R1a}^\dagger f_{R2b} | \Psi_0 \rangle \quad (14)$$

and the superscript $T$ indicates the transpose.

It is also convenient to introduce the so-called “matrix of slave-boson amplitudes”, see [15 28 65 68 69], which is defined as follows:

$$\phi_R = \Lambda_R \sqrt{\rho_R^0} , \quad (15)$$

where

$$[\rho_R^0]_{nRn'} = \langle n_R | \rho_R^0 | n_R\rangle . \quad (16)$$

Following Refs. [15 68], we also introduce the so-called “embedding mapping”, which relates the matrix $\phi_R$ to the states $|\Phi_R\rangle$ belonging to an auxiliary impurity model with a bath site of size equal to the size of the impurity. The definition of the embedding mapping is the following:

$$|\Phi_R\rangle = \sum_R \exp \left( i \frac{\pi}{2} N(\hat{n}_R) (N(\hat{n}_R) - 1) \times \times |\Phi_R\rangle |\Gamma_n U_{PH} |\hat{\Gamma}_R \rangle |\hat{n}_R\rangle , \quad (17)$$

where

$$|\hat{\Gamma}_R\rangle = (\hat{c}_{R1}^\dagger \ n_1(\hat{f},R) \ldots (\hat{c}_{RN}^\dagger \ n_N(\hat{f},R) |0,R\rangle ,$$

$$|\hat{n}_R\rangle = (\hat{f}_{R1}^\dagger \ n_{1(\hat{f},R)} \ldots (\hat{f}_{RN}^\dagger \ n_{N(\hat{f},R)} |0,R\rangle . \quad (18)$$

Here $n_{\alpha}(\hat{f}, R), n_{\alpha}(\hat{n}, R) \in \{0,1\}$ represent the occupation numbers of the states $|\hat{n}_R\rangle$, $|\hat{\Gamma}_R\rangle$ respectively, and

$$N(\hat{n}_R) = \sum_{a=1}^N n_{\alpha}(\hat{n}, R) \quad (19)$$

is the sum of the occupation numbers of the single particle states for the bath. Furthermore $U_{PH}$ is defined as follows:

$$U_{PH} \hat{c}_{Ra} \hat{c}_{Ra}^\dagger U_{PH} = \hat{c}_{Ra}$$

$$U_{PH} \hat{c}_{Ra} \hat{c}_{Ra}^\dagger U_{PH} = \hat{c}_{Ra}$$

$$U_{PH} \hat{f}_{Ra} \hat{f}_{Ra}^\dagger U_{PH} = \hat{f}_{Ra}$$

$$U_{PH} \hat{f}_{Ra} \hat{f}_{Ra}^\dagger U_{PH} = \hat{f}_{Ra} . \quad (20)$$

Here the fact that $[P_R, \hat{N}] = 0$ implies that the state $|\Phi_R\rangle$ is at half filling, i.e.:

$$\sum_{\alpha} \hat{c}_{Ra}^\dagger \hat{c}_{Ra} + \sum_{\alpha} \hat{f}_{Ra}^\dagger \hat{f}_{Ra} = N |\Phi_R\rangle . \quad (22)$$

Note that, within the definitions above, the Gutzwiller constraints in Eq. (4) can be written as [15 60 65 68]:

$$|\Phi_R \rangle = 1$$

$$|\Phi_R \rangle \hat{f}_{Ra} \hat{f}_{Ra}^\dagger |\Phi_R \rangle = \langle \Psi_0 | \hat{f}_{Ra} \hat{f}_{Ra}^\dagger | \Psi_0 \rangle \quad (23)$$
B. Fermionic Equivalences

Let us derive the equivalence relations for all local operators in Eq. (7) that increase the number of electrons by one, i.e., \( c_R^+ c_R \) and \( c_{R\alpha}^+ c_{R\beta} c_{R\gamma} \).

As demonstrated in the Appendices B and D3a at the leading order of the \(1/z\) expansion the following Gutzwiller equivalences hold:

\[
P_R^f c_R^+ P_R \sim \sum_a \mathcal{R}_{Raa} f_R^a,
\]

\[
P_R^+ c_{R\alpha}^+ c_{R\beta} c_{R\gamma} P_R \sim \sum_a \mathcal{S}_{R\alpha\beta\gamma a} f_R^a.
\]  

(24)

Here \( \mathcal{R}_R \) and \( \mathcal{S}_R \) are examples of the coefficients \( Z_{R\mu} \). The Hermitian conjugate of Eq. (24) also holds. Here the coefficients \( \mathcal{R}_{Raa}, \mathcal{S}_{R\alpha\beta\gamma a} \) are determined by the following equations:

\[
\langle \Psi_0 | P_R^f c_R^+ P_R f_R | \Psi_0 \rangle = \langle \Psi_0 | \sum_b \mathcal{R}_{Rab} f_R^b \rangle f_R^a | \Psi_0 \rangle
\]

\[
\langle \Psi_0 | P_R^+ c_{R\alpha}^+ c_{R\beta} c_{R\gamma} P_R f_R | \Psi_0 \rangle = \langle \Psi_0 | \sum_b \mathcal{S}_{R\alpha\beta\gamma b} f_R^b \rangle f_R^a | \Psi_0 \rangle.
\]  

(25)

Furthermore in Appendix D3a we solve explicitly these equations and show that:

\[
\mathcal{R}_{Raa} = \sum_b \langle \Phi_R | \hat{c}_{Ra} \hat{f}_{Rb} | \Phi_R \rangle
\]

\[
\mathcal{S}_{R\alpha\beta\gamma a} = \sum_b \langle \Phi_R | \hat{c}_{Ra} \hat{c}_{R\beta} \hat{c}_{R\gamma} \hat{f}_{Rb} | \Phi_R \rangle \times
\]

\[
\times \left[ \frac{1}{(I - \Delta_{RR}) \Delta_{RR}} \right]^{1/2}_{ba}.
\]  

(27)

In summary, at the leading order of the \(1/z\) expansion we have that:

\[
\frac{\langle \Psi | H_{\text{Ferm}} \rangle | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \langle \Psi_0 | \hat{H}_{\text{Ferm}} | \Psi_0 \rangle,
\]  

(28)

where:

\[
H_{\text{Ferm}} = \sum_{R_1 \neq R_2} N \sum_{\alpha, \beta, \gamma = 1} t_{R_1; R_2} \hat{c}_{R_1 \alpha} \hat{c}_{R_2 \beta} + \left( \sum_{R_1 \neq R_2} \sum_{\alpha, \beta, \gamma, \delta = 1} x_{R_1; R_2} \hat{c}_{R_1 \alpha} \hat{c}_{R_2 \beta} \hat{c}_{R_1 \gamma} \hat{c}_{R_2 \delta} + h.c. \right),
\]  

(29)

\[
\hat{H}_{\text{Eff}} = \sum_{R_1 \neq R_2} N \sum_{\alpha, \beta, \gamma, \delta = 1} t_{R_1; R_2} \hat{f}_{R_1 a} \hat{f}_{R_2 b} + \left( \sum_{R_1 \neq R_2} \sum_{\alpha, \beta, \gamma, \delta = 1} \sum_{a, b, d = 1} x_{R_1; R_2} \hat{f}_{R_1 a} \hat{f}_{R_2 b} \hat{f}_{R_1 d} \hat{f}_{R_2 d} + h.c. \right).
\]  

(30)

Here the coefficients \( \mathcal{R}_R, \mathcal{S}_R \) are explicitly expressed in terms of the Gutzwiller variational parameters in Eqs. (27) and (27).

In terms of the notation introduced in Eq. (2) all of the above equations can be schematically represented as follows:

\[
P_R^f O_{R\mu} P_R \sim \sum_a \mathcal{Z}_{R\mu a} f_R^a.
\]  

(31)

Here \( \mathcal{R}_R \) and \( \mathcal{S}_R \) are specific instances of the coefficients \( Z_{R\mu} \). Here the \( Z_{R\mu a} \) are determined by the equation:

\[
\langle \Psi_0 | P_R^f O_{R\mu} P_R f_R | \Psi_0 \rangle = \langle \Psi_0 | \sum_b \mathcal{Z}_{R\mu b} f_R^b \rangle f_R^a | \Psi_0 \rangle.
\]  

(32)

The explicit solution of the equation above is the following:

\[
\mathcal{Z}_{R\mu a} = - \sum_b \langle \Phi_R | \hat{O}_{R\mu} \hat{f}_{Rb} | \Phi_R \rangle \left[ \frac{1}{(I - \Delta_{RR}) \Delta_{RR}} \right]^{1/2}_{ba}.
\]  

(33)

C. Bosonic Equivalences (fermion number conserving operators)

Let us derive the equivalence relations for all local operators of Eq. (7) that do not change the number of electrons, i.e., \( c_R^+ c_R \). We note that something similar can be done for the operators \( c_{R\alpha}^+ c_{R\beta} c_{R\gamma} c_{R\delta} \) though they do not appear as a single site term as a part of two site terms in the Hamiltonian in Eq. (1).

As demonstrated in the Appendices B, D3a and D3a at the leading order of the \(1/z\) expansion the following
Gutzwiller equivalences hold:

\[ P_{R}^{\dagger}c_{R\alpha}c_{R\beta}P_{R} \sim \sum_{ab} T_{Ra\beta ba}f_{Ra}f_{Rb} + T_{Ra\beta I} \]

\[ P_{R}^{\dagger}c_{R\alpha}c_{R\beta}c_{R\gamma}c_{R\delta}P_{R} \sim \sum_{ab} T_{Ra\beta \gamma \delta ba}f_{Ra}f_{Rb} + T_{Ra\beta \gamma \delta I} . \]

Here \( T_{R} \) is an example of the coefficients \( Z_{R_{ij}} \). In this case we show in Appendix D3b that \( T_{Ra\beta cd}, T_{Ra\beta I} \) are determined by the following equations:

\[ \langle \Psi_{0} | P_{R}^{\dagger}c_{R\alpha}c_{R\beta}P_{R}f_{Ra}f_{Rb} | \Psi_{0} \rangle = \]

\[ \langle \Psi_{0} | \sum_{cd} T_{Ra\beta dc}f_{Ra}f_{Rc} + T_{Ra\beta I} I | \Psi_{0} \rangle = \]

\[ \langle \Psi_{0} | P_{R}^{\dagger}c_{R\alpha}c_{R\beta}P_{R} \cdot I | \Psi_{0} \rangle = \]

\[ \langle \Psi_{0} | \sum_{cd} T_{Ra\beta dc}f_{Ra}f_{Rc} + T_{Ra\beta I} I \rangle . \]

Furthermore in Appendix D3b we solve these equations explicitly and show that:

\[ T_{Ra\beta dc} = \sum_{ab} \left[ \frac{1}{(1 - \Delta_{RR})} \right]_{ab}^{1/2} \langle \Phi_{R} | c_{Ra}^{\dagger}c_{R\beta}f_{Ra}f_{Rd} | \Phi_{R} \rangle \]

\[ \times \left[ \frac{1}{(1 - \Delta_{RR})} \right]_{bc}^{1/2} - \langle \Phi_{R} | c_{Ra}^{\dagger}c_{R\beta} | \Phi_{R} \rangle \times \left[ \frac{1}{(1 - \Delta_{RR})} \right]_{cd} . \]

In summary, at the leading order of the 1/z expansion we have that:

\[ \frac{\langle \Psi | H^{Con} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \cong \langle \Psi_{0} | \hat{H}^{Con} | \Psi_{0} \rangle \]

where:

\[ H^{Con} = \sum_{R_{1} \neq R_{2}} \sum_{\alpha, \beta, \gamma, \delta = 1}^{N} V_{R_{1}, R_{2}}^{\alpha \beta \gamma \delta} \left[ c_{R_{1} \alpha}^{\dagger}c_{R_{2} \beta} \right] \left[ c_{R_{2} \gamma}^{\dagger}c_{R_{1} \delta} \right] , \]

\[ \hat{H}^{Con} = \sum_{R_{1} \neq R_{2}} \sum_{\alpha, \beta, \gamma, \delta = 1}^{N} V_{R_{1}, R_{2}}^{\alpha \beta \gamma \delta} \left[ \sum_{\alpha, \beta = 1}^{N} T_{Ra\beta ab}f_{Ra}f_{Rb} + T_{Ra\beta I} I \right] \times \left[ \sum_{\beta, \gamma, \delta = 1}^{N} T_{R\gamma \delta cd}f_{Rc}f_{Rd} + T_{R\gamma I} I \right] . \]

Here the coefficients \( T_{R} \) are explicitly expressed in terms of the Gutzwiller variational parameters in Eqs. (36) and (37).

In terms of the notation introduced in Eq. (2) all of the above equations can be schematically represented as follows:

\[ P_{R}^{\dagger}O_{R_{i}}P_{R} \sim \sum_{ab} Z_{R_{i}ab}f_{Ra}f_{Rb} + Z_{R_{i}I} I . \]

Here \( T_{R} \) is a specific instance of the coefficients \( Z_{R_{i}ab} \).

The explicit solution of the equation above is the following, see Appendix D3b.
\[ Z_{R\mu dc} = \sum_{ab} \left[ \frac{1}{\langle \bar{1} - \Delta_{RR} \Delta_{RR} \rangle_{ab}} \langle \Phi_R | \hat{O}_{R\mu} \hat{f}_{R\beta} \hat{f}_{R\gamma} \hat{f}_{R\delta} | \Phi_R \rangle \right]^{1/2} \times \left[ \frac{1}{\langle \bar{1} - \Delta_{RR} \Delta_{RR} \rangle_{bc}} \right]^{1/2} - \langle \Phi_R | \hat{O}_{R\mu} | \Phi_R \rangle \times \left[ \frac{1}{\langle \bar{1} - \Delta_{RR} \Delta_{RR} \rangle_{dc}} \right], \]

D. Bosonic Equivalences (fermion number changing operators)

Let us derive the equivalence relations for all local operators of Eq. (7) that increase the number of electrons by two, i.e., \( c_{R\alpha} c_{R\beta} \). We note that something similar can be done for the operators \( c_{R\alpha} c_{R\beta} c_{R\gamma} c_{R\delta} \) though they do not appear as any single site terms as a part of two site terms in the Hamiltonian in Eq. (1).

As demonstrated in the Appendices D 3c and D 3a at the leading order of the \( 1/z \) expansion the following Gutzwiller equivalences hold:

\[ P_R^\dagger c_{R\alpha} c_{R\beta} P_R \sim \sum_{ab} U_{R\alpha \beta ab} f_{R\alpha} f_{R\beta} \]

\[ P_R^\dagger c_{R\alpha} c_{R\beta} c_{R\gamma} c_{R\delta} P_R \sim \sum_{ab} U_{R\alpha \beta \gamma \delta ab} f_{R\alpha} f_{R\beta} f_{R\gamma} f_{R\delta}. \]  

Furthermore in Appendix D 3c we solve these equations explicitly and show that:

\[ \langle \Psi_0 | P_R^\dagger c_{R\alpha} c_{R\beta} P_R f_{R\alpha} f_{R\beta} | \Psi_0 \rangle = \langle \Psi_0 | \sum_{cd} U_{R\alpha \beta cd} f_{Rc} f_{Rd} | \Psi_0 \rangle. \]

In summary, at the leading order of the \( 1/z \) expansion we have that:

\[ \frac{\langle \Psi | H^{Chan} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \frac{\langle \Psi_0 | H^{Chan}_{Eff} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}, \]

where:

\[ H^{Chan}_{Eff} = \sum_{R_1 \neq R_2} \sum_{\alpha, \beta, \gamma, \delta = 1}^N Y_{R_1; R_2}^{\alpha \beta; \gamma \delta} \left[ U_{R\alpha \beta \gamma \delta ab} f_{R\alpha} f_{R\beta} f_{R\gamma} f_{R\delta} \right] \times \sum_{c, d = 1}^N U_{R\gamma \delta cd} f_{Rc} f_{Rd}. \]

Here the coefficients \( U_R \) are explicitly expressed in terms of the Gutzwiller variational parameters in Eqs. (47).

In terms of the notation introduced in Eq. (2) all of the above equations can be schematically represented as

\[ Z_{R\mu I} = \langle \Phi_R | \hat{O}_{R\mu} | \Phi_R \rangle - \sum_{cd} Z_{R\mu dc} [\Delta_{RR}]_{cd}. \]
Here the $\tilde{Z}_{R_{\alpha b}}$ are determined by the equations:

$$ (\Psi_0 | P_R^b O_{P_R} P_R f_{R_a} f_{R_b} | \Psi_0) = $$

$$ = (\Psi_0 | \sum_{cd} \tilde{Z}_{R_{\mu cd} f_{R_c} f_{R_d}} f_{R_a} f_{R_b} | \Psi_0) \ . $$

(52)

The explicit solution of the equation above is the following, see Appendix D.3.e

$$ \tilde{Z}_{\mu ab} = - \sum_{\gamma \delta} \left[ \frac{1}{(\gamma - \Delta_{RR}) \Delta_{RR}^c} \right]^{1/2}_{a c} \times $$

$$ \times (\Phi_R | \tilde{\Omega}_{R_{\mu}} \tilde{f}_{R_c} \tilde{f}_{R_d} | \Phi_R) \times \left[ \frac{1}{(\gamma - \Delta)} \Delta \right]^{1/2}_{b d} \ . $$

(53)

Within this strategy, the energy minimization problem amounts to calculate the saddle points of the following Lagrange function:

$$ \mathcal{L}_N \left( \{ D_R, E_R, F_R, G_R \}, \{ D^*_R, E^*_R, F^*_R, G^*_R \}, \{ R_R, S_R, T_R, U_R \}, \{ R^*_R, S^*_R, T^*_R, U^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \{ \lambda^b_{\alpha \beta 3} \}_{\alpha \beta 3} \right) = $$

$$ = \mathcal{L}_{QP} \left( \{ R_R, S_R \}, \{ R^*_R, S^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \mu, \Phi_0 \right) + $$

$$ + \mathcal{L}_{\text{Embed}} \left( \{ D_R, E_R, F_R, G_R \}, \{ D^*_R, E^*_R, F^*_R, G^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \lambda^b_{\alpha \beta 3}, \lambda_{R_{\alpha 2}}, \mu \right) + $$

$$ + \mathcal{L}_{\text{Mix}} \left( \{ D_R, E_R, F_R, G_R \}, \{ D^*_R, E^*_R, F^*_R, G^*_R \}, \{ R_R, S_R, T_R, U_R \}, \{ R^*_R, S^*_R, T^*_R, U^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \lambda^b_{\alpha \beta 3}, \lambda_{R_{\alpha 2}}, \mu \right) + $$

$$ + \mathcal{L}_{\text{HF}} \left( \{ T_R, U_R \}, \{ T^*_R, U^*_R \}, \{ \Delta_{R_{\alpha 2}} \}_{\alpha 2}, \mu \right) \ . $$

(54)

The explicit solution of the equation above is the following, see Appendix D.3.e

$$ \tilde{Z}_{\mu ab} = - \sum_{\gamma \delta} \left[ \frac{1}{(\gamma - \Delta_{RR}) \Delta_{RR}^c} \right]^{1/2}_{a c} \times $$

$$ \times (\Phi_R | \tilde{\Omega}_{R_{\mu}} \tilde{f}_{R_c} \tilde{f}_{R_d} | \Phi_R) \times \left[ \frac{1}{(\gamma - \Delta)} \Delta \right]^{1/2}_{b d} \ . $$

(53)

V. GUTZWILLER LAGRANGE FUNCTION

In the previous section we have expressed explicitly the total energy as a function of the variational parameters at the leading order of the $1/z$ and the $P_R^b P_R - I$ expansions.

Here we consider the problem of minimizing the variational energy with respect to the variational parameters $|\Psi_0\rangle$ and $\{\Phi_R\}$. To achieve this goal we need to take into account that: (1) the energy has to be minimized satisfying the constraints, (2) the renormalization coefficients $\{ R_R, S_R, T_R, U_R \}$ depend on the variational parameters non-linearly, see Eqs. (53), (36), (37) and (47). Following Refs. (15, 65, 68), these problems can tackled introducing Lagrange multipliers both for enforcing the Gutzwiller constraints (Eq. (23) as well as for promoting the coefficients $\{ R_R, S_R, T_R, U_R \}$ in Eqs. (53), (36), (37) and (47)) and $\{ \Delta_{R_{\alpha 2}} \}_{\alpha 2}$ to independent variables. Furthermore, we promote to independent variable the coefficients $\theta_{R_{\alpha 2}} = \{ \Phi_R \} C^\dagger_{R_{\alpha}} C_{R_{\beta}} | \Phi_R \rangle$.

Within this strategy, the energy minimization problem amounts to calculate the saddle points of the following Lagrange function:

$$ \mathcal{L}_N \left( \{ D_R, E_R, F_R, G_R \}, \{ D^*_R, E^*_R, F^*_R, G^*_R \}, \{ R_R, S_R, T_R, U_R \}, \{ R^*_R, S^*_R, T^*_R, U^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \{ \lambda^b_{\alpha \beta 3} \}_{\alpha \beta 3} \right) = $$

$$ = \mathcal{L}_{QP} \left( \{ R_R, S_R \}, \{ R^*_R, S^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \mu, \Phi_0 \right) + $$

$$ + \mathcal{L}_{\text{Embed}} \left( \{ D_R, E_R, F_R, G_R \}, \{ D^*_R, E^*_R, F^*_R, G^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \lambda^b_{\alpha \beta 3}, \lambda_{R_{\alpha 2}}, \mu \right) + $$

$$ + \mathcal{L}_{\text{Mix}} \left( \{ D_R, E_R, F_R, G_R \}, \{ D^*_R, E^*_R, F^*_R, G^*_R \}, \{ R_R, S_R, T_R, U_R \}, \{ R^*_R, S^*_R, T^*_R, U^*_R \}, \{ \lambda_{R_{\alpha 2}} \}_{\alpha 2}, \lambda^b_{\alpha \beta 3}, \lambda_{R_{\alpha 2}}, \mu \right) + $$

$$ + \mathcal{L}_{\text{HF}} \left( \{ T_R, U_R \}, \{ T^*_R, U^*_R \}, \{ \Delta_{R_{\alpha 2}} \}_{\alpha 2}, \mu \right) \ . $$

(54)
\[ H_{\text{embed}}^R = \sum_{\alpha \beta \delta} U_R^{\alpha \beta \gamma \delta} \hat{c}_{R\alpha}^\dagger \hat{c}_{R\beta}^\dagger \hat{c}_{R\gamma} \hat{c}_{R\delta} + \sum_{\alpha \beta} E_R^{\alpha \beta} \hat{c}_{R\alpha}^\dagger \hat{c}_{R\beta} + \sum_{\alpha \beta} \lambda_{R\alpha}^{\alpha \beta} \hat{f}_{R\alpha} \hat{f}_{R\beta} + \sum_{\alpha \beta} [D_{R\alpha}]_b \hat{c}_{R\alpha}^\dagger \hat{f}_{Rb} + \text{h.c.} \]

\[ + \sum_{\alpha \beta \gamma \delta} \left[ E_{R\alpha}^{\gamma \delta} \right]_d \hat{c}_{R\alpha}^\dagger \hat{c}_{R\beta} \hat{c}_{R\gamma} \hat{f}_{Rd} + \text{h.c.} \]
Hubbard model \[37–46, 70 \linebreak[1] \[15, 50, 60, 61, 66–68\]:

\[
H_{SB} = -t \sum_{\langle R, R' \rangle, \sigma = \pm} \left( c_{R \sigma}^\dagger c_{R' \sigma} + h.c. \right) + U \sum_R n_{R \uparrow} n_{R \downarrow}
\]

\[
+ V \sum_{\langle R, R' \rangle} n_R n_{R'} - J \sum_{\langle R, R' \rangle} \hat{S}_R \cdot \hat{S}_{R'} + \ 
\]

\[
+ X \sum_{\langle R, R' \rangle, \sigma = \pm} \left( c_{R \sigma}^\dagger c_{R' \sigma} + h.c. \right) \left( n_{R - \sigma} + n_{R' - \sigma} \right)
\]

\[
+ Y \sum_{\langle R, R' \rangle} \left( c_{R \uparrow}^\dagger c_{R' \downarrow}^\dagger c_{R' \uparrow} + h.c. \right) - \mu \sum_{R \sigma} n_{R \sigma},
\]

where \( \langle R, R' \rangle \) denotes nearest neighbors \( R \) and \( R' \). In the next section we will write the single-band Hubbard model Gutzwiller Lagrange function, assuming translational invariance.

For clarity, here we briefly review the definitions outlined above in relation with the notation utilized in previous work \[26, 50 \linebreak[1] 60\]. We consider the projector \[15, 50, 60 \linebreak[1] 61, 65, 68\]:

\[
\Lambda_R = \begin{pmatrix}
    a_{00} & 0 & 0 & 0 \\
    0 & a_{\uparrow 0} & 0 & 0 \\
    0 & 0 & a_{0 \downarrow} & 0 \\
    0 & 0 & 0 & g
\end{pmatrix},
\]

which we assume does not depend on \( R \) as we have assumed that translational invariance is preserved. Here the basis set we use is:

\[
\left\{ |\Gamma_R \rangle \right\} = \{ |0 \rangle, |\uparrow \rangle, |\downarrow \rangle, |\uparrow \downarrow \rangle \},
\]

\[
\left\{ |n_R \rangle \right\} = \{ |0 \rangle, |\uparrow \rangle, |\downarrow \rangle, |\uparrow \downarrow \rangle \}.
\]

We now assume that \( F_R^0 \) (with respect to the same basis set) is given by \[15, 50 \linebreak[1] 60 \linebreak[1] 61, 65, 68\]:

\[
F_R^0 = \begin{pmatrix}
    (1 - n_\uparrow) & (1 - n_\downarrow) & 0 & 0 \\
    0 & n_\uparrow & (1 - n_\downarrow) & 0 \\
    0 & 0 & n_\downarrow & (1 - n_\uparrow) \\
    0 & 0 & 0 & n_\uparrow n_\downarrow
\end{pmatrix},
\]

which we assume does not depend on \( R \) as we have assumed that translational invariance is preserved. Following Kotliar and Ruckenstein \[26\] we define the matrix of slave boson amplitudes \[15, 50 \linebreak[1] 60 \linebreak[1] 61, 65, 68\]:

\[
\phi_R = \begin{pmatrix}
    c & 0 & 0 & 0 \\
    0 & p_\uparrow & 0 & 0 \\
    0 & 0 & p_\downarrow & 0 \\
    0 & 0 & 0 & d
\end{pmatrix} = \Lambda_R \sqrt{F_R^0}.
\]

**B. Gutzwiller Lagrange function**

Following our derivations in Section \[\Box\] the single band Gutzwiller Lagrange function is given by:

\[
\mathcal{L}_N \left( \{D_\sigma, E_\sigma, F_\sigma, G\}, \{D_\sigma^*, E_\sigma^*, F^*, G^*\}, \{R_\sigma, S_\sigma, T_\sigma, U\}, \{R_\sigma^*, S_\sigma^*, T^*, U^*\} \right)
\]

\[
\lambda_\sigma, \lambda_\sigma^{(n,n)}, \lambda_\sigma^b, \Delta_\sigma, \Delta_\sigma^{(n,n)}, o_\sigma, E, \mu, |\Psi_0\rangle, |\Phi\rangle
\]

\[
= \mathcal{L}_{QP} \left( \{R_\sigma, S_\sigma\}, \{R_\sigma^*, S_\sigma^*\}, \lambda_\sigma, E, \mu, |\Psi_0\rangle \right) = \ 
\]

\[
+ \mathcal{L}_{Embed} \left( \{D_\sigma, E_\sigma, F_\sigma, G\}, \{D_\sigma^*, E_\sigma^*, F^*, G^*\}, E^c, \lambda_\sigma^b, \Delta_\sigma, |\Phi\rangle \right) + \ 
\]

\[
+ \mathcal{L}_{Mix} \left( \{D_\sigma, E_\sigma, F_\sigma, G\}, \{D_\sigma^*, E_\sigma^*, F^*, G^*\}, \{R_\sigma, S_\sigma, T_\sigma, U\}, \{R_\sigma^*, S_\sigma^*, T^*, U^*\}, \lambda_\sigma, \lambda_\sigma^{(n,n)}, \lambda_\sigma^b, \Delta_\sigma^{(n,n)}, o_\sigma \right) + \ 
\]

\[
+ \mathcal{L}_{HF} \left( \{T_\sigma, U\}, \{T^*, U^*\}, \Delta_\sigma^{(n,n)}, o_\sigma \right).
\]

Where:

\[
\mathcal{L}_{QP} \left( \{R_\sigma, S_\sigma\}, \{R_\sigma^*, S_\sigma^*\}, \lambda_\sigma, E, \mu, |\Psi_0\rangle \right) = \ 
\]

\[
= |\Psi_0\rangle - t \sum_{\langle R'R \rangle \sigma} R_\sigma R_{R'}^\dagger f_{R_\sigma_R}^\dagger f_{R'_{\sigma'}} + \left[ X \sum_{\langle R'R \rangle \sigma} S_\sigma R_{R'}^\dagger f_{R_\sigma_R}^\dagger f_{R'_{\sigma'}} + h.c. \right] + \ 
\]

\[
+ \sum_{\langle RR' \rangle \sigma} \lambda_\sigma^{(n,n)} f_{R_\sigma_R}^\dagger f_{R'_{\sigma'}} + \sum_{R \sigma} \lambda_\sigma^b f_{R_\sigma_R}^\dagger f_{R_\sigma_R} - \mu \sum_{R \sigma} f_{R_\sigma_R}^\dagger f_{R_\sigma_R} |\Psi_0\rangle + E \left( 1 - (|\Psi_0\rangle |\Psi_0\rangle) + \mu N \right.
\]

\[
+ \mathcal{L}_{Embed} \left( \{D_\sigma, E_\sigma, F_\sigma, G\}, \{D_\sigma^*, E_\sigma^*, F^*, G^*\}, E^c, \lambda_\sigma^b, \Delta_\sigma, |\Phi\rangle \right) = \langle \Phi | H_{Embed} |\Phi\rangle + E^c \left( 1 - (|\Phi\rangle |\Phi\rangle) \right),
\]
\[ H_{\text{embed}} = U| \hat{c}_i \rangle \langle \hat{c}_i | + \sum_{\sigma} \lambda^c_{\sigma} f_{\sigma}^\dagger f_{\sigma}^\ast + \left[ \sum_{\sigma} D_{\sigma} c_{\sigma}^\dagger f_{\sigma}^\ast + \text{h.c.} \right] + \left[ \sum_{\sigma} E_{\sigma} c_{\sigma}^\dagger \hat{c}_\sigma f_{\sigma}^\ast + \text{h.c.} \right] + \sum_{\sigma a} F_{\sigma a} \left( c_{\sigma a}^\dagger f_{\sigma}^\ast f_{\sigma}^\dagger - c_{\sigma a}^\dagger c_{\sigma a} \Delta_{\sigma a} \right) + \left[ G \left( c_{\sigma}^\dagger f_{\sigma}^\ast f_{\sigma}^\dagger + \text{h.c.} \right) + \sum_{\sigma} \lambda^b_{\sigma} c_{\sigma}^\dagger \hat{c}_\sigma, \right] \tag{74} \]

\[ \mathcal{L}_{\text{Mix}} \left( \{ D_{\sigma}, E_{\sigma}, F_{\sigma a}, F, G \}, \{ D_{\sigma}^\ast, E_{\sigma}^\ast, F^\ast, G^\ast \}, \{ R_{\sigma}, S_{\sigma}, T_{\sigma a}, T, U \}, \{ R_{\sigma}^\ast, S_{\sigma}^\ast, T^\ast, U^\ast \} \right), \lambda_{\sigma}, \lambda^{(n.n.)}_{\sigma}, \lambda^c_{\sigma}, \Delta_{\sigma}, (\Delta^{(n.n.)}_{\sigma}, o_{\sigma}) \]

\[ = - \sum_{\sigma} \left( \lambda_{\sigma} + \lambda_{\sigma}^c \right) \Delta_{\sigma} - \sum_{\sigma} \lambda^{(n.n.)}_{\sigma} \Delta^{(n.n.)}_{\sigma} - \sum_{\sigma} \lambda^{b}_{\sigma} o_{\sigma} - \sum_{\sigma} \left[ D_{\sigma} \left( R_{\sigma} \sqrt{1 - \Delta_{\sigma}} \Delta_{\sigma} \right) + \text{c.c.} \right] - \sum_{\sigma a} F_{\sigma a} (1 - \Delta_{a}) \Delta_{a} T_{\sigma a} - \left[ F \sqrt{(1 - \Delta_{T})} \Delta_{T} \sqrt{(1 - \Delta_{T})} \Delta_{T} + \text{c.c.} \right] - \left[ G \sqrt{(1 - \Delta_{T})} \Delta_{T} U \sqrt{(1 - \Delta_{T})} \Delta_{T} + \text{c.c.} \right], \tag{75} \]

In Appendix \( \text{G} \) we show that, for this single-band problem, it is possible to reduce the problem of extremizing the Lagrange function \( \mathcal{L} \) to the problem of minimizing the Gutzwiller energy as a function of the double occupancy \( \eta \equiv d^2 \).

### C. Mott gap: first benchmark

Here we consider the extended single-band Hubbard model, see Eq. \((66)\), for an arbitrary Bravis lattice (e.g., square, cubic, triangular, body centered cubic (BCC), face centered cubic (FCC)). We define \( z \) the number of nearest neighbors to each site and \( \Delta^{(n.n.)} \equiv \langle \Psi_0 | c_{\vec{R}_a}^\dagger c_{\vec{R} \sigma} | \Psi_0 \rangle \equiv \chi \), where \( R \) and \( R' \) are nearest neighbors.

As a first benchmark of our theory, in this subsection we calculate the Mott gap (defined as the jump in chemical potential across the Mott transition) and compare our results with Ref. [81]. As shown in Appendix \( \text{G} \) extremizing Eq. \((71)\), we obtain that the Mott gap is given by:

\[ \Delta \mu = \tilde{U} \sqrt{1 - \frac{\tilde{U}_c}{\tilde{U}}}, \tag{77} \]

where

\[ \tilde{U} = U + 12 J z \chi^2 \]
\[ \tilde{U}_c = 16 \chi (1 - X). \tag{78} \]

We note that Eq. \((77)\) reduces to the result of Ref. [81] for the standard Hubbard model when we set the intersite interactions to zero, where, by definition, \( \tilde{U} = U \) and \( \tilde{U}_c = U_c \).

### D. Extended Hubbard model: half filling

To assess the influence of inter-site interactions on the Mott physics, in this subsection we study the Hamiltonian in Eq. \((66)\) at half filling. As mentioned above, we will focus exclusively on the normal phase, i.e., we will not consider phases such as superconductivity, spin density wave (SDW) or charge density wave (CDW). Note that, because we are at half filling in the normal phase, we have that \( n_\uparrow = n_\downarrow = \frac{1}{2} \).

As shown in Appendix \( \text{G} \) for this system we obtain following operator equivalences:

\[ P^\dagger_{R \sigma} c_{R \sigma} P_R \sim 2 \sqrt{2 \eta (1 - 2 \eta)} c_{R \sigma} \]
\[ P^\dagger_{R \sigma} n_{R \sigma} P_R \sim 4 \eta m_R + (1 - 4 \eta) I \]
\[ P^\dagger_{R \sigma} c_{R \sigma}^\dagger c_{R \sigma} P_R \sim 4 \eta c_{R \sigma}^\dagger c_{R \sigma} \]
\[ P^\dagger_{R \sigma} \tilde{S}_R P_R \sim 2 (1 - 2 \eta) \tilde{S}_R \]
\[ P^\dagger_{R \sigma} n_{R \sigma} c_{R \sigma} P_R \sim 2 \sqrt{2 \eta (1 - 2 \eta)} c_{R \sigma}^\dagger. \tag{79} \]
This leads to the result that extremizing Eq. (71) amounts to minimize the following energy function of the local double occupancy $\eta \equiv d^2$:

$$
\langle H \rangle = \eta^2 \left[ 32 (t-X) z \chi - 16 (V-Y) z \chi^2 - 12 z J \chi^2 \right] + \eta \left[ -16 (t-X) z \chi + 12 z J \chi^2 + U \right] + \frac{1}{2} V z - 3 z J \chi^2 - \mu_{1/2}. 
$$

Here $\mu_{1/2}$ is the chemical potential needed to enforce that the system is at half filling. For simplicity, from now on we will assume that $J = 0$, as typically $J \ll t - X, V - Y, U$.

In Fig. (1) we show the phase diagram of this system, which is conveniently expressed in terms of the following dimensionless quantities:

$$
u = \frac{U}{16 (t-X) z \chi}, \quad v = \frac{16 (V-Y) z \chi^2}{16 (t-X) z \chi}. 
$$

Consistently with the fact that our theory reduces to the ordinary GA in the limit of vanishing intersite interactions, at $v = 0$ we recover the Brinkman Rice transition [12], where $\eta = 0$ (i.e., the charge fluctuations are frozen) for all $u \geq 1$. More generally the Brinkman Rice phase occurs when $u > 1$ and $v < 2u$.

1. Metallic phase: enhanced-valence crossover

Minimizing the energy function [Eq. (80)] it can be readily shown that for $u < 1$ and $v < v_c = 1 + u$ the system remains metallic and that, in this phase, the double occupancy is given by:

$$
\eta = \frac{1 - u}{4 (1 - v/2)}.
$$

Eq. (82) shows that the intersite Coulomb interaction can enhance dramatically charge fluctuations. In particular, we note that $\eta$ can even exceed $\frac{1}{4}$ for $v_c > v > 2u$ while this is impossible in the half-filled single-band Hubbard model with only local Hubbard repulsion. The points where $\eta = \frac{1}{4}$, which here we refer to as the "enhanced-valence crossover," are marked by a dotted line in Fig. (1).

2. Valence-skipping phase

Remarkably, we find that the non-local Coulomb interaction can induce a phase transition into a phase with double occupancy $\eta = \frac{1}{2}$, which is stable for $v > 1 + u$ and $v > 2u$.

In this work we refer to this region as the "valence-skipping phase". For $v > 2$ there is a first order phase transition between the Brinkman Rice phase [12] and the valence skipping phase while for $v < 2$ there is a second order phase transition between the metallic phase and the valence skipping phase. $(u, v) = (1, 2)$ is a multicritical point.

It is insightful to compare our phase diagram with the DMFT+GW study in Fig. (5) of Ref. [37], where CDW and SDW symmetry breaking was allowed. We observe that the main qualitative difference with respect to our phase diagram is that in Ref. [37] at large $v$ the valence skipping phase is replaced by a charge ordered-phase, while the Brinkman Rice phase is replaced by a spin-ordered phase. The valence-skipping phase can be interpreted as the normal-phase precursor of the CDW [37] [38].
E. Quasiparticle dispersion

In this Section we restore \( J \neq 0 \). We have that the quasiparticle dispersion is given by (see Appendix A):

\[
H_{QP} = \sum_{\langle R, R' \rangle, \sigma} c_{R\sigma}^\dagger c_{R'\sigma} [-8\eta (1 - 2\eta) (t - X) \nonumber
- (3(1 - 2\eta)^2 J + 16\eta^2 (V - Y)) \chi] \nonumber
- Z \sum_{\langle R, R' \rangle, \sigma} c_{R\sigma}^\dagger c_{R'\sigma} + \Delta t \sum_{\langle R, R' \rangle, \sigma} c_{R\sigma}^\dagger c_{R'\sigma},
\]

where

\[
Z = 8\eta (1 - 2\eta) \nonumber
X = -3(1 - 2\eta)^2 \frac{J}{t} + 16\eta^2 \frac{(V - Y)}{t} \chi.
\]

Now we follow \[15, 20\] and write

\[
G = \frac{Z}{i\omega_n - Z\varepsilon(k) + \Delta\varepsilon(k) + \mu_{1/2}} \nonumber
= \frac{1}{i\omega_n - \varepsilon(k) + \mu_{1/2} - \Sigma(k, \omega)},
\]

where \( \mu_{1/2} \) is the chemical potential at half filling for the quasiparticle Hamiltonian, so that:

\[
\Sigma(k, \omega_n) = -\frac{\Delta}{Z} \varepsilon(k) + \mu_{1/2} + i\omega_n \left[ 1 - \frac{1}{Z} \right] - \frac{\mu_{1/2}}{Z}.
\]

We note that, consistently with previous GW+DMFT studies of the two dimensional extended Hubbard model \[37, 38\], the self energy is a function of both momentum and frequency.

VII. CONCLUSIONS

In this work we have introduced a new method to study the GA for a broad class of multi-band extended Hubbard Hamiltonians with two site interactions by combing the large \( z \) and the \( P_R^1 P_R - I \) expansions. We have presented the final result in terms of a Gutzwiller Lagrange function valid for multi-band Hubbard models. Using this formalism, we have have studied the single band extended Hubbard model, showing that this method is highly practical and leads to new qualitative results. In particular, we have recovered a Brinkman-Rice transition \[12\] for the extended Hubbard model and observed that a valence skipping phase emerges for large intersite interactions. Our work can enable a more refined treatment of intersite interactions in the ab-initio calculations. In the future this may lead to parameter free theories of realistic solids and molecules.

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Appendix A: \( P_R^1 P_R - I \) expansion

In this Appendix we will describe the \( P_R^1 P_R - I \) expansion used in Section III and use it to derive Eq. \[5\] at leading order in the \( P_R^1 P_R - I \) expansion. We will focus on the case of the two point operator, though higher point operators may be handled similarly. Corrections to Eq. \[5\] appear as higher order terms in the \( P_R^1 P_R - I \) expansion parameter \( x \), which we now introduce through the following relation:

\[
P_R^1 P_R \equiv I + x \left( P_R^1 P_R - I \right) \equiv I + x \Theta_R.
\]

The correct value of \( x \) is given by \( x = 1 \), but we will treat \( x \) as a small parameter; which stems from the physical assumption that all the eigenvalues of \( \Theta_R \ll 1 \). As such we will drop all terms proportional to any positive power of \( x \).

1. The case with two sites

Consider the simplest case where the system is composed of just two sites \( R \) and \( R' \). In this case we have that:

\[
\frac{\langle \Psi | O_R O_{R'} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\langle \Psi_0 | P_R^1 O_R P_R^1 O_{R'} | \Psi_0 \rangle}{\langle \Psi_0 | P_R^1 P_R^1 O_R O_{R'} | \Psi_0 \rangle} \nonumber
= \frac{\langle \Psi_0 | P_R^1 O_R P_R^1 O_{R'} | \Psi_0 \rangle}{\langle \Psi_0 | P_R^1 O_R P_R^1 O_{R'} | \Psi_0 \rangle}
\]

where

\[
\mathcal{D} = 1 + x \langle \Psi_0 | \Theta_R | \Psi_0 \rangle
+ x \langle \Psi_0 | \Theta_{R'} | \Psi_0 \rangle + x^2 \langle \Psi_0 | \Theta_R \Theta_{R'} | \Psi_0 \rangle.
\]

We see that

\[
\frac{\langle \Psi | O_R O_{R'} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \approx \langle \Psi_0 | P_R^1 O_R P_R^1 O_{R'} | \Psi_0 \rangle
\]

with corrections being order \( x \) or higher. It is not too hard to see that this is still true in the general case of many sites. Indeed any terms not in the form of the right hand side of Eq. \[A4\] in the expansion of \( \frac{\langle \Psi | O_R O_{R'} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \), both in the denominator and the numerator, come with positive powers of \( x \), and therefore are neglected in the \( P_R^1 P_R - I \) approximation.
Appendix B: 1/z scaling

1. 1/z Scaling for a single particle

As a first step to understand the various terms that enter the Gutzwiller energy function in Eq. (2), we will consider the single particle Hamiltonian in the limit of large dimensions. We will follow closely [10]. We will show that:

\[ t_n^{α,β} \sim \frac{1}{z^{n/2}} \]
\[ \langle \Psi_0 | f_{R_α}^1 f_{R_β}^b | \Psi_0 \rangle \sim \frac{1}{z^{n/2}}. \]  

(B1)

For simplicity we assume a hypercubic lattice. Here \( n \) is the Manhattan distance between \( R \) and \( R' \). Where the Manhattan distance, \( D(R, R') \), is the shortest distance between two points \( R \) and \( R' \) that can be travelled by a particle that can only move on the edges of the hypercubic lattice.

For simplicity we will consider a spinless, single band, tight binding Hamiltonian on the hypercubic lattice (orbital and spin degrees may be added straightforwardly):

\[ H = -\sum_{R \neq R'} t_{RR'} c_{R}^\dagger c_{R'} + h.c. \]  

(B2)

Let's decompose the Hamiltonian into pieces with equal Manhattan distance:

\[ H = -\sum_{n=1}^{\infty} \sum_{D(R, R') = n} t_n c_{R}^\dagger c_{R'} + h.c. \equiv H_n \]  

(B3)

The eigenvalues of the Hamiltonian \( H_n \) are given by:

\[ E_n (k_1, k_2, \ldots, k_d) = -t_n \sum_{P_n} \left[ \exp (i \vec{P}_n \cdot \vec{k}) + \exp (-i \vec{P}_n \cdot \vec{k}) \right] \]
\[ = -t_n \sum_{P_n} E_{P_n} (\vec{k}) \]  

(B4)

Here the \( P_n \) are all the Manhattan paths of total length \( n \) with distinct endpoints (we choose only one path for each endpoint) and \( \vec{P}_n \) is the vector displacement of the Manhattan path (note we are grouping path \( \vec{P}_n \) and \( -\vec{P}_n \) together to obtain a real value for the energy). It is not too hard to see that there are:

\[ 2^{n-1} \binom{d+n-1}{n} \equiv \mathcal{N}(n) \sim z^n \]  

(B5)

such paths. We now have that:

\[ \int \frac{d^d k}{(2\pi)^d} E_{P_n} (\vec{k}) = 0 \]
\[ \int \frac{d^d k}{(2\pi)^d} E_{P_n} (\vec{k}) E_{P_n}^* (\vec{k}) = 2\delta_{P_n, P_n^\dagger} \]  

(B6)

Therefore by the central limit theorem we have that the energy has a distribution given by:

\[ \mathcal{P}_n (E) \equiv \int \frac{d^d k}{(2\pi)^d} \delta \left( -t_n \sum_{P_n} E_{P_n} (\vec{k}) - E \right) \]
\[ \equiv \frac{1}{\mathcal{Z}} \exp \left( -t_n^2 \mathcal{N}(n) \cdot E^2 \right) \]  

(B7)

Here \( \mathcal{Z} \) is a normalization constant. We now demand that \( \mathcal{P}_n (E) \) be independent of \( z \) in which case we must have that:

\[ t_n \sim \frac{1}{\sqrt{\mathcal{N}(n)}} \sim \frac{1}{z^{n/2}} \]  

(B8)

We now have that:

\[ \int_{-\infty}^0 E \cdot \mathcal{P}_n (E) = \langle H_n \rangle \sim 1 \]  

(B9)

We further have that

\[ \langle H_n \rangle = -t_n \cdot 2 \cdot \mathcal{N}(n) \cdot \langle \Psi_0 | c_{R}^\dagger c_{R'} | \Psi_0 \rangle \sim 1 \]  

(B10)

This means that:

\[ \langle \Psi_0 | c_{R}^\dagger c_{R'} | \Psi_0 \rangle \sim \frac{1}{z^{n/2}} \]  

(B11)

from which Eq. (B1) follows. Below we use these results to show how the various terms in the main Hamiltonian in Eq. (2) scale.

2. Scaling of operator expectation values

We will consider the large co-ordination number, large \( z \), approximation. As a first step towards obtaining the results in Appendices [B3] and [C1] (which present key results needed in the main text in Section [IV]), we calculate the scaling of various operators in the large \( z \) limit. We will also only take the leading order in the \( P_R^b P_R - I \) expansion.

a. Scaling fermionic operators

We now used Wick’s theorem to obtain the scaling for the expectation values of various terms in Eq. (2). Let's assume that the Hamiltonian contains \( J_{R_α R_β} O_{R_α} O_{R_β^\dagger} \), with \( O_{R_α} \) and \( O_{R_β^\dagger} \) fermionic, then we know that the lowest order contribution to \( \langle J_{R_α R_β^\dagger} (\Psi) | O_{R_α} O_{R_β^\dagger} | \Psi \rangle / \langle \Psi | \Psi \rangle \) may be written as:

\[ J_{R_α R_β} \int \langle \Psi | O_{R_α} O_{R_β^\dagger} | \Psi \rangle / \langle \Psi | \Psi \rangle \]
\[ \sim J_{R_α R_β} \sum_{\alpha \beta=1}^{\cal N} Z_{\alpha}^{\dagger} Z_{\beta} \langle \Psi_0 | f_{R_α}^1 f_{R_β}^b | \Psi_0 \rangle \]
\[ \sim J_{R_α R_β} \frac{1}{z^{n/2}}. \]  

(B12)
Here we have used the operator equivalences in Section IV. Now there $N(n) \sim z^n$ such terms (see Appendix B1) so we have the total contribution for such terms scales as:

$$\sim J^{\mu\nu}_{R;R'} \cdot \frac{1}{z^{n/2}} \cdot z^n \sim 1. \quad (B13)$$

In which case we have that:

$$J^{\mu\nu}_{R;R'} \sim \frac{1}{z^{n/2}}. \quad (B14)$$

b. Scaling Bosonic operator that changes fermion number by two

Lets assume that the Hamiltonian contains $J^{\mu\nu}_{R;R'} O_{R_0} O_{R'_0}$, with $O_{R_0}$ and $O_{R'_0}$, bosonic and changing fermion number by two, then we know that the lowest order contribution to $J^{\mu\nu}_{R;R'} \langle \Psi | O_{R_0} O_{R'_0} | \Psi \rangle / \langle \Psi | \Psi \rangle$ may be written as:

$$J^{\mu\nu}_{R;R'} \langle \Psi | O_{R_0} O_{R'_0} | \Psi \rangle / \langle \Psi | \Psi \rangle \sim J^{\mu\nu}_{R;R'} \sum_{a,b,c,d=1}^N \bar{Z}_{\mu ac} \bar{Z}_{\nu bc} \langle \Psi_0 | f_{Ra} f_{R'b} | \Psi_0 \rangle \times$$

$$\times \langle \Psi_0 | f_{R_c} f_{R'd} | \Psi_0 \rangle \sim J^{\mu\nu}_{R;R'} \cdot \frac{1}{z^n}. \quad (B15)$$

Now there $N(n) \sim z^n$ such terms, so we have the total contribution for such terms scales as:

$$\sim J^{\mu\nu}_{R;R'} \cdot \frac{1}{z^n} \cdot z^n \sim 1. \quad (B16)$$

In which case we have that:

$$J^{\mu\nu}_{R;R'} \sim 1. \quad (B17)$$

c. Scaling Bosonic operator that does not change fermion number

Hartree Term  Let's assume that the Hamiltonian contains $J^{\mu\nu}_{R;R'} O_{R_0} O_{R'_0}$, with $O_{R_0}$ and $O_{R'_0}$, bosonic and fermion number conserving, then we know that the lowest order, Hartree term for $J^{\mu\nu}_{R;R'} \langle \Psi | O_{R_0} O_{R'_0} | \Psi \rangle / \langle \Psi | \Psi \rangle$ may be written as:

$$J^{\mu\nu}_{R;R'} \langle \Psi | O_{R_0} O_{R'_0} | \Psi \rangle / \langle \Psi | \Psi \rangle \sim J^{\mu\nu}_{R;R'} \langle \Psi_0 | P_{R_0} P_R | \Psi_0 \rangle \langle \Psi_0 | P_{R'_0} P_{R'} | \Psi_0 \rangle \sim J^{\mu\nu}_{R;R'} \quad (B18)$$

Now there $N(n) \sim z^n$ such terms so we have the total contribution for such terms is:

$$\sim J^{\mu\nu}_{R;R'} \cdot z^n \sim 1. \quad (B19)$$

In which case we have that:

$$J^{\mu\nu}_{R;R'} \sim \frac{1}{z^n} \quad (B20)$$

Fock term  The scaling of the Fock term may be given by:

$$J^{\mu\nu}_{R;R'} \langle \Psi | O_{R_0} O_{R'_0} | \Psi \rangle / \langle \Psi | \Psi \rangle \sim J^{\mu\nu}_{R;R'} \sum_{a,b,c,d=1}^N \bar{Z}_{\mu ac} \bar{Z}_{\nu bc} \langle \Psi_0 | f_{Ra} f_{R'b} | \Psi_0 \rangle \times$$

$$\times \langle \Psi_0 | f_{R_c} f_{R'd} | \Psi_0 \rangle \sim J^{\mu\nu}_{R;R'} \cdot \frac{1}{z^n} \cdot z^n \sim \frac{1}{z^n} \to 0. \quad (B21)$$

Now there $N(n) \sim z^n$ such terms so we have the total contribution for such terms is:

$$\sim J^{\mu\nu}_{R;R'} \cdot \frac{1}{z^n} \cdot z^n \sim \frac{1}{z^n} \to 0. \quad (B22)$$

This means that the Fock term is highly suppressed, however we still are able to keep its effects in the Gutzwiller Lagrange function in Eq. (54).

d. Discussion

We would like to note that these scaling arguments are very interesting from a formal and theoretical point of view, but need to be significantly modified for the case of realistic extended Hubbard model Hamiltonians. For example, the coefficients in $V_{R_1;R_2}$ which are proportional to a Coulomb mediated density density interaction scale as $\sim 1/\sqrt{n}$ which is not $z$ dependent, which is markedly different then Eq. (B20). We note that the reason for the square root in the previous formula is that for $z \gg n$ the typical Manhattan path makes $n - 1$ turns in different directions. Furthermore our scaling analysis shows that the order of magnitude of the density density terms is the same as those for spin spin interactions, all $V_{R_1;R_2}$ scale the same way with $z$. However because one term involves the overlap between electron wavefunctions on different sites while the other doesn’t; as such the spin spin interaction is exponentially suppressed with distance while the density density is not. This is true even though the exponent has nothing to do with the coordination number $z$. This is true even though the overlap between electron wavefunctions on different sites is exponentially decaying with distance which is given by the overlap of various Wannier functions. As such, realistic Hamiltonians do not scale exactly as in the limit that $z \to \infty$. More precisely, as the various terms in $J^{\mu\nu}_{R;R'}$, $J^{\mu\nu}_{R;R'}$, and $J^{\mu\nu}_{R;R'}$ do not follow the scaling needed for a rigorous $1/z$ expansion in realistic materials. As such we will scale each different type of term separately and maintain only leading order term or terms in the $1/z$ expansion for each type of interaction. More explicitly the terms we keep in the equivalences in Eqs. (31), (36), (37).
and (47) are leading order for each individual term in the Hamiltonian in Eq. (1). We note that in Eqs. (36), (37) we keep both the Hartree and the Fock terms, despite the fact that the Fock terms are subleading. This is done because the bosonic fermion number conserving terms in the Hamiltonian in Eq. (1) are usually the biggest terms as in many cases they do not involve overlaps of Wannier functions on different sites and as such must be handled as carefully as possible. Furthermore the Hartree term is handled exactly by our formalism (see Appendix D3b) so no corrections to the Hartree term effect the precision to which the Fock terms may be handled.

3. Leading order in $1/z$ terms for Gutzwiller (failure of Eq. (5) without additional assumptions besides large co-ordination number)

a. Manhattan path example

In this section we will motivate the need for the $P_R^1 P_R - I$ expansion used in Section III. We show that already at leading order Eq. (5) fails without additional assumptions, besides the Gutzwiller constraints and the $1/z$ expansion, for the extended GA presented in the main text. In particular, the usual arguments [15, 60, 61, 66–68] about the validity of Eq. (5) based on the Gutzwiller constraints in Eq. (4) and the large co-ordination limit, which work for the regular Hubbard model, fails without additional assumptions, such as the $P_R^1 P_R - I$ expansion. We now consider the pair hopping terms — those that change the particle number by two. We show that already at leading order for these terms Eq. (5) fails without additional assumptions, as we need terms where we insert projectors of the form $P_R^1 P_R$ at various sites to obtain the correct expectation value for the left hand side of Eq. (5) to make the equality true even at leading order. Indeed, if we take the pair hopping operator $J^{\mu\nu}_{R_1 R_2} O_{R_1 \mu} O_{R_2 \nu}$ and consider any Manhattan path between $R_1$ and $R_2$: $P_{R_1} P_{R_2}$. Then for every Manhattan path $P_{R_1} P_{R_2}$ we may insert an arbitrary number of operators $P_{R_i} P_{R_j}$ at any set of sites (with at most one insertion per site) along this path with and obtain an operator:

$$J^{\mu\nu}_{R_1 R_2} [P_{R_1}^1 O_{R_1 \mu} P_{R_1}^1] \prod_i P_{R_i}^1 P_{R_i} [P_{R_2}^1 O_{R_2 \nu} P_{R_2}^1].$$ (B23)

We now contract the operators along the Manhattan path with nearest neighbors being contracted with each other (two contractions per neighbor) and obtain a term on the left hand side of Eq. (5) which is of the same order of magnitude as the terms on the right hand side in Eq. (5), but not included on the right hand side (as such the equation fails). This is pictured in Fig. (2). We see that Eq. (5) fails even in the large coordination limit without additional assumptions. In Section III we make such an assumption: the $P_R^1 P_R - I$ expansion.

b. Tadpole example

We notice that the example presented in Section B3a does not apply for nearest neighbor sites. Here we will show that, using just the $1/z$ expansion, the Fock terms in Eq. (40) have the same scaling in $1/z$ as additional multisite terms not considered on the right hand side in Eq. (5) but needed for the left hand side, making an additional assumption, such as the $P_R^1 P_R - I$ expansion, necessary for Eq. (5) to be true for them. We now assume that $P_{R_1} O_{R_1} P_{R_1}$ and $P_{R_2} O_{R_2} P_{R_2}$ are operators on nearest neighbor sites which conserve fermion number. We again consider Eq. (5) for these operators. We now consider site $R_3$ which is a nearest neighbor of site $R_1$ where there are four contractions between $P_{R_1} O_{R_1} P_{R_1}$ and $P_{R_3} O_{R_3} P_{R_3}$ on the right hand side of Eq. (5). This term scales as $\sim 1/z^2$ and there are $\sim z$ such terms which means that the total scaling of such terms is $\sim z \times 1/z^2 \sim 1/z$ which means that it has the same scaling as any Fock term on the right hand side of Eq. (5). This is true for both for bosonic fermion number conserving operators and bosonic fermion number changing operators (in the case of superconductivity, not considered in this work). As such an additional assumption such as the $P_R^1 P_R - I$ expansion is mandatory for those terms even for nearest neighbors. This is illustrated in Fig. (2).

Appendix C: Towards ab initio research

In order to perform true ab initio research one needs to deal with all of the terms in Eq. (1), not just the one and two site terms as in Eq. (7) studied in the main text. In this Appendix we outline a method to do just that.
1. The need for three Wick’s contractions for calculating expectation values with three and four point operators

As a first step towards handling three and four site terms, we will describe why the treatment presented in the main text fails for them.

\[
\mathcal{L}_{HF} \left( \{ R_R, T_R, U_R \} \right) = \mathcal{L}_{HF} (\{ R_R, T_R, U_R \} ) + \mathcal{L}_{HF} (\{ \Delta_R, \Delta_R \} )
\]

\[
= \sum_{R_1 \neq R_2} V^{\alpha \beta \gamma \delta}_{R_1 R_2} o_{\alpha \beta} o_{\gamma \delta} + \sum_{R_1 \neq R_2} \sum_{\alpha \beta} \sum_{\gamma \delta} \sum_{abcd} V^{\alpha \beta \gamma \delta}_{R_1 R_2} \left( \Delta_{R_1 R_2} \right)_{ac} \left( \Delta_{R_1 R_2} \right)_{db} \left( T^\beta_{R_1 \alpha} \right)_{ba} \left( T^\gamma_{R_2 \delta} \right)_{cd} + \nonumber
\]

\[
+ \sum_{R_1 \neq R_2} \sum_{\alpha \beta} \sum_{\gamma \delta} \sum_{abcd} \left( \Delta_{R_1 R_2} \right)_{ad} \left( \Delta_{R_1 R_2} \right)_{bc} - \left( \Delta_{R_1 R_2} \right)_{ac} \left( \Delta_{R_1 R_2} \right)_{bd} \left[ U_{R \alpha \beta} \right]_{ab} \left[ U^*_{R \gamma \delta} \right]_{cd} + \nonumber
\]

\[
+ \sum_{R_1 \neq R_2 \neq R_3} \sum_{\alpha \beta} \sum_{\gamma \delta} \sum_{abcd} \left( \Delta_{R_1 R_2 R_3} \right)_{ab} \left( R_{R_2} \right)_{a} \left( R^*_R \right)_{b} \left( R_{R_3} \right)_{a} o_{R_1 \alpha \beta}.
\]

(a. Three site terms)

Fock contribution  We would like to show an example of the need for three fermion contractions to evaluate the expectation value of the Hamiltonian in Eq. (1) for three point operators, even in leading order in the $1/z$ expansion and the $P_{P_R} P_R - I$ expansion. Consider two single fermion operators and one bosonic operator on three neighbor sites such that $R_2$ (fermionic site) is the nearest neighbor of both $R_1$ (fermionic site) and $R_3$ (bosonic site). We will consider the terms \[
\sum_{R_1 \neq R_2 \neq R_3} \sum_{R_{R_2}} V^{\alpha \beta \gamma \delta}_{R_1 R_2 R_3} \left[ c_{R_1} c_{R_2} c_{R_3} \right] \left[ c_{R_2} c_{R_3} \right].
\]

In Eq. (1) (one can check that the terms of the form \[
\sum_{R_1 \neq R_2 \neq R_3} \sum_{R_{R_2}} V^{\alpha \beta \gamma \delta}_{R_1 R_2 R_3} \left[ c_{R_1} c_{R_2} c_{R_3} \right] \left[ c_{R_2} c_{R_3} \right] + h.c.
\]

have a similar scaling problem). We now consider the Fock terms (those with at least one contraction between each site). We now consider possible contractions relevant to this scenario. Both diagrams shown in figure 4 contribute to order $\sim \frac{1}{z^{2r-2}}$ (which is leading order for the Fock term). Here we are ignoring the scaling for the prefactor for this diagram as well as the number of similar diagrams (see Appendix B2) which is the same for both sets of contractions. However the first diagram has three contractions on the central site and therefore is higher order then we considered until now (as such we need the terms described in Section C3 below).

Hartree terms One can check that the Hartree contribution to the terms \[
\sum_{R_1 \neq R_2 \neq R_3} \sum_{R_{R_2}} V^{\alpha \beta \gamma \delta}_{R_1 R_2 R_3} \left[ c_{R_1} c_{R_2} c_{R_3} \right] \left[ c_{R_2} c_{R_3} \right] \]

and there is no Hartree piece. To see this clearly, note that the Hartree contribution for the example in Fig. 1 scales as $\sim \frac{1}{z}$ while the Fock and the three contractions diagram scale as $\frac{1}{z^{2r}}$ meaning that the Hartree is dominant. To keep this term, one needs only modify the Lagrange function in Section V by changing $\mathcal{L}_{HF}$ to:
As compared to Eq. \( (10) \). Below we will see the problem gets worse for four site terms as there are no Hartree terms and there is no way to keep the Fock piece consistently.

nearest neighbors to each other). We now consider the two possible sets of contractions shown in Figure 5 both sets of contractions contribute to order \( \sim 1/2^{N/2} \) (which is leading order for this diagram). Here we are ignoring the scaling for the prefactor for this diagram as well as the number of similar diagrams, so that the total scaling for both terms can be made order \( \sim 1 \) (see Appendix B2). However the first diagram has three contractions on the central site and therefore is higher order then we considered so far. As such we need to add three contraction terms to the site \( R_2 \) as is described in Section C3.

### 2. Approximate approach

The procedure, to properly account for the terms considered in Appendix C1 described in Appendix C3 below, is rather cumbersome. In this Appendix in order to perform crude ab-initio research we present a simplified method to treat multisite interactions to deal with all terms in Eq. \( (1) \). To do this very quickly but crudely one needs an effective Hamiltonian much like Eq. \( (10) \) but for the generalized model given by the Hamiltonian in Eq. \( (1) \). One natural guess for such an effective Hamiltonian is that:

\[
\langle \Psi_0 | H_F | \Psi_0 \rangle \cong \langle \Psi_0 | H_{\text{Eff}} | \Psi_0 \rangle .
\]

Where \( H_{\text{Eff}} \) is given by:

\[
H_{\text{Eff}} = \sum_\mathcal{R} \sum_\mathcal{R} P_R^\dagger H_P^\text{loc} P_R + \sum_{\mathcal{R}_1 \neq \mathcal{R}_2} \sum_{\mu\nu} J_{\mathcal{R}_1;\mathcal{R}_2}^{\mu\nu} \left[ \sum_i Z_{\mathcal{R}_1, \mu i} O_{\mathcal{R}_1 i} \right] \left[ \sum_j Z_{\mathcal{R}_2, \nu j} O_{\mathcal{R}_2 j} \right] + \nonumber \]

\[
+ \sum_{\mathcal{R}_1 \neq \mathcal{R}_2 \neq \mathcal{R}_3} \sum_{\mu\nu\eta\rho} J_{\mathcal{R}_1;\mathcal{R}_2;\mathcal{R}_3}^{\mu\nu\eta\rho} \left[ \sum_i Z_{\mathcal{R}_1, \mu i} O_{\mathcal{R}_1 i} \right] \left[ \sum_j Z_{\mathcal{R}_2, \nu j} O_{\mathcal{R}_2 j} \right] \left[ \sum_k Z_{\mathcal{R}_3, \eta k} O_{\mathcal{R}_3 k} \right] + \nonumber \]

\[
+ \sum_{\mathcal{R}_1 \neq \mathcal{R}_2 \neq \mathcal{R}_3 \neq \mathcal{R}_4} \sum_{\mu\nu\eta\rho} J_{\mathcal{R}_1;\mathcal{R}_2;\mathcal{R}_3;\mathcal{R}_4}^{\mu\nu\eta\rho} \left[ \sum_i Z_{\mathcal{R}_1, \mu i} O_{\mathcal{R}_1 i} \right] \left[ \sum_j Z_{\mathcal{R}_2, \nu j} O_{\mathcal{R}_2 j} \right] \left[ \sum_k Z_{\mathcal{R}_3, \eta k} O_{\mathcal{R}_3 k} \right] \left[ \sum_l Z_{\mathcal{R}_4, \rho l} O_{\mathcal{R}_4 l} \right].
\]

We again note that as explained in Appendices C1a and C1b this is not completely satisfactory, even for the leading order in the \( P_R^d P_R - I \) expansion and the leading order in the \( 1/z \) expansion. There are terms of the same order of magnitude in the \( 1/z \) expansion as the terms in the Hamiltonian in Eq. \( (C3) \) which are missed by the Hamiltonian in Eq. \( (C3) \). However using the effective Hamiltonian in Eq. \( (C3) \) is a very simple approach and may be good enough for preliminary calculations. If this approximate approach is chosen, then the Lagrange function in Section V need

Figure 5. Two diagrams for four sites as described in the main text with a different number of contractions but the same \( 1/z \) scaling. Lines indicate Wick’s theorem contractions.

b. Four site terms

We would like to present an example where, despite making both the large coordination number assumption and the leading order in \( P_R^d P_R - I \) expansion assumption, one needs three fermion contractions to obtain the leading order term for four site operators. Consider four single fermion operators on four neighbor sites such that \( R_2 \) is nearest neighbor to \( R_1, R_3 \) and \( R_4 \) (which are all next
only be modified by changing \( \mathcal{L}_{HF} \), which now should be given by:

\[
\mathcal{L}_{HF} \{ \{ R_{\mu}, T_{\mu}, U_{\mu} \}, \{ R_{\mu}^\dagger, T_{\mu}^\dagger, U_{\mu}^\dagger \}, [\Delta R_{1\mu},\Delta R_{2\mu}]_{ab},\alpha_R \beta \}\ =
\]

\[
\sum_{R_1 R_2 \alpha \beta \gamma \delta} V_{R_1 R_2}^{\alpha \beta \gamma \delta} O_{\alpha \gamma \delta} O_{\beta \gamma \delta} - \sum_{R_1 \neq R_2} \sum_{\alpha \beta \gamma \delta} \sum_{abcd} V_{R_1 R_2}^{\alpha \beta \gamma \delta} [\Delta R_{1 R_2}]_{ac} [\Delta R_{2 R_1}]_{bd} \left[ T_{1 \alpha}^{\beta} \right]_{ba} \left[ T_{2 \gamma}^{\delta} \right]_{dc} +
\]

\[
\sum_{R_1 \neq R_2} \sum_{\alpha \beta \gamma \delta} \left[ V_{R_1 R_2}^{\alpha \beta \gamma \delta} \Delta R_{1 R_2} \Delta R_{2 R_1} \right]_{ab} \left[ U_{R_\alpha \beta} \right]_{ab} \left[ U_{R_\gamma \delta} \right]_{cd} +
\]

\[
\sum_{R_1 \neq R_2} \sum_{\alpha \beta \gamma \delta} \sum_{abcd} \left[ V_{R_1 R_2}^{\alpha \beta \gamma \delta} \Delta R_{1 R_2} \Delta R_{2 R_1} \right]_{ab} \left[ R_{R_\alpha \beta} \right]_{ab} \left[ R_{R_\gamma \delta} \right]_{cd} \alpha_R \alpha_R \beta \beta_R \gamma \gamma_R \delta \delta_R -
\]

\[
\sum_{R_1 \neq R_2} \sum_{\alpha \beta \gamma \delta} \sum_{abcd} \left[ V_{R_1 R_2}^{\alpha \beta \gamma \delta} \Delta R_{1 R_2} \Delta R_{2 R_1} \right]_{ab} \left[ R_{R_\alpha \beta} \right]_{ab} \left[ R_{R_\gamma \delta} \right]_{cd} \alpha_R \alpha_R \beta \beta_R \gamma \gamma_R \delta \delta_R +
\]

\[
\sum_{R_1 \neq R_2} \sum_{\alpha \beta \gamma \delta} \sum_{abcd} \left[ V_{R_1 R_2}^{\alpha \beta \gamma \delta} \Delta R_{1 R_2} \Delta R_{2 R_1} \right]_{ab} \left[ R_{R_\alpha \beta} \right]_{ab} \left[ R_{R_\gamma \delta} \right]_{cd} \alpha_R \alpha_R \beta \beta_R \gamma \gamma_R \delta \delta_R .
\]

As compared to Eq. (59). With this modification the Lagrange function can be minimized directly.

\[ \tag{C4} \]

### 3. Extended approach

A rigorous approach to the problem of three contractions outlined in Section [C1](#) is to replace some of the terms of the form \( P_R^\dagger O_R P_R \) on various site sites in our Hamiltonian (the precise sites to be chosen are explained in Section [C1](#)) with three and four fermion terms instead of the one and two fermion terms found in the equivalences in Eqs. (31), (33), (34) and (53). This allows one to reproduce the three and four contraction terms shown in Section [C1](#). This approach is needed only for some of the three and four site terms in Eq. (1) and the two site analysis done previously is unaffected. One then uses the generalized equivalences which will be given below for these sites and proceeds much like in the main text. We now describe the more general equivalences needed for these three and four fermion equivalences.

#### a. Fermionic Equivalences

We consider fermionic single site operators \( O_R \). In Appendix [D4a](#) we will show that there is an equivalence:

\[
P_R^\dagger O_R P_R \sim \sum_a \hat{Z}_{R\alpha a} f_{Ra}^\dagger f_{Ra} + \sum_a \hat{Z}_{R\alpha b} f_{Ra} f_{Rb} f_{Rc} \tag{C5}
\]

and similarly for its Hermitian conjugate. In Appendix [D4a](#) we show that the coefficients \( \hat{Z}_{R\alpha a}, \hat{Z}_{R\alpha b} \) are determined by the following equations:

\[
\langle \Psi_0 | P_R^\dagger O_R P_R f_{Rd} | \Psi_0 \rangle = \langle \Psi_0 | \left[ \sum_b \hat{Z}_{R\alpha b} f_{Rb}^\dagger + \sum_a \hat{Z}_{R\alpha b} f_{Ra} f_{Rb} f_{Rc} \right] f_{Rd} | \Psi_0 \rangle ;
\]

\[
\langle \Psi_0 | P_R^\dagger O_R P_R f_{Rd} f_{Rf} | \Psi_0 \rangle = \langle \Psi_0 | \left[ \sum_b \hat{Z}_{R\alpha b} f_{Rb}^\dagger + \sum_a \hat{Z}_{R\alpha b} f_{Ra} f_{Rb} f_{Rc} \right] f_{Rd} f_{Rf} | \Psi_0 \rangle \tag{C6}
\]

#### b. Bosonic Equivalences (fermion number conserving operators)

We consider bosonic operators that conserve fermion number. In Appendix [D4b](#) we show the following equivalence:

\[
P_R^\dagger O_R P_R \sim \sum_{abcd} \hat{Z}_{R\alpha b} f_{Ra} f_{Rb} f_{Rc} f_{Rd} +
\]

\[
+ \sum_{ab} \hat{Z}_{R\alpha b} f_{Ra} f_{Rb} + \hat{Z}_{R\alpha b} I \tag{C7}
\]
We show that $\hat{Z}_{R_{\mu ab}}$, $\hat{Z}_{R_{\mu ac}}$, $\hat{Z}_{R_{\mu td}}$ are determined by the following equations (see Appendix [D4b]):

\[
\langle \Psi_0 | P^\dagger_R O_{R_{\mu}} P_{R_{\rho}} f^\dagger_{R_{\eta}} f_{R_{\mu}} | \Psi_0 \rangle = \\
= \langle \Psi_0 | \sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} + \\
\sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} | \Psi_0 \rangle ;
\]

\[
\langle \Psi_0 | P^\dagger_R O_{R_{\mu}} P_{R_{\rho}} f^\dagger_{R_{\eta}} f_{R_{\mu}} | \Psi_0 \rangle = \\
= \langle \Psi_0 | \sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} + \\
\sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} | \Psi_0 \rangle .
\]

We now consider bosonic operators that change the total number of electrons by two, such as pair hopping terms. In Appendix [D4c] we show that:

\[
P^\dagger_R O_{R_{\mu}} P_R \sim \sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} + \sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} f_{R_{ab} R_{\mu}}
\]

and similarly for its complex conjugate. We show that $\hat{Z}_{R_{\mu abc}}$ and $\hat{Z}_{R_{\mu ab}}$ are determined by the following equations (see Appendix [D4b]):

\[
\langle \Psi_0 | P^\dagger_R O_{R_{\mu}} P_{R_{\rho}} f^\dagger_{R_{\eta}} f_{R_{\mu}} f^\dagger_{R_{ab}} f_{R_{ab}} | \Psi_0 \rangle = \\
= \langle \Psi_0 | \sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} + \\
\sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} f_{R_{ab} R_{\mu}} | \Psi_0 \rangle .
\]

\[
\langle \Psi_0 | P^\dagger_R O_{R_{\mu}} P_{R_{\rho}} f^\dagger_{R_{\eta}} f_{R_{\mu}} | \Psi_0 \rangle = \\
= \langle \Psi_0 | \sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} + \\
\sum_{ab} \hat{Z}_{R_{\mu ab}} f^\dagger_{R_{\mu} R_{ab}} f_{R_{\mu} R_{ab}} f_{R_{ab} R_{\mu}} f_{R_{ab} R_{\mu}} | \Psi_0 \rangle .
\]

\[
\text{c. Bosonic Equivalences (fermion number changing operators)}
\]

Appendix D: Derivations of equivalence relations

1. Useful identities

In this section we drop the index $R$ as only one site is considered and $\Delta = \Delta_{R,R}$. Below to derive the Lagrangian in Section [D3] we will need the functions:

\[
\frac{1}{\sqrt{\rho_0}} O_i \sqrt{\rho_0} = \sum_k G_i,k (\Delta) O_k
\]

For $O_i \subset I, f_a, f_a^\dagger, f_b^\dagger f_b, f_a f_b, f_b^\dagger f_a^\dagger$. Indeed we have by Wick's theorem:

\[
Tr \{ \rho_0 f_a^\dagger f_b \} = \Delta_{ab}
\]

\[
Tr \{ \rho_0 f_a^\dagger f_b f_a f_b \} = (I - \Delta)_{ba}
\]

\[
Tr \{ \rho_0 f_a^\dagger f_b f_c f_d \} = \Delta_{ac} \Delta_{bd} + \Delta_{bc} \Delta_{ad}
\]

\[
Tr \{ \rho_0 f_a f_b f_c f_d \} = -(I - \Delta)_{ca} (I - \Delta)_{db}
\]

We further have that:

\[
\frac{1}{\sqrt{\rho_0}} f_a \sqrt{\rho_0} = \sum_b \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{ab}^{1/2} f_b
\]

\[
\frac{1}{\sqrt{\rho_0}} f_a^\dagger \sqrt{\rho_0} = \sum_b \left[ \frac{1 - \Delta^T}{\Delta^T} \right]_{ba}^{1/2} f_b^\dagger
\]

\[
\frac{1}{\sqrt{\rho_0}} f_a f_b \sqrt{\rho_0} = \sum_{cd} \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{cd}^{1/2} \left[ \frac{1 - \Delta^T}{\Delta^T} \right]_{ca}^{1/2} f_c f_d
\]

\[
\frac{1}{\sqrt{\rho_0}} f_a^\dagger f_b^\dagger \sqrt{\rho_0} = \sum_{cd} \left[ \frac{1 - \Delta^T}{\Delta^T} \right]_{cd}^{1/2} \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{ca}^{1/2} f_c^\dagger f_d^\dagger
\]

\[
\frac{1}{\sqrt{\rho_0}} f_a f_b \sqrt{\rho_0} = \sum_{cd} \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{cd}^{1/2} \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{bd}^{1/2} f_c f_d
\]

Where repetitive use of Eq. (13) has been made. Explicitly this means that:
2. Operators in the embedding mapping

\[ G_{f_a; f_b} (\Delta) = \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{ab}^{1/2} \]

\[ G_{f_a^1; f_b^1} (\Delta) = \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{ba}^{1/2} \]

\[ G_{f_a f_a^1; f_b f_b^1} (\Delta) = \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{bd}^{1/2} \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{ac}^{1/2} \]

\[ G_{f_a f_b; f_a^1 f_b^1} (\Delta) = \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{bd}^{1/2} \left[ \frac{\Delta^T}{I - \Delta^T} \right]_{ac}^{1/2} \] (D4)

In this section we have suppressed the site index \( R \) in our notation as we will be dealing with a single site only. We would like to show that:

\[ Tr \left[ \phi \hat{O}_\mu \hat{O}_\mu \phi \right] = \langle \Phi | \hat{O}_\mu \hat{O}_\mu^R | \Phi \rangle \exp \left[ \frac{\pi}{2} \left[ (N (n') - N (n))^2 - (N (n') - N (n))^2 \right] \right] \] (D5)

Here we define:

\[ O_i = \prod_{i=0}^{m} f_{a_i}^{(1)} \], \( \hat{O}_i^R = \prod_{i=0}^{m} \hat{f}_{a_{m-i}}^{(1)} \] (D6)

and

\[ O_\mu = \prod_{i=0}^{K} c_{\alpha_i}^{(1)} \], \( \hat{O}_\mu = \prod_{i=0}^{K} \hat{c}_{\alpha_i}^{(1)} \)

Here \( R \) stands for reverse order. Here (†) means that there may or may not be Hermitian conjugation (so that Eq. [D5] can be used to handle strings of both creation and annihilation operators). We have that:

\[ \langle \Phi | \hat{O}_\mu \hat{O}_\mu | \Phi \rangle \]

\[ = \sum_{n', \Gamma} \langle \hat{n}' | \hat{\Gamma} | \phi_{n^* \Gamma}^* \hat{\mu} \times \]

\[ \times \sum_{\Gamma, n} \phi_{\Gamma n} U_{\mu \Gamma}^R \hat{O}_i U_{\mu \Gamma} \left| \hat{n} \right> \exp \left( i \frac{\pi}{2} N (n) (N (n) - 1) \right) \]

\[ \times \exp \left( -i \frac{\pi}{2} N (n') (N (n') - 1) \right) \]

\[ = \sum_{n', \Gamma} \phi_{\Gamma n} \langle \hat{n}' | \hat{\Gamma} | \phi_{n^* \Gamma}^* \hat{\mu} \hat{O}^{R \Gamma} | \hat{n} \rangle \times \exp \left( i \frac{\pi}{2} N (n) (N (n) - 1) \right) \]

\[ \times \exp \left( -i \frac{\pi}{2} N (n') (N (n') - 1) \right) \]

\[ = \sum_{n', \Gamma} \sum_{\Gamma, n} \exp \left( i \frac{\pi}{2} N (n) (N (n) - 1) - i \frac{\pi}{2} N (n') (N (n') - 1) \right) \left( -1 \right)^{[N(\Gamma)][m+1]}

\[ \times \phi_{n^* \Gamma}^* \phi_{\Gamma n} \times \langle \hat{n}' | \hat{\Gamma} | \hat{\mu} \hat{O}^{R \Gamma} | \hat{n} \rangle \] (D7)

Now we have that:

\[ N (\Gamma) = N (n) \] (D8)

This means that \((-1)^{[N(\Gamma)][m+1]} = (-1)^{[N(n)][m+1]}\). Furthermore we have that:

\[ m + 1 = N (n') - N (n) \mod 2 \] (D9)
This means that
\[
= \exp \left( i \frac{\pi}{2} (N(n) (N(n) - 1) - i \frac{\pi}{2} (N(n') (N(n') - 1)) \right) (-1)^{[N(\Gamma)][m+1]} \\
= \exp \left( i \frac{\pi}{2} (N(n) (N(n) - 1) - N(n') (N(n') - 1) - 2 [N(n') - N(n)] [N(n)] \right)
\]
\text{(D10)}

We now write:
\[
N(n') = N(n) + [N(n') - N(n)]
\]
\text{(D11)}

This means that:
\[
\exp \left[ i \frac{\pi}{2} (N(n) (N(n) - 1) - N(n') (N(n') - 1)) \right] \\
-2 [N(n') - N(n)] [N(n)] \\
= \exp \left[ i \frac{\pi}{2} \left( [N(n') - N(n)]^2 - [N(n') - N(n)] \right) \right] \\
= \left\{ \begin{array}{l}
1, \quad N(n') - N(n) = 0 \mod 4 \\
1, \quad N(n') - N(n) = 1 \mod 4 \\
-1, \quad N(n') - N(n) = 2 \mod 4 \\
-1, \quad N(n') - N(n) = 3 \mod 4
\end{array} \right.
\]
\text{(D12)}

We now write:
\[
= \sum_{n', \Gamma, \Gamma_n} \sum \exp \left[ i \frac{\pi}{2} \left( [N(n') - N(n)]^2 - [N(n') - N(n)] \right) \right] \\
\times \phi_{n', \Gamma, \Gamma_n} \times \langle \hat{n} | \hat{O}_\mu | \hat{n} \rangle \\
= TR \left[ \phi^R_{\mu \nu} \phi^R_{\mu \nu} \right] \\
\times \exp \left[ i \frac{\pi}{2} \left( [N(n') - N(n)]^2 - [N(n') - N(n)] \right) \right]
\]
\text{(D13)}

and relation [D5] follows. We have also assumed that
\[
\langle \hat{n}' | \hat{O}^R_{\mu} | \hat{n} \rangle = \langle \hat{n} | \hat{O}^R | \hat{n}' \rangle, \quad \text{e.g. the operator } \hat{O}^R \text{ is real,}
\]
however all operators of the form in Eq. [D6] are of this form.

3. Derivations of equivalence relations

We will focus on the case of two point operators. The general case in Eq. [10] can not be done similarly, as was shown in Appendix C.1.

a. Fermionic operators

Equivalence results By Wicks theorem in the limit of large dimensions we may write that:
\[
\langle \Psi_0 | P_R^\dagger O_{R,R} P_R^\dagger O_{R',R'} P_R | \Psi_0 \rangle = \\
= [P_R^\dagger O_{R,R} P_R][P_R^\dagger O_{R',R'} P_R] \\
\times \left( 1 + O \left( \frac{1}{z} \right) \right)
\]
\text{(D14)}

Where $[P_R^\dagger O_{R,R} P_R][P_R^\dagger O_{R',R'} P_R]$ means perform all intra-site contractions and then a single intersite contractions between $R$ and $R'$. Terms with more then one contraction between $R$ and $R'$ are higher order in $1/z$. We may write that [15] [60] [65][68]:
\[
[P_R^\dagger O_{R,R} P_R][P_R^\dagger O_{R',R'} P_R] \\
= \sum_{ab} T_{R_{a} R_{b}} T_{R'_{a} R'_{b}} \langle f_{R_a} f_{R'_b} \rangle
\]
\text{(D15)}

For some coefficients $T_{R_{a} R_{b}}$. Indeed to obtain the expectation in the first line of Eq. [D14] we can contract the operators $P_R^\dagger O_{R,R} P_R$ and $P_R^\dagger O_{R',R'} P_R$ in all possible ways while leaving only one operator uncontracted. We can then write contractions between the two remaining single fermion terms. Since this is a well defined procedure there is unique $T_{R_{a} R_{b}}$, $T_{R'_{a} R'_{b}}$ that represent the final states after all but one of the contractions have been made. As such to derive that Eq. [10] is reproduced to order $1/z$ we need only show that:
\[
Z_{R_{a} R_{b}} = T_{R_{a} R_{b}}
\]
\text{(D16)}

However we have that:
\[
\langle \Psi_0 | \sum_{a} Z_{R_{a} R_{b}} f_{R_a}^\dagger f_{R_b} \rangle f_{R_b} | \Psi_0 \rangle = \\
\langle \Psi_0 | P_R^\dagger O_{R,R} P_R f_{R_b} | \Psi_0 \rangle = \\
= \langle \Psi_0 | \sum_{a} T_{R_{a} R_{b}} f_{R_a}^\dagger f_{R_b} \rangle f_{R_b} | \Psi_0 \rangle.
\]
\text{(D17)}

From which Eq. [D16] follows.

solutions to equivalence relations In this Appendix we have suppressed the site index $R$ in our notation as we will be dealing with a single site only and $\Delta = \Delta_{R,R}$. We will also not distinguish between linear operators and their matrices in the natural basis. We know that the equivalence relationship may be written as:
\[
TR \left[ \sqrt{\rho_0} P_R^\dagger O_\mu P_R f_a \sqrt{\rho_0} \right] = \sum_b Z_{\mu b} \langle f_b^\dagger f_a \rangle
\]
\text{(D18)}

We have that
\[
\sum_{b} Z_{\mu b} \langle f_b^\dagger f_a \rangle = \sum_{b} Z_{\mu b} \Delta_{ba}
\]
\text{(D19)}
Gutzwiller equivalences are set up so that if more precise. Explicitly below we show that the Hartree Fock term only renormalizes weakly:

$$\langle \psi_0 | P_R^I O_{R_\mu} P_R^I O_{R'\nu} P_{R'} \psi_0 \rangle_{\text{Fock}} =$$

$$= \langle \psi_0 | \left[ \sum_i Z_{R_{i\mu}} O_{R_i} \right] \left[ \sum_j Z_{R'_{i\nu}} O_{R'_{i\nu}} \right] | \psi_0 \rangle_{\text{Fock}} \times$$

$$\times \left( 1 + O \left( \frac{1}{z} \right) \right)$$

(D26)

Here Fock means that there are two or more intersite Wick contractions (or equivalently all the terms not included in the Hartree piece). Here $z$ is the number of nearest neighbors. In some sense the Gutzwiller equivalence procedure is designed to change as little of the expectation values as possible and use the simplest operators possible to do so.

Hartree contributions We would like to show that the Hartree contribution to correlation functions does not renormalize under the equivalences in Eq. (35). For this we first consider the equation (see Eq. (35)):

$$\langle \psi_0 | P_R^I O_{R_\mu} P_R \cdot I \rangle =$$

$$= \langle \psi_0 | \left[ \sum_{cd} Z_{R_d c} f_{R_c} I_{R_d} + Z_{R_{i\mu}} I \right] \cdot I \rangle$$

(D27)

That says that trace of an operator with respect to the non-interacting density matrix is preserved under equivalences. This means that the Hartree term does not renormalize under these equivalences, indeed the Hartree term may be written as:

$$\langle \psi_0 | P_R^I O_{R_\mu} P_R^I O_{R'\nu} P_{R'} \psi_0 \rangle_{\text{Hartree}} =$$

$$= \langle \psi_0 | \left[ \sum_i Z_{R_{i\mu}} O_{R_i} \right] \left[ \sum_j Z_{R'_{i\nu}} O_{R'_{i\nu}} \right] \psi_0 \rangle_{\text{Hartree}}$$

(D25)

with no corrections of any form. Here Hartree means that only intersite Wick contractions are done. Furthermore we will show that the Fock term only renormalizes weakly:

$$\langle \psi_0 | P_R^I O_{R_\mu} P_R^I O_{R'\nu} P_{R'} \psi_0 \rangle_{\text{Fock}} =$$

$$= \langle \psi_0 | \left[ \sum_i Z_{R_{i\mu}} O_{R_i} \right] \left[ \sum_j Z_{R'_{i\nu}} O_{R'_{i\nu}} \right] \psi_0 \rangle_{\text{Fock}} \times$$

$$\times \left( 1 + O \left( \frac{1}{z} \right) \right)$$

(D26)

Furthermore using the results in Section D1

$$\text{Tr} \left[ \sqrt{\rho_0} P_R^I O_{R_\mu} P_R f_a \sqrt{\rho_0} \right]$$

$$= \sum_b \left[ \frac{\Delta}{1 - \Delta} \right]^{1/2}_{ba} \text{Tr} \left[ \phi^I O_{R_\mu} \phi f_b \right]$$

$$= \Gamma \sqrt{\frac{\Delta}{1 - \Delta}}$$

(D20)

Here $\Gamma_b$ is the vector $[\phi^I O_{R_\mu} \phi f_b]$ and we are using matrix notation. We now have that in matrix notation

$$Z_{\mu} \Delta = \Gamma \sqrt{\frac{\Delta}{1 - \Delta}}$$

$$Z_{\mu a} = \sum_b \text{Tr} \left[ \phi^I O_{R_\mu} \phi f_b \right] \left[ \frac{1}{1 - \Delta} \right]^{1/2}_{ab}$$

(D22)

Now using Eq. (D5) we have Eq. (33) follows. Or alternatively:

$$\left[ Z [1 - \Delta] \Delta \right]^{1/2} = \text{Tr} \left[ \phi^I O_{R_\mu} \phi f_b \right]$$

(D23)

We note that by the complex conjugation property in Eq. (E7) we have that:

$$\hat{Z}^{\mu a} = Z^{\mu a} = \Gamma^{\mu I} \sqrt{\frac{\Delta}{1 - \Delta}}^{1/2}$$

$$= \sum_b \text{Tr} \left[ \phi^I O_{R_\mu} \phi f_b \right] \left[ \frac{1}{1 - \Delta} \right]^{1/2}_{ab}$$

(D24)

Here we have used the following notation:

$$P_R^I O_{R_\mu} P_R \sim \sum_a Z_{R_{\mu a}} f_{Ra}$$

b. Bosonic operators with same number of creation operators as annihilation operators

Equivalence results We would like to make Eq. (10) more precise. Explicitly below we show that the Gutzwiller equivalences are set up so that if $P_R^I O_{R_\mu} P_R \sim \sum_i Z_{R_{i\mu}} O_{R_i}$ then:

$$\langle \psi_0 | P_R^I O_{R_\mu} P_R^I O_{R'\nu} P_{R'} | \psi_0 \rangle_{\text{Hartree}} =$$

$$= \langle \psi_0 | \left[ \sum_i Z_{R_{i\mu}} O_{R_i} \right] \left[ \sum_j Z_{R'_{i\nu}} O_{R'_{i\nu}} \right] | \psi_0 \rangle_{\text{Hartree}}$$

(D25)

Fock contributions Consider bosonic operators with an equal number of creation and annihilation operators: $O_{R_\mu}$ and $O_{R'\nu}$. By Wicks theorem in the limit of large
dimensions we may write that:
\[
\langle \Psi_0 | P^\dagger_R O_{R_R} P_{R^\prime} f_{R^\prime}^\dagger O_{R^\prime} \rho \rho R | \Psi_0 \rangle = \\
= \langle \Psi_0 | P^\dagger_R O_{R_R} P_{R^\prime} f_{R^\prime}^\dagger O_{R^\prime} | \Psi_0 \rangle_{\text{Hartree}} + \\
+ [P^\dagger_R O_{R_R} P^\dagger_R O_{R^\prime} P_{R^\prime}] \times \\
\times \left( 1 + O \left( \frac{1}{z} \right) \right) \\
\tag{D28}
\]

Where \([P^\dagger_R O_{R_R} P^\dagger_R O_{R^\prime} P_{R^\prime}]\) means perform all intrasite contractions and then two intersite contractions between \(R\) and \(R'\). Terms with more than two contractions between \(R\) and \(R'\) are higher order in \(1/z\). We may write that \([\mathbf{15} \ 60 \ 65-68]\):
\[
[P^\dagger_R O_{R_R} P^\dagger_R O_{R^\prime} P_{R^\prime}] = \\
= \sum_{abcd} \rho_{abcd} T_{R_{R_{ab}}} T_{R_{R_{cd}} \rho} \langle f^\dagger_{R \rho} f_{R_{ab}} f^\dagger_{R_{cd}} f_{R_{cd}} \rangle_{\text{Fock}} \\
\tag{D29}
\]

For some coefficients \(T_{R_{R_{ab}}}\). Indeed to obtain the expectation in the first line of Eq. \([\mathbf{14}]\) we can contract the operators \(P^\dagger_R O_{R_R} P_{R} \) and \(P^\dagger_{R'} O_{R^\prime} P_{R^\prime}\) in all possible ways while leaving only two operator uncommented. We can then write contractions between the four remaining single fermion terms. Since this is a well defined procedure there is unique \(T_{R_{R_{ab}}}\) represent the final states after all but two of the contractions have been made. Now the Hartree terms in Eq. \([\mathbf{25}]\) are exactly reproduced by Eq. \([\mathbf{25}]\) as derived in Section \([\mathbf{3}]\) as such we need only derive that the Fock terms are reproduced to order \(1/z\) or:
\[
Z_{R_{R_{ab}}} = T_{R_{R_{ab}}} \\
\tag{D30}
\]

However we have that:
\[
= \langle \Psi_0 | \sum_{ab} Z_{R_{R_{ab}}} f^\dagger_{R_{ab}} f_{R_{ab}} + Z_{R_{R}} \rho | \Psi_0 \rangle \\
+ \langle \Psi_0 | \sum_{ab} \rho_{abcd} T_{R_{ab}} f^\dagger_{R_{ab}} f_{R_{ab}} | \Psi_0 \rangle_{\text{Fock}} \\
= \langle \Psi_0 | P^\dagger_R O_{R_R} P_{R^\prime} f_{R^\prime}^\dagger O_{R^\prime} | \Psi_0 \rangle = \\
= \langle \Psi_0 | P^\dagger_R O_{R_R} P_{R} | \Psi_0 \rangle \langle \Psi_0 | f^\dagger_{R_{ab}} f_{R_{ab}} | \Psi_0 \rangle_{\text{Fock}} \\
+ \langle \Psi_0 | \sum_{ab} \rho_{abcd} T_{R_{R_{ab}}} f^\dagger_{R_{ab}} f_{R_{ab}} | \Psi_0 \rangle_{\text{Fock}} \\
\tag{D31}
\]

From which Eq. \([\mathbf{30}]\) follows.

**Solutions to equivalence relations** In this Appendix we have suppressed the site index \(R\) in our notation as we will be dealing with a single site only and \(\Delta = \Delta_{R R}\). We will also not distinguish between linear operators and their matrices in the natural basis. With this definition due to the relations in Section \([\mathbf{D31}]\) we know that the equivalence relationship may be written as:
\[
Tr \left[ \sqrt{\rho_0} P^\dagger_R O_{\rho} P_{R^\prime} f_{R^\prime}^\dagger f_{R^\prime} \right] \\
= Tr \left[ \sqrt{\rho_0} P^\dagger_R O_{\rho} P_{R^\prime} \right] \cdot Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \\
\tag{D32}
\]

We now have that:
\[
Tr \left[ \sqrt{\rho_0} P^\dagger_R O_{\rho} P_{R^\prime} \right] \cdot Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \\
= Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \\
\tag{D34}
\]

Furthermore we have that:
\[
\sum_{\gamma \delta} Z_{\mu \nu} f_{\mu}^\dagger f_{\nu} f_{\nu} f_{\nu} = \\
\sum_{\gamma \delta} Z_{\mu \nu} \Delta_{\gamma \delta} (\mathbb{I} - \Delta_{\gamma \delta}) \\
= \left( \mathbb{I} - \Delta \right) Z_{\mu \nu} \Delta_{\gamma \delta} \\
\tag{D35}
\]

Furthermore by the results of Section \([\mathbf{D4}]\) we have that:
\[
Tr \left[ \sqrt{\rho_0} P^\dagger_R O_{\rho} P_{R^\prime} f_{R^\prime}^\dagger f_{R^\prime} \right] \\
= \sum_{\gamma} \left[ \frac{\Delta}{\mathbb{I} - \Delta} \right]^{1/2} \sum_{\gamma} \left[ \frac{\Delta}{\mathbb{I} - \Delta} \right]^{1/2} \cdot Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \\
= \sum_{\gamma} \left[ \frac{\Delta}{\mathbb{I} - \Delta} \right]^{1/2} \sum_{\gamma} \left[ \frac{\Delta}{\mathbb{I} - \Delta} \right]^{1/2} \cdot \Upsilon_{\gamma \delta} \\
= \left( \frac{\Delta}{\mathbb{I} - \Delta} \right) \sqrt{\frac{\Delta}{\mathbb{I} - \Delta}} \Upsilon_{\gamma \delta} \\
\tag{D36}
\]

Here we have defined the matrix \(\Upsilon_{\gamma \delta} = Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right].\) This means that:
\[
(\mathbb{I} - \Delta) Z_{\mu \nu} \Delta = \left( \frac{\Delta}{\mathbb{I} - \Delta} \right) \left( \frac{\Delta}{\mathbb{I} - \Delta} \right) \sqrt{\frac{\Delta}{\mathbb{I} - \Delta}} \\
- Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \cdot \Delta \\
\tag{D37}
\]

Or equivalently:
\[
Z_{\mu \nu} = \sqrt{\frac{1}{(\mathbb{I} - \Delta) \Delta}} \sqrt{\frac{1}{(\mathbb{I} - \Delta) \Delta}} \\
- Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \left( \frac{\Delta}{\mathbb{I} - \Delta} \right) \Delta \\
\tag{D38}
\]

Furthermore we have that in index notation:
\[
Z_{\mu \nu} = \sum_{ab} \left[ \frac{1}{(\mathbb{I} - \Delta) \Delta} \right]^{1/2} \cdot Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \times \\
\times \left[ \frac{1}{(\mathbb{I} - \Delta) \Delta} \right]^{1/2} - Tr \left[ \rho_0 f_{R}^\dagger f_{R} \right] \left( \frac{\Delta}{(\mathbb{I} - \Delta) \Delta} \right) \\
\tag{D39}
\]
Now using Eq. (D5) we have Eqs. (43) and (44) follow. Or alternatively:
\[
\left([\mathbb{1} - \Delta] \Delta^{1/2} Z [\mathbb{1} - \Delta] \Delta^{1/2}\right)_{ab} = Tr \left[ \phi^\dagger O_\mu \phi f_d^\dagger f_b \right] - Tr \left[ \phi^\dagger O_\mu \phi \right] \cdot [\mathbb{1}]_{ab}
\] (D40)

Furthermore we have that
\[
Z_{\mu \ell} = Tr \left[ \phi^\dagger O_\mu \phi \right] - \sum_{\gamma \delta} Z_{\mu \delta \epsilon} \Delta_{\epsilon \delta}
\] (D41)

c. Bosonic operators with two more creation operators than annihilation operators

**Equivalence results** By Wicks theorem in the limit of large dimensions we may write that:
\[
\langle \Psi_0 | P_R^\dagger O_{R\nu} P_{R'}^\dagger O_{R'\nu} P_{R''} | \Psi_0 \rangle = \left[ P_R^\dagger O_{R\nu} P_{R'}^\dagger O_{R'\nu} P_{R''} \right]
\]
\[
\times \left( 1 + O \left( \frac{1}{z} \right) \right)
\] (D42)

Where \([ P_R^\dagger O_{R\nu} P_{R'}^\dagger O_{R'\nu} P_{R''} \] means perform all intrasite contractions and then two intersite contractions between \( R \) and \( R' \). Terms with more than two contraction between \( R \) and \( R' \) are higher order in \( 1/z \). We may write that [15 60 65 68]:
\[
[ P_R^\dagger O_{R\nu} P_{R'}^\dagger O_{R'\nu} P_{R''} ]
\]
\[
= \sum_{abc} T_{R_{ab}} T'_{R'_{cd}} \left\langle f_{R_a}^\dagger f_{R_b}^\dagger f_{R_c} f_{R_d} \right\rangle
\] (D43)

For some coefficients \( T_{R_{ab}} \). Indeed to obtain the expectation in the first line of Eq. (D14) we can contract the operators \( P_R^\dagger O_{R\nu} P_R \) and \( P_{R'}^\dagger O_{R'\nu} P_{R'} \) in all possible ways while leaving only two operator uncontraction. We can then write contractions between the four remaining single fermion terms. Since this is a well defined procedure there is unique \( T_{R_{ab}} \), \( T'_{R'_{cd}} \) that represent the final states after all but two of the contractions have been made. As such to derive that Eq. (10) is reproduced to order \( 1/z \) we need to show that:
\[
\bar{Z}_{R_{ab}} = T_{R_{ab}}
\] (D44)

However we have that:
\[
\langle \Psi_0 | \sum_{ab} \bar{Z}_{R_{ab}} c_{R_a}^\dagger c_{R_b} \Psi_0 \rangle = \langle \Psi_0 | P_R^\dagger O_{R\nu} P_{R'c} c_{R_c} \Psi_0 \rangle = \langle \Psi_0 | \sum_{ab} T_{R_{ab}} c_{R_a}^\dagger c_{R_b} \Psi_0 \rangle
\] (D45)

From which Eq. (D44) follows.

**Solutions to equivalence relations** In this Appendix we have suppressed the site index \( R \) in our notation as we will be dealing with a single site only and \( \Delta = \Delta_{R,R} \). We will also not distinguish between linear operators and their matrices in the natural basis. We know that the equivalence relationship may be written as:
\[
Tr \left[ \sqrt{\rho_0} P_R^\dagger O_{\mu} P_{R} f_a f_b \sqrt{\rho_0} \right] = \sum_{c>d} \bar{Z}_{\mu cd} \left\langle f_c f_d^\dagger f_a f_b \right\rangle_{Fock}
\] (D46)

Now we have that:
\[
\sum_{c>d} \bar{Z}_{\mu cd} \left\langle f_c f_d^\dagger f_a f_b \right\rangle_{Fock} = \sum_{c>d} \bar{Z}_{\mu dc} \times \left( -\Delta_{ca} \Delta_{db} + \Delta_{cb} \Delta_{da} \right)
\] (D47)

Now define:
\[
\bar{Z}_{\mu cd} = -\bar{Z}_{\mu dc}
\] (D48)

This means that:
\[
\sum_{c>d} \bar{Z}_{\mu cd} \left\langle f_c f_d^\dagger f_a f_b \right\rangle_{Fock} = \sum_{c>d} \bar{Z}_{\mu dc} \Delta_{ca} \Delta_{da}
\]
\[
= \left[ \Delta^T Z_{\mu} \Delta \right]_{ab}
\]

Furthermore by the results of Section D1 we have that:
\[
Tr \left[ \sqrt{\rho_0} P_R^\dagger O_{\mu} P_{R} f_a f_b \sqrt{\rho_0} \right] = \sum_{\gamma} \left[ \frac{\Delta^T}{\mathbb{1} - \Delta^T} \right]_{ac}^{1/2} \left[ \frac{\Delta^T}{\mathbb{1} - \Delta^T} \right]_{bd}^{1/2} Tr \left[ \phi^\dagger O_{\mu} \phi f_c f_d \right]
\]
\[
= \sum_{\gamma} \left[ \frac{\Delta^T}{\mathbb{1} - \Delta^T} \right]_{ac}^{1/2} \left[ \frac{\Delta^T}{\mathbb{1} - \Delta^T} \right]_{bd}^{1/2} \Omega_{cd}
\]
\[
= \left[ \sqrt{\frac{\Delta^T}{\mathbb{1} - \Delta^T}} \cdot \Omega \cdot \sqrt{\frac{\Delta}{\mathbb{1} - \Delta}} \right]_{ab}
\] (D49)

Here we have defined the matrix \( \Omega_{cd} = Tr \left[ \phi^\dagger O_{\mu} \phi f_c f_d \right] \). This means that
\[
\bar{Z}_{\mu} = \sqrt{\frac{1}{\mathbb{1} - \Delta^T} \Delta^T} \cdot \Omega \cdot \sqrt{\frac{1}{\mathbb{1} - \Delta}}
\] (D50)

Or equivalently:
\[
\bar{Z}_{\mu ab} = \sum_{cd} \left[ \frac{1}{\mathbb{1} - \Delta^T} \Delta^T \right]_{ac}^{1/2} \cdot \left[ \frac{1}{\mathbb{1} - \Delta} \Delta \right]_{db}^{1/2}
\] (D51)

Now using Eq. (D5) we have Eq. (53) follows. Or alternatively:
Now we know that:

$$\hat{Z}_{\mu^* ba} = \hat{Z}_{\mu ba} = \sum_{cd} \left[ \frac{1}{(1 - \Delta)} \right]_{ac}^{1/2} \cdot \frac{1}{(1 - \Delta^T)^T} \right]_{db}^{1/2} \tag{D53}$$

We would like to show that the equivalences presented in Section C3 represent all three contraction terms. We will show this for an example of just two operators, where these terms may be used to generate higher order terms in $1/z$, but they can directly be generalized to three and four site terms where they can be used as part of the leading order contribution.

### 4. Proofs for Section C3

We have that:

$$\langle \Psi_0 | P_R^I O_{R\mu} P_R P_R^I O_{R\nu} P_R^I P_R O_R^I P_R^I | \Psi_0 \rangle = \left[ P_R^I O_{R\mu} P_R^I O_{R\nu} P_R^I P_R O_R^I P_R^I \right] \times \left( 1 + O \left( \frac{1}{z} \right) \right) \tag{D54}$$

From this it is clear that all we have to show for Eq. C6 is to show that all zero, two and four contraction terms are reproduced. However the Equations in Eq. C7 are linear combinations of these equations with invertible coefficients (for generic contractions $\langle f_a f_b \rangle$) from which Eq. C7 follows.

#### b. Bosonic equivalences (fermion number preserving)

We have that:

$$\langle \Psi_0 | P_R^I O_{R\mu} P_R P_R^I O_{R\nu} P_R^I | \Psi_0 \rangle = \left[ P_R^I O_{R\mu} P_R^I O_{R\nu} P_R^I P_R O_R^I P_R^I \right] \times \left( 1 + O \left( \frac{1}{z} \right) \right) \tag{D55}$$

From this it is clear that all we have to show for Eq. C10 is to show that all two and four contraction terms are reproduced. However the Equations in Eq. C10 are linear combinations of these equations with invertible coefficients (for generic contractions $\langle f_a f_b \rangle$) from which Eq. C10 follows.

#### c. Bosonic equivalences (fermion number changing)

We have that:

$$\langle \Psi_0 | P_R^I O_{R\mu} P_R P_R^I O_{R\nu} P_R^I P_R O_R^I P_R^I | \Psi_0 \rangle = \left[ P_R^I O_{R\mu} P_R^I O_{R\nu} P_R^I P_R O_R^I P_R^I \right] \times \left( 1 + O \left( \frac{1}{z} \right) \right) \tag{D56}$$

From this it is clear that all we have to show for Eq. C10 is to show that all two and four contraction terms are reproduced. However the Equations in Eq. C10 are linear combinations of these equations with invertible coefficients (for generic contractions $\langle f_a f_b \rangle$) from which Eq. C10 follows.

### Appendix E: Sanity checks

#### 1. Gutzwiller constraints: the identity operator

So far we have not used the Gutzwiller constrains in Eq. 4 in our derivations. We would like to use these constraints to show that it is possible to insert an identity operators in Eq. 10 without changing the ground state energy within our calculations and as such provide a consistency check. More precisely we would like to show that:

$$O_{R\mu} = \kappa I, \quad (E1)$$
we have that
\[ Z_{R \mu I} = \kappa, \ Z_{R \mu ba} = 0, \]  
(E2)
and as such
\[ P_R^\dagger I P_R \sim I. \]  
(E3)
To do so, let’s rewrite the Gutzwiller constraints in Eq. (32) in the following suggestive way:
\[
\langle \Psi_0 | P_R^\dagger \kappa I P_R f_{R a} f_{R b} | \Psi_0 \rangle = \\
\langle \Psi_0 | \sum_{cd} 0 \cdot f_{R c} f_{R d} + \kappa I \rangle f_{R a} f_{R b} | \Psi_0 \rangle \\
\langle \Psi_0 | P_R^\dagger \kappa I P_R \cdot I | \Psi_0 \rangle = \\
\langle \Psi_0 | \sum_{cd} 0 \cdot f_{R c} f_{R d} + \kappa I \cdot I | \Psi_0 \rangle.
\]
(E4)
From which Eqs. (E2) and (E3) follow.

2. Hermicity check

We would like to show that under the equivalence in Eqs. (31), (43), (44) and (53) Hermitian Hamiltonians are mapped onto Hermitian Hamiltonians. The main idea will be to show that the Hermitian conjugate of an operator is equivalent to the Hermitian conjugate of the equivalent operator. Below in Appendix E2d we will show that this is sufficient for the Hamiltonian in Eq. (10) to be Hermitian.

a. Fermionic operators

We start with the case where the operator \( O_{R \mu} \) is fermionic. For this case we would like to check that if:
\[
P_R^\dagger O_{R \mu} P_R \sim \sum_a Z_{R \mu a} f_{R a} \]  
(E5)
then
\[
P_R^\dagger O_{R \mu}^\dagger P_R \sim \sum_a Z_{R \mu a}^* f_{R a}^\dagger \]  
(E6)
More precisely we would like to show that:
\[
Z_{R \mu a} = \tilde{Z}_{R \mu a}. \]  
(E7)
To do so, we notice that Eq. (32) may be rewritten as:
\[
\langle \Psi_0 | f_{R a} P_R^\dagger O_{R \mu} P_R | \Psi_0 \rangle = \langle \Psi_0 | f_{R a} \sum_b Z_{\mu b} f_{R b} | \Psi_0 \rangle. 
\]  
(E8)
Indeed after we perform all contractions and reduced \( P_R^\dagger O_{R \mu} P_R \) to a single annihilation operator in every possible way using Wick’s theorem we get that
\[
P_R^\dagger O_{R \mu} P_R \sim \sum_a Z_{R \mu a} f_{R a} \]  
(E9)
and it does not matter which order we put the operators \( f_{R a} \) in order to determine the coefficients \( Z_{R \mu a} \), e.g., \( Z_{R \mu a} \) are unique and it does not matter which of the two types of equations we use to determine them. Taking the Hermitian conjugate of this equation (Eq. (E8)) we get that:
\[
\langle \Psi_0 | P_R^\dagger O_{R \mu} P_R f_{R a} | \Psi_0 \rangle = \langle \Psi_0 | \sum_b Z_{R \mu b}^* f_{R b} \rangle f_{R a}^\dagger | \Psi_0 \rangle. 
\]  
(E10)
As such Eq. (E7) follows. The bosonic Hermicity checks are highly similar and done below.

b. Bosonic operator with the same number of creation and annihilation operators

We continue with the case where the operator \( O_{R \mu} \) is bosonic number conserving operator. For this case we would like to check that if:
\[
P_R^\dagger O_{R \mu} P_R \sim \sum_{\alpha \beta} Z_{R \mu \alpha b} f_{R a}^\dagger f_{R b} + Z_{R \mu I} I \]  
(E11)
then
\[
P_R^\dagger O_{R \mu}^\dagger P_R \sim \sum_{\alpha \beta} Z_{R \mu \beta a}^* f_{R b}^\dagger f_{R a} + Z_{R \mu I}^* I \]  
(E12)
e.g.
\[
Z_{R \mu ab}^* = Z_{R \mu ba}, \quad Z_{R \mu I}^* = Z_{R \mu I}. \]  
(E13)
However, in a manner similar to Appendix E2d we can show that \( Z_{R \mu cd}, Z_{R \mu l} \) satisfy the following equations:
\[
\langle \Psi_0 | f_{R b}^\dagger f_{R a} P_R^\dagger O_{R \mu} P_R | \Psi_0 \rangle = \\
\langle \Psi_0 | f_{R b}^\dagger f_{R a} \sum_{cd} Z_{R \mu cd} f_{R d}^\dagger f_{R c} + Z_{R \mu I} I | \Psi_0 \rangle \\
\langle \Psi_0 | I \cdot P_R^\dagger O_{R \mu} P_R | \Psi_0 \rangle = \\
\langle \Psi_0 | I \cdot \sum_{cd} Z_{R \mu cd} f_{R d}^\dagger f_{R c} + Z_{R \mu I} I | \Psi_0 \rangle. 
\]  
(E14)
Taking the Hermitian conjugate of these equations we get that:
\[
\langle \Psi_0 | P_R^\dagger O_{R \mu} P_R f_{R b}^\dagger f_{R a} | \Psi_0 \rangle = \\
\langle \Psi_0 | \sum_{cd} Z_{R \mu cd}^* f_{R d}^\dagger f_{R c} + Z_{R \mu I}^* I | \Psi_0 \rangle \\
\langle \Psi_0 | P_R^\dagger O_{R \mu} P_R \cdot I | \Psi_0 \rangle = \\
\langle \Psi_0 | \sum_{cd} Z_{R \mu cd}^* f_{R d}^\dagger f_{R c} + Z_{R \mu I}^* I \cdot I | \Psi_0 \rangle. 
\]  
(E15)
and Eqs. [E12] and [E13] follow.

c. Bosonic operators that change fermion number by two

We continue with the case where the operator \( O_{R_R} \) is bosonic operator that changes the fermion number by two. For this case we would like to check that if:

\[
P_R^\dagger O^\dagger_R P_R \sim \sum_{\alpha\beta} \tilde{Z}_{R_{\alpha\beta}} f^\dagger_{R_{\alpha}} f^\dagger_{R_{\beta}} \tag{E16}
\]

then:

\[
P_R^\dagger O^\dagger_R P_R \sim \sum_{\alpha\beta} \tilde{Z}^*_{R_{\alpha\beta}} f_{R_{\alpha}} f_{R_{\beta}} \tag{E17}
\]

e.g.

\[
\tilde{Z}^*_{R_{\alpha\beta}} = \tilde{Z}_{R^{-1}_{\mu\nu}} ba. \tag{E18}
\]

However we have that \( \tilde{Z}_{R_{\alpha\beta}} \) satisfy the following equations:

\[
\langle \Psi_0 | f_{R_R} f_{R_a} P^\dagger_R O^\dagger_R P_R | \Psi_0 \rangle = \langle \Psi_0 | f_{R_R} f_{R_a} \left[ \sum_{cd} \tilde{Z}_{R_{\alpha\beta}} f^\dagger_{R_{\alpha}} f^\dagger_{R_{\beta}} \right] | \Psi_0 \rangle. \tag{E19}
\]

Taking the hermitian conjugate of this equation we get that:

\[
\langle \Psi_0 | P^\dagger_R O^\dagger_R f^\dagger_{R_R} f_{R_R} | \Psi_0 \rangle = \langle \Psi_0 | \sum_{cd} \tilde{Z}^*_{R_{\alpha\beta}} f_{R_{\alpha}} f_{R_{\beta}} | \Psi_0 \rangle \tag{E20}
\]

and Eqs. [E17] and [E18] follow.

d. Explicit hermicity proof

We note that for a hermitian Hamiltonian we may write

\[
H = \frac{1}{2} (H + H^\dagger)
\]

\[
= \frac{1}{2} \left[ \sum_{n} \sum_{R_1 \ldots R_n} \sum_{\mu_1 \ldots \mu_n} J^\mu_1 \ldots \mu_n O_{R_1 \mu_1} \ldots O_{R_n \mu_n} \right] \\
+ \frac{1}{2} \left[ \sum_{n} \sum_{R_1 \ldots R_n} \sum_{\mu_1 \ldots \mu_n} J^\mu_1 \ldots \mu_n^* O^\dagger_{R_1 \mu_1} \ldots O^\dagger_{R_n \mu_n} \right]. \tag{E21}
\]

In which case

\[
H \sim H_{\text{eff}} = \frac{1}{2} \left[ \sum_n \sum_{R_1 \ldots R_n} \sum_{\mu_1 \ldots \mu_n} J^\mu_1 \ldots \mu_n \left[ \sum_{i_1} \tilde{Z}_{R_1 \mu_1 i_1} O_{R_1 \mu_1 i_1} \right] \ldots \left[ \sum_{i_n} \tilde{Z}_{R_n \mu_n i_n} O_{R_n \mu_n i_n} \right] \right] \\
+ \frac{1}{2} \left[ \sum_n \sum_{R_1 \ldots R_n} \sum_{\mu_1 \ldots \mu_n} J^\mu_1 \ldots \mu_n^* \left[ \sum_{i_n} \tilde{Z}^*_{R_n \mu_n i_n} O^\dagger_{R_n \mu_n i_n} \right] \ldots \left[ \sum_{i_1} \tilde{Z}^*_{R_1 \mu_1 i_1} O^\dagger_{R_1 \mu_1 i_1} \right] \right]. \tag{E22}
\]

Which is clearly Hermitian.

Appendix F: Short Lagrangian

We can now obtain and analog of Eq. [E4] by replacing the various constraints by Lagrange multipliers and the main Hamiltonian by the embedding Hamiltonian. As such we have the following action (which is for simplicity specialized to the case where we only consider the first two lines of Eq. [P]):

\[
\mathcal{L}_N \left( D_{R\mu i}, E_R^c, Z_{R\mu i}, \phi_R, \left[ \lambda_{R_1 R_2}^\alpha \right]_{ab}, \left[ \Delta_{R_1 R_2} \right]_{ab}, \left[ \Delta_R \right]_{ab}, |\Psi_0 \rangle \right) = \langle \Psi_0 | \varepsilon_{HF} + \left[ \lambda_{R_1 R_2}^\alpha \right]_{ab} - \mu |\Psi_0 \rangle \\
+ \sum_{R} E^c_R - \sum_{R_{ab}} \left( \left[ \lambda_{R_R}^\alpha \right]_{ab} + \left[ \lambda_{R_R}^* \right]_{ab} \right) [\Delta_{RR}]_{ab} - \mathcal{F}_D (\{ [\Delta_{R_1 R_2}]_{ab} \}) - \sum_{R_{R_{ij}}} D_{R_{ij}} Z_{R_{ij}} F_{ij} (\{ [\Delta_{RR}]_{ab} \}) - \\
- \sum_{R_{1 \neq R_{2}} \neq R_{ab}} \left[ \lambda_{R_1 R_2}^\alpha \right]_{ab} [\Delta_{R_1 R_2}]_{ab} + \mathcal{L}_{\text{embed}} + \mu N \tag{F1}
\]
Where we define define $L_{embed} = \sum_R \langle \Phi_R | H_{embed}^R | \Phi_R \rangle + \sum_R E_R^S$, where:

$$H_{embed} = \sum_{\mu i} D_{\mu i} \left( \sum_k \hat{\Omega}_{\mu i}^R \hat{\Omega}_{\mu i}^R G_{i k} (\Delta R) \right) \exp \left[ i \frac{\pi}{2} \left[ (N (n')) - N (n) \right]^2 - \Delta (n') \right]$$

$$+ H_{elas}^R - \sum_R E_R^S + \sum_{ab} [\lambda_R^S]_{ab} \hat{f}_{Rb} \hat{\phi}_{Ra}$$

(F2)

Where $\varepsilon$ is the Hartree Fock energy, e.g.,

$$\varepsilon_{HF} = \sum_{\mu} \sum_{R_1, R_2} \sum_{ij} J_{\mu}^{R_1; R_2} Z_{R_1, \mu} Z_{R_2, \nu} [O_{R_1} O_{R_2}]_{HF}$$

(F3)

Where for example

$$\left[ f_{R_1 a}^d f_{R_2 c}^+ f_{R_3 d}^+ \right]_{HF} = \left[ \Delta_{R_1 R_2} \right]_{ab} f_{R_1 a}^d f_{R_2 c}^+ f_{R_3 d}^+$$

(F4)

And

$$\mathcal{F}_D ([\Delta_{R_1 R_2}], ) \supset J_{\mu}^{R_1; R_2} [\Delta_{R_1 R_2} \right]_{ab} \left[ \Delta_{R_1 R_2} \right]_{cd} = \left[ \Delta_{R_1 R_2} \right]_{cd} [\Delta_{R_1 R_2}]_{bc}$$

(F5)

The extremization is carried out over all variables including Lagrange multipliers $[15, 60, 65, 68]$. We have that at saddle point $[\lambda_{R_1, \neq R_2}]_{ab} = 0$, see Appendix [F1]. We note that the Lagrangian in Eq. (F1) is not real so it cannot be minimized only extremizing (the saddle point energy is real though). For a more complex but completely real Lagrangian that is specialized to the Hamiltonian in Eq. [11] see Section [V] which is our main result.

1. Quasiparticle energies

   a. Argument why $[\lambda_{R_1, \neq R_2}]_{ab} = 0$ at saddle point

In the formulation in Appendix [F] we have that the energy functional is given by:

$$\mathcal{L}_N = \langle \Psi_0 | \varepsilon_{HF} + [\lambda_{R_1, R_2}]_{ab} - \mu | \Psi_0 \rangle$$

$$- \sum_{R_1, \neq R_2, ab} [\lambda_{R_1, R_2}]_{ab} [\Delta_{R_1 R_2}]_{ab} - \sum_{R_1, \neq R_2, \mu, \nu} J_{\mu}^{R_1; R_2} Z_{R_1, \mu} Z_{R_2, \nu} [\Delta_{R_1 R_2}]_{ab}$$

$$\cdot [\Delta_{R_1 R_2}]_{cd} + ...$$

(F6)

Where $+,...$ will not effect our derivations. We now have that extremizing with respect to the variables in the Lagrange function:

$$0 = \frac{\partial \mathcal{L}_N}{\partial [\Delta_{R_1, \neq R_2}]_{ab}} = \sum_{\mu} \sum_{i, j} J_{\mu}^{R_1; R_2} Z_{R_1, \mu} Z_{R_2, \nu} [\Delta_{R_1 R_2}]_{ab}$$

$$+ \sum_{\mu} \sum_{i, j} J_{\mu}^{R_1; R_2} Z_{R_1, \mu} Z_{R_2, \nu} \left( f_{i, R_2}^+ f_{j, R_1} \right) - [\lambda_{R_1, R_2}]_{ab}$$

(F7)

This greatly simplifies the saddle point, and in particular the quasiparticle Hamiltonian $H_{QP}$ see below.

b. Excitations

We know that the proper way to study the quasiparticle energy is to take the thermodynamic limit and to study the following wave function:

$$P_G \sum_{\alpha} | \psi_{\alpha} \rangle = P_G | \Psi_{Slater} \rangle$$

(F8)

Now the single particle density matrix $\Delta_{R_3 \alpha, \beta}$ for $| \Psi_{Slater} \rangle$ is almost the same as for $| \Psi_{Slater} \rangle$ plus $1/N$ corrections (here $N$ is the number of atoms which blows up in the thermodynamic limit). This means that the equivalence relations

$$O_{Ri} \sim \sum_i Z_{Ri, \alpha} O_{Ri} = \sum_i Z_{Ri, \alpha} O_{Ri} + O \left( \frac{1}{N} \right)$$

(F9)

$$Z_{Ri, \alpha} = 0 + O \left( \frac{1}{N} \right)$$

(F10)

However we know that the energy functional is stationary with respect to variations of $Z_{Ri, \alpha}$ which means that:

$$Z \mathcal{L}_N (Z_{Ri, \alpha}) = \mathcal{L}_N (Z_{Ri, \alpha}) + O \left( \frac{N}{N^2} \right)$$

(F11)

This means that we may as well ignore the changes in $Z_{Ri, \alpha}$ and set

$$Z_{Ri, \alpha} \cong Z_{Ri, \alpha}$$

(F12)
As such the Hamiltonian for the original problem
\[ H = \sum_{R,R',\mu\nu} J_{R_i;R_j}^{R_i;R_j} O_{R_i\mu} O_{R_j\nu} H_{\text{loc}} \]

While \( H_{\text{loc}} \) and the other terms in \( L_N \) depend on \([\Delta_{R_i,R_j}]_{ab}\) because of the stationarity conditions their effect may be neglected. As such the problem of excitations maps onto the problem of excitations of the following Hamiltonian:
\[ H_{\text{eff}} = \sum_{R,R',\mu\nu} J_{R_i;R_j}^{R_i;R_j} \sum_{i,j} Z_{R_i\mu} Z_{R'_{\nu}} [O_{R_i;R_j} O_{R_j\nu}] + \sum_{Rab} [\lambda^{RR}_{ab}] f^\dagger_{Ra} f_{Rb} \]

Which has no dependence on \( \psi \) of any form. This means that the excitation energy for the Gutzwiller Lagrange function is the same as the excitation energy of \( H_{\text{eff}} \) which is the Hartree Fock excitation energy which is given by the eigenenergies of the Hamiltonian:
\[ H_{QP} = \sum_{R,R',\mu\nu} J_{R_i;R_j}^{R_i;R_j} \sum_{i,j} Z_{R_i\mu} Z_{R'_{\nu}} [O_{R_i;R_j} O_{R_j\nu}] H_F + \sum_{Rab} [\lambda^{RR}_{ab}] f^\dagger_{Ra} f_{Rb} \]

### Appendix G: Mott Gap

1. Expectation values and equivalence relationships

We want to solve for the Mott gap in the Brinkman Rice transition. The Gutzwiller constraints are:
\[ p_{\uparrow}^2 + d^2 = \Delta_{\uparrow} \equiv \langle \Psi_0 | f^\dagger_{R_i} f_{R_i \uparrow} | \Psi_0 \rangle \]
\[ p_{\downarrow}^2 + d^2 = \Delta_{\downarrow} \equiv \langle \Psi_0 | f^\dagger_{R_i} f_{R_i \downarrow} | \Psi_0 \rangle \]
\[ e^2 + p_{\uparrow}^2 + p_{\downarrow}^2 + d^2 = 1 \]  

Furthermore as \([P_R, \rho_{R0}] = 0\) (this is not the case in general) we have that:
\[ \langle \Phi_R | c_{R_i \uparrow} c_{R_i \uparrow} | \Phi_R \rangle \equiv n_{\uparrow} = \Delta_{\uparrow} \]
\[ \langle \Phi_R | c_{R_i \downarrow} c_{R_i \downarrow} | \Phi_R \rangle \equiv n_{\downarrow} = \Delta_{\downarrow} \]  

We note that the solutions to the Gutzwiller equivalences depend only on \( e, p_{\uparrow}, p_{\downarrow}, d \) as well as \( \Delta_{\uparrow} \) and \( \Delta_{\downarrow} \). Now because of Eq. (G2) we have that \( \Delta_{\uparrow} \) and \( \Delta_{\downarrow} \) are fixed for all states with a fixed magnetization and occupation. Furthermore because of the Gutzwiller constraints we have that \( e, p_{\uparrow}, p_{\downarrow} \) are functions of \( d \) and the occupation and magnetization. As such the renormalization coefficients \( R_{\mu_i} \) depend only on \( d \) and on the occupation and magnetization (which are fixed) and not explicitly on the wavefunction \( |\Psi_0\rangle \). This greatly facilitates analytic calculations in this special case. In particular we may set \( c_0 = f_\alpha \).

We will consider the generic single band Hubbard Hamiltonian with nearest neighbor interactions given in Eq. (66). We will assume that
\[ p_{\uparrow} = p_{\downarrow} = p \]  

In this case the Gutzwiller equivalences (which may be obtained from the Lagrange multiplier terms in the Lagrangian in Eq. (71)) are given by:
\[ P_{R_i}^\dagger c_{\alpha_i}^\dagger P_R \sim \frac{(e + d) p}{\sqrt{1 - d^2 - p^2}} \sqrt{1 - e^2 - p^2 c_\alpha} \]
\[ P_{R_i}^\dagger n P_R \sim \frac{[e^2 - d^2 + \frac{d^2}{p^2 + d^2}] n + \left[ + 2p^2 + 2d^2 - 2 \left[ \frac{e^2 - d^2 + \frac{d^2}{p^2 + d^2}}{(1 - p^2 - d^2)} \right] (p^2 + d^2) \right] I \]
\[ P_{R_i}^\dagger c_{\alpha_i}^\dagger P_R \sim \frac{d e}{(1 - p^2 - d^2)} (p^2 + d^2) c_{\alpha_i}^\dagger \]
\[ P_{R_i}^\dagger \bar{S} P_R \sim \frac{p^2}{(1 - p^2 - d^2)} (p^2 + d^2) \bar{S} \]
\[ P_{R_i}^\dagger n \bar{c}_{\alpha_i} P_R \sim \frac{d p}{\sqrt{1 - p^2 - d^2}} \sqrt{1 - e^2 - p^2 c_\alpha} \]
\[ P_{R_i}^\dagger n \bar{c}_{\alpha_i} P_R \sim \left( \frac{d^2}{p^2 + d^2} \right) n - d^2 I \]

Indeed one can take derivatives with respect to \( D_\sigma, E_\sigma, F_{\sigma \sigma'}, F \) and set them to zero to obtain Eq. (G4).

2. Gutzwiller Lagrange function
We now replace terms enforcing the Gutzwiller constraints as they are of Lagrange multiplier form and do not contribute to the total energy and replaced the coefficients (G9). Using the Gutzwiller constraints we have that

\[\langle \hat{H} \rangle = -2 \left( \sqrt{1-n+d^2} + d \right) \frac{\left( \frac{1}{2} - d^2 \right)}{(1 - \frac{u}{2})} \right) \frac{\left( n \right)}{Vz\chi} + Ud^2
\]

\[\langle \hat{H} \rangle = -8 \left( \sqrt{d^2 - \delta + d} \right) \frac{\left( 1 + \delta \right) - d^2}{1 - \delta^2} \right) \frac{\left( 1 + \delta \right) - d^2}{1 - \delta^2} \right) \frac{\left( n \right)}{Vz\chi} + Ud^2
\]

Now we introduce the variable \( x = e + d \) then we have that

\[d^2 = \left( \frac{x^2 + \delta}{2x} \right)^2 \quad \text{(G10)}\]

\[p^2 = \frac{1 + \delta}{2} - \left( \frac{x^2 + \delta}{2x} \right)^2 \quad \text{(G11)}\]

\[e^2 = \left( \frac{x^2 + \delta}{2x} \right)^2 - \delta \quad \text{(G11)}\]
Then we have that [88]:

\[
\langle H \rangle = -2 \left[ 1 - \frac{(1 - x^2)^2}{1 - \delta^2} \right] t z \chi + U \left( \frac{x^2 + \delta}{2x} \right)^2 + \frac{1}{2} V (1 + \delta)^2 z - \frac{3}{4} \left[ \frac{2x^2 - (x^4 + \delta^2)}{x^2 [1 - \delta^2]} \right]^2 z J \chi^2 - \left( \frac{-\delta^2 x^2 + (x^4 + \delta^2)}{(1 - \delta^2) x^2} \right)^2 V z \chi^2 + Y z \left( \frac{(y^2 - \delta^2)^2}{(1 - \delta^2)^2 y^2} \right)^2 + 2 \left( \frac{(x^2 + \delta^2)}{y^2} \right)^2 + 2 \left( \frac{(x^2 + \delta^2)}{y^2} \right)^2 \left( \frac{1 - (1 - y^2)}{1 - \delta^2} \right) \right] z \chi X
\]

(G12)

We now introduce \( y = x^2 \) and write:

\[
\langle H \rangle = -2 \left[ 1 - \frac{(1 - y)^2}{1 - \delta^2} \right] t z \chi + U \left( \frac{y}{4} + \frac{\delta}{2} + \frac{\delta^2}{4y} \right) + \frac{1}{2} V (1 + \delta)^2 z - \frac{3}{4} \left[ \frac{2y - (y^2 + \delta^2)}{y [1 - \delta^2]} \right]^2 z J \chi^2 - \left( \frac{-\delta^2 2y + (y^2 + \delta^2)}{(1 - \delta^2) y} \right)^2 V z \chi^2 + Y z \left( \frac{(y^2 - \delta^2)^2}{(1 - \delta^2)^2 y^2} \right)^2 + 2 \left( \frac{(y^2 - \delta^2)}{y^2} \right)^2 + 2 \left( \frac{(y^2 - \delta^2)}{y^2} \right)^2 \left( \frac{1 - (1 - y^2)}{1 - \delta^2} \right) \right] z \chi X
\]

(G13)

Now minimizing the energy with respect to \( y \) we get that:

\[
\frac{\partial H}{\partial y} = -4 \left[ \frac{(1 - y)^2}{1 - \delta^2} \right] (t - X) z \chi + U \left( \frac{1}{4} - \frac{\delta^2}{4y^2} \right) - 3 \left[ \frac{(-y^2 + \delta^2)}{y^2} \right] z J \chi^2 = 0
\]

(G14)

We now take \( y, \delta \ll 1 \), with this \( \frac{\partial H}{\partial y} \) is approximately given by:

\[
\frac{\partial H}{\partial y} = -4 (t - X) z \chi + U \left( \frac{1}{4} - \frac{\delta^2}{4y^2} \right) - 3 \left[ \frac{(-y^2 + \delta^2)}{y^2} \right] z J \chi^2 = 0
\]

(G15)

Where we have taken:

\( y = O(\delta) \),

(G16)

and have kept only the order one terms, the rest will not contribute to the Mott gap. Where we used approximations like:

\[
-2 \frac{\delta}{y^2} \left[ 1 - \frac{(1 - y)^2}{1 - \delta^2} \right] \approx -4 \frac{\delta}{y}
\]

(G17)

We now rewrite Eq. (G15) as:

\[
y^2 \left[ -4 (t - X) z \chi + \frac{U}{4} + 3 z J \chi^2 \right] = \delta^2 \left[ \frac{U}{4} + 3 z J \chi^2 \right]
\]

(G18)

In this case:

\[
y = |\delta| \sqrt{\frac{|U + 12 z J \chi^2|}{|U + 12 z J \chi^2|}} = |\delta| \frac{\varsigma}{c}
\]

(G19)

From this we see that

\[
U_c = 16 \left( t - X \right) z \chi - 12 z J \chi^2
\]

(G20)

is the critical onsite Hubbard interaction where the Mott gap opens. This matches with Eq. (78) from the main text. We now write [81]

\[
y_\pm = \frac{|\delta|}{\varsigma}
\]

\[
e^2 = \left( \frac{y}{4} + \frac{\delta}{2} + \frac{\delta^2}{4y} \right) - \delta = \left( \frac{|\delta|}{4\varsigma} + \frac{|\delta| \varsigma}{4} - \frac{\delta}{2} \right) = \varsigma_{\pm} |\delta|
\]

\[
d^2 = \left( \frac{y}{4} + \frac{\delta}{2} + \frac{\delta^2}{4y} \right) = \left( \frac{|\delta|}{4\varsigma} + \frac{|\delta| \varsigma}{4} + \frac{\delta}{2} \right) = \varsigma_{\pm d} |\delta|
\]

\[
p^2 = \frac{1}{2} \left( \frac{|\delta|}{4\varsigma} + \frac{|\delta| \varsigma}{4} \right)
\]

(G21)
We then have that
\[ \sqrt{\xi_d} = \sqrt{\frac{1}{4\epsilon_0} + \frac{\xi}{4} + \frac{1}{2}} \]
\[ \sqrt{\xi_e} = \sqrt{\frac{1}{4\epsilon_0} + \frac{\xi}{4} + \frac{1}{2}} \] (G22)

3. The Mott gap

Now going back to Eq. (G5) we get that:
\[ \langle H \rangle = \langle H_0 \rangle + \lambda^{(1)} (e^2 + 2p^2 + d^2 - 1) + \lambda^{(2)} (2p^2 + 2d^2 - 2 \langle f^d f \rangle) - \mu (n - 2 \langle f^d f \rangle) \]

We then have that
\[ \langle H_0 \rangle = -2 \left( \frac{(e + d)^2 - 2p^2}{1 - d^2 - p^2} \right) tz\chi + Ud^2 + 2V ((c^d c)^2 - \frac{3}{4} \left( \frac{p^2}{1 - p^2} (p^2 + d^2) \right)^2 z\chi^2 \]
\[ - \left( \frac{e^2 - d^2 + \frac{d^2}{(p^2 + d^2)}}{1 - p^2 - d^2} \right) V z\chi^2 + \frac{YZ}{z^2} \left( \frac{d^2}{1 - p^2 - d^2} (1 - e^2 - p^2) z\chi X \right) \]
\[ + 4 \left( \frac{1}{1 - d^2 - p^2} (1 - e^2 - p^2) z\chi X \right) \] (G23)

Furthermore:
\[ 0 = \frac{\partial \langle H \rangle}{\partial \langle f^d f \rangle} \Rightarrow \mu = \lambda^{(2)} \] (G24)

Therefore:
\[ \lambda^{(2)} = \text{const} - 2 (t - X) z\chi \left[ \frac{e}{d} - \frac{d}{e} \right] + \ldots \]
\[ = \text{const} - 2 (t - X) z\chi \left( \frac{\sqrt{\xi_d}}{\sqrt{\xi_e}} - \frac{\sqrt{\xi_e}}{\sqrt{\xi_d}} \right) \] (G27)

Form this we see that:
\[ \Delta \mu = \lambda^{(2)} - \lambda^{(2)} \] (G28)

This means that
\[ \Delta \mu = 4 (t - X) z\chi \left[ \frac{\sqrt{\xi_d}}{\sqrt{\xi_e}} - \frac{\sqrt{\xi_e}}{\sqrt{\xi_d}} \right] \]
\[ = \frac{16 ((t - X) z\chi)}{\sqrt{U + 12zJ^2} - \sqrt{U - 16z^2}} \] (G29)

a. Simplifying the expressions

We write:
\[ \bar{U} = U + 12Jz\chi^2 \]
\[ \bar{t} = t - X \] (G30)

Then
\[ \Delta \mu = 16z\chi \bar{t} \]
\[ \sqrt{U - 16z^2} \] (G31)

We now introduce
\[ \bar{U}_c = 16z\chi \bar{t} \] (G32)

Then
\[ \Delta \mu = \sqrt{\bar{U}_c} \sqrt{\bar{U}} \] (G33)

We note that this result matches Eq. (??). Then there are two cases to consider \( \delta \bar{U} \equiv \bar{U} - \bar{U}_c \ll \bar{U}_c \) and \( \bar{U} \gg \bar{U}_c \)

Case \( \delta \bar{U} \ll \bar{U}_c \) Then
\[ \Delta \mu \approx \bar{U}_c \sqrt{\delta \bar{U}} \] (G34)

Case \( \bar{U} \gg \bar{U}_c \) Then
\[ \Delta \mu \approx \bar{U} - \frac{1}{2} \bar{U}_c \] (G35)

Appendix H: Calculating the embedding Hamiltonian

We would like to qualitatively motivate the results of the previous section that the gap does not depend on \( V \) and \( Y \) by studying the embedding Hamiltonian (48) (49). To do so we note that for cases when some of the variables \( \{ R_\sigma, S_\sigma, T_\sigma, T, U \} \), \( \{ R_\sigma^*, S_\sigma^*, T^*, U^* \} \) become zero the corresponding piece of the embedding Hamiltonian becomes zero. Indeed taking derivatives we get that:
Indeed, taking appropriate combinations of derivatives of the Lagrange function, we get:
\[
\begin{align*}
\frac{\partial L}{\partial R_\sigma} &= 0 \Rightarrow 0 = \langle \Psi_0 | -t \sum_{(RR')\sigma} R^*_R f^\dagger_{RR'} f_{RR'} + X \sum_{(RR')\sigma} S^*_R f^\dagger_{RR'} f_{RR'} | \Psi_0 \rangle = D_\sigma \sqrt{(1 - \Delta_\sigma)} \Delta_\sigma \\
\frac{\partial L}{\partial S_\sigma} &= 0 \Rightarrow 0 = \langle \Psi_0 | X \sum_{(RR')\sigma} R^*_R f^\dagger_{RR'} f_{RR'} | \Psi_0 \rangle = E_\sigma \sqrt{(1 - \Delta_\sigma)} \Delta_\sigma \\
\frac{\partial L}{\partial T} &= 0 \Rightarrow 0 = -z J \Delta^\alpha_{(n,n)} \Delta^\beta_{(n,n)} T^* = F \sqrt{(1 - \Delta_T)} \Delta_T \sqrt{(1 - \Delta_\xi)} \Delta_\xi \\
\frac{\partial L}{\partial U} &= 0 \Rightarrow 0 = \frac{z}{2} Y \left( \sum_\sigma \Delta^\alpha_{(n,n)} \Delta^\beta_{(n,n)} \right) U = G \sqrt{(1 - \Delta_T)} \Delta_T \sqrt{(1 - \Delta_\xi)} \Delta_\xi
\end{align*}
\] (H1)

From this we see that \( G, F, E_\sigma, D_\sigma \) vanish whenever \( U, T, S_\sigma, R_\sigma \) vanish. The situation with \( F_a \) is more complex. The coefficients \( T_{\sigma a} \) do not vanish simultaneously anywhere in the phase diagram but instead satisfy \( T_{\uparrow \uparrow} = -T_{\uparrow \downarrow} = T_{\downarrow \uparrow} = -T_{\downarrow \downarrow} \) when \( \eta = 0 \), \( \Delta^\alpha_{(n,n)} = \Delta^\beta_{(n,n)} = \Delta_{(n,n)} = \chi \) and \( \Delta_a = \Delta_\bar{a} = \Delta = n_a = n_\bar{a} = n = \frac{1}{2} \) (we note that \( \Delta_\bar{a} = n_a \) is a direct consequence of our assumption that \( [\Lambda_R, F^0_R] = 0 \)). We will now show that this implies the following relations between the coefficients \( F_{\sigma a} \):
\[
F_{\uparrow \uparrow} = -F_{\uparrow \downarrow} = F_{\downarrow \uparrow} = -F_{\downarrow \downarrow} = \hat{F}
\] (H2)

Indeed, taking appropriate combinations of derivatives of the Lagrange function, we get that:
\[
\begin{align*}
\frac{\partial L}{\partial T_{\sigma a}} + \frac{\partial L}{\partial \tilde{T}_{\sigma a}} &= 0 \Rightarrow 0 = -2 z V \sum_{\sigma'} \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} T_{\sigma a} + \frac{z}{4} \sum_{\sigma'} (\sigma + \tilde{\sigma}) \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} + \frac{z}{4} \sum_{\sigma'} (\sigma + \tilde{\sigma}) \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} \\
&= F_{\sigma a} (1 - \Delta_a) \Delta_a + F_{\tilde{\sigma} a} (1 - \Delta_\bar{a}) \Delta_\bar{a} \\
\frac{\partial L}{\partial T_{\sigma a}} + \frac{\partial L}{\partial \tilde{T}_{\sigma a}} &= 0 \Rightarrow 0 = -2 \sum_{\sigma'} \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} T_{\sigma a} - 2 \sum_{\sigma'} \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} + 2 \sum_{\sigma'} \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} \\
&+ \frac{z}{4} \sum_{\sigma'} \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} + \frac{z}{4} \sum_{\sigma'} \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} + \frac{z}{4} \sum_{\sigma'} \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} \\
&= F_{\sigma a} (1 - \Delta_a) \Delta_a + F_{\tilde{\sigma} a} (1 - \Delta_\bar{a}) \Delta_\bar{a}
\end{align*}
\] (H3)

From this we get that Eq. (H2) follows. In particular at half filling for \( \eta = 0 \) we have that
\[
H_{\text{embed}} = U c^\dagger_a c^\dagger_\bar{a} c_\bar{a} + \sum_\sigma \lambda^a_\sigma f_\sigma f^\dagger_\sigma + \left[ F c^\dagger_\sigma c_\sigma + \tilde{F} \sum_\sigma \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} \tilde{T}_{\sigma a} + \sum_\sigma \bar{\lambda}^a_{\sigma} c^\dagger_{\sigma a} \tilde{c}^\dagger_{\bar{a}} \right] \] (H4)

We see that there is no density density type of interaction or pair hopping. We note that we can get a relation between \( F \) and \( \hat{F} \) via:
\[
F = \frac{-z J \Delta^\alpha_{(n,n)} \Delta^\beta_{(n,n)} T^*}{\sqrt{(1 - \Delta_T)} \Delta_T \sqrt{(1 - \Delta_\xi)} \Delta_\xi} = \frac{-z J \chi^2 T^*}{(1 - \Delta) \Delta}
\]
\[
\frac{\delta L}{\delta T_{\uparrow \uparrow}} = 0 \Rightarrow -\frac{1}{4} \sum_{\sigma \sigma'} \sigma' \Delta^\alpha_{\sigma a} \Delta^\beta_{\sigma a} T_{\sigma a} = \hat{F} (1 - \Delta_T) \Delta_T \Rightarrow \hat{F} = -\frac{-z J \chi^2 T^*}{2 (1 - \Delta)} \] (H5)

We now use that \( T_{\uparrow \uparrow} = \frac{\hat{T}}{2} = 1 \). Therefore we have that:
\[
H_{\text{embed}} = U c^\dagger_a c^\dagger_\bar{a} c_\bar{a} + \sum_\sigma \lambda^a_\sigma f_\sigma f^\dagger_\sigma - 8 z J \chi^2 \left( \tilde{S}_c \cdot \tilde{S}_f \right) + \sum_\sigma \lambda^b_\sigma c^\dagger_{\sigma a} \tilde{c}^\dagger_{\bar{a}} \] (H6)

Here \( \tilde{S}_c \) is the spin operator for the impurity and \( \tilde{S}_f \) is the spin operator for the bath. We note that the term:
\[
- \sum_\sigma F_a \bar{c}_\sigma c^\dagger_\sigma \Delta_a = 0
\] (H7)
due to Eq. (H2). We note that the parameters \( V \) and \( Y \) do not enter the embedding Hamiltonian at half filling in the Brinkman Rice phase.
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