Low-energy effective Hamiltonians for correlated electron systems beyond density functional theory

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We propose a refined scheme of deriving an effective low-energy Hamiltonian for materials with strong electronic Coulomb correlations beyond density functional theory (DFT). By tracing out the electronic states away from the target degrees of freedom in a controlled way by a perturbative scheme we construct an effective model for a restricted low-energy target space incorporating the effects of high-energy degrees of freedom in an effective manner. The resulting effective model can afterwards be solved by accurate many-body solvers. We improve this “multi-scale ab initio scheme for correlated electrons” (MACE) primarily in two directions: (1) Double counting of electronic correlations between the DFT and the low-energy solver is avoided by using the constrained GW scheme. (2) The frequency dependence of the interaction emerging from the partial trace summation is taken into account as a renormalization to the low-energy dispersion. The scheme is successfully tested on the example of SrVO₃. Our work opens unexplored ways to understanding the electronic structure of strongly correlated systems beyond current DFT methods.

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I. INTRODUCTION

Strongly correlated electron systems are widely found in condensed matter and have proven to generate many attractive phenomena and fundamental concepts including quantum phase transitions and fluctuations such as superconducting and metal-insulator phenomena with potential applications to future technology. Their accurate and ab initio theoretical treatment with predictive power is therefore one of the grand challenges of nowadays condensed matter physics. However, conventional ab initio computational schemes based on density functional theory (DFT) or many-body perturbation theory in the so-called GW approximations are known to encounter serious difficulties when electronic correlation effects are crucial.

Recently proposed versatile multi-scale methods that make use of the hierarchical energy structure of strongly correlated electrons (hereafter abbreviated as MACE, for “multi-scale ab initio schemes for correlated electrons”) have opened the way to the design of increasingly accurate methods, which are now overtaking the conventional ones. In strongly correlated electron systems in condensed matter, the low-energy degrees of freedom (L part) represented by the bands near the Fermi level in the DFT or GW scheme are typically sparse and isolated from the high-energy degrees of freedom (H part) obtained as dense bands away from the Fermi level. This is not accidental because the isolation of the H and sparse L part is a necessary condition for the strong electron correlation. (Otherwise, it would be a weakly correlated system because of the screening by the H part or by self-screening by the L part. For a more extended discussion, see Ref. ⁴). MACE schemes take advantage of this hierarchical separation in the energy space to treat the L part within highly accurate but relatively expensive numerical techniques that could not be used directly for the full space in contrast to molecules and clusters treated in quantum chemistry and nuclear physics. For the H part on the other hand, cheaper techniques can be employed thanks to less significant quantum fluctuations.

Motivated by the fact that the H part behaves effectively as an insulator with a gap around the Fermi level once the dynamics within the L part is excluded, one can treat it in a controllable and accurate way by conventional methods such as the DFT within the local density approximation (LDA) or GW. This is not in contradiction to the fact that our target materials are strongly correlated electron systems and perturbative approaches do not work as a whole, because strong correlation effects appear prominently in the excitations within the L part that will be treated and solved afterwards beyond the LDA or GW. Thanks to their mutual isolation, effects of the H part on the L part can be safely calculated perturbatively in the spirit of the constrained random phase approximation (cRPA). Unlike a partial trace summation only over the H part is taken, effectively determining the renormalization of the L part by the H part.

Physical properties of interest live in most cases on the energy scale of room temperature or below, and certainly within the L part. Therefore, an accurate treatment of the degrees of freedom in the L part is required. This low-energy system (L part) can in fact be solved using nonperturbative many-body tools such as quantum Monte Carlo (QMC) methods and various renormalization group schemes in particular the variational
Monte Carlo (VMC)\textsuperscript{4,9,10,17} – or dynamical mean field theory (DMFT), and related methods\textsuperscript{5,6,13,20} – obtaining results beyond the DFT or standard GW schemes by the combination of the DFT and DMFT (DFT+DMFT)\textsuperscript{21,22}.

Such an \textit{ab initio} hierarchical scheme has proven useful and successful for a wide range of materials questions\textsuperscript{24–26}, from transition metals\textsuperscript{24–26}, their oxides\textsuperscript{27–35}, sulphides\textsuperscript{36}, pnictides\textsuperscript{37–45}, rare earths\textsuperscript{46–48} and their compounds\textsuperscript{49–52}, including heavy fermions\textsuperscript{53–54}, actinides\textsuperscript{55,56} and their compounds\textsuperscript{57} to organics\textsuperscript{58,59}, correlated semiconductors\textsuperscript{60,61}, spin-orbit materials\textsuperscript{62,63} and correlated surfaces and interfaces\textsuperscript{64,65}. In this hierarchical scheme such as the DFT+DMFT, an effective Hamiltonian within a low-energy window around the Fermi level is obtained using the DFT, and this Hamiltonian is then solved by a low-energy solver. This construction thus makes explicit use of the “separability” of high- and low-energy degrees of freedom. However, in most current schemes, little effort is devoted to the electronic structure of the higher energy degrees of freedom – which are simply described at the DFT level – and their influence on the low-energy part.

In practice, examples where electron correlation effects were overestimated have also been found: a typical case are organic conductors\textsuperscript{59,61}, where many-body calculations using cRPA values for the interaction – even after “dimensional downfolding”\textsuperscript{70} – overestimate correlation effects as compared to experiments. Along the same lines, it has been argued that, in iron pnictide compounds, the ratio of the effective Coulomb interactions as estimated within the cRPA to the effective bandwidth of the Kohn-Sham band structure of the DFT is slightly overestimated as compared to experimental results\textsuperscript{71,72}. On the other hand, it is known that the neglect of dynamical effects in the screening by the H part leads to an underestimation of correlation effects\textsuperscript{73} (since the effective bandwidth is overestimated\textsuperscript{74}). It was proposed that this subtlety has relevance to the low-temperature metallic and non-magnetic state of FeSe as well as the so-called bicollinear antiferromagnetic order of FeTe\textsuperscript{75}. A further example is the transition metal pnictide BaCo\textsubscript{2}As\textsubscript{2} where dynamical screening effects have been invoked to explain the puzzling absence of ferromagnetism despite a large LDA density of states at the Fermi level\textsuperscript{76}. We will come back to these observations in the discussion section at the end of this paper.

In MACE schemes, the accurate derivation of the effective low-energy models is crucially important for the quantitative level of the predictive power of the calculations. Therefore, the DFT or GW calculations for the global electronic structure including both the L and H part must be consistently bridged to the effective models in the L part. The main challenge consists in avoiding double counting of the electronic correlations and screening already taken into account at the DFT or GW level: In the DFT, Coulomb interactions are treated through the construction of an effective potential, the (Kohn-Sham) exchange correlation potential, while the GW scheme constructs a frequency-dependent many-body self-energy (albeit in a perturbative manner). On the other hand, the low-energy effective models are solved by low-energy solvers, where the electron correlation effects are more accurately treated within this low-energy degrees of freedom. Therefore, there exists overlap in treating the low-energy part of the electron correlation. This is known as the “double counting problem”, and a careful and improved treatment to avoid double counting is required.

At the DFT level, the nonlinear dependence of the exchange-correlation potential on the electronic density makes the formal separation of the correlation energy contributions stemming from a subset of orbitals an ill-defined problem. On a conceptual level, strictly double counting-free schemes are therefore only possible when avoiding the use of the DFT altogether. Double-counting-free schemes can be defined e.g. based on many-body perturbation theory: in this case, the exchange-correlation potential is replaced by a perturbative self-energy, calculated directly in a Green’s function language. The combined “GW+DMFT” scheme\textsuperscript{74} illustrates the advantages of such an approach. A simpler scheme, derived from the GW+DMFT, is the recently proposed “screened exchange dynamical mean field theory”\textsuperscript{75,76}, where the DFT exchange-correlation potential is eliminated and replaced by a screened exchange term. We also mention a recent attempt to transfer this concept to the LDA+DMFT scheme\textsuperscript{77}.

These considerations motivate the construction of effective low-energy Hamiltonians based on many-body perturbation theory for the H part, rather than on the Kohn-Sham Hamiltonian of the DFT. As we already mentioned, the perturbative treatment of the H part is indeed justified by the fact that the exclusion of excitations within the L part makes the system “insulating” with the suppressed vertex correction.

A disadvantage is, however, that the resulting effective models are naturally first given as models with frequency-dependent parameters. Indeed, integrating out the high energy degrees of freedom generically generates frequency-dependent effective interactions and hopping. It is very useful to further reduce such models to effective Hamiltonian forms because low-energy solvers for frequency-independent Hamiltonians are computationally less demanding. In this paper, we develop a consistent and accurate \textit{ab initio} framework of deriving the low-energy effective Hamiltonian of the L part in view of the construction of a complete MACE scheme. Our aim in the present article is to derive low-energy effective models for the L-space that are as accurate as possible and can be treated by sophisticated low-energy solvers in the subsequent step.

The paper is organized as follows: In Section II A, we describe the general strategy to be employed. In section III we give a first outline of the equations, followed by the detailed derivations in Section IV. Section V presents a concise summary of the obtained scheme, while
Section IV explains variants of the scheme. In Section IV, we present calculations on the perovskite oxide SrVO$_3$, illustrating how the scheme works and giving practical information on the relative importance of the different terms. Finally, we present our conclusions and perspectives in Section VII.

II. OUTLINE OF DERIVATION OF
LOW-ENERGY EFFECTIVE HAMILTONIAN

A. General strategy

We decompose the full Hilbert space into low-energy (the L space) and high-energy subspaces (the H part) thanks to the hierarchical structure of strongly correlated electron systems as described in Sec. II. Our construction for the decomposition and bridging between the two parts will be based on the GW scheme, since this allows for a well-defined way to avoid double-counting. Indeed, at the DFT level, after identifying the H- and L-spaces, the partial trace summation and the elimination of the H-space can be performed by means of the cRPA$^{12}$, as described below. However, when the low-energy part is solved by a refined many-body solver, some part of the interactions are counted twice since the initial DFT calculation already contains the correlation effects for the L part. Indeed, the DFT considers the exchange correlation contribution without distinguishing the L- and H-spaces, and it is impossible to disentangle the two spaces at this level. The GW scheme, instead, allows for the subtraction of the double counting by calculating a constrained self-energy as constructed in Ref. 78. This constrained self-energy incorporates the interactions in the form of a self-energy from which the contribution of the L part has been excluded.

After eliminating the H-space, the L-space is expressed by single-, two-, three-particles, and even higher terms. However, the effective many-body interaction higher than the two-particle channel is expected to be small if the target L-space is isolated from the H-space. This is true in typical strongly correlated systems, and motivates a perturbative treatment of the H-L-coupling. In this article, we ignore multi-particle effective interactions of higher order than the two-body terms.

The single-particle (kinetic energy) terms are modified (renormalized) by the constrained self energy. The two-particle (effective Coulomb interaction) terms are represented as the partially screened interaction obtained from the cRPA$^{12}$. In general, the self-energy and the screened interaction are frequency-dependent, thus not allowing for a representation in a Hamiltonian form.

As mentioned above, in this paper, we focus on methods that derive the low-energy effective models described in the form of Hamiltonians

\[ H_{\text{eff}} = \sum_q T_{\text{eff}}(q)c_q^\dagger c_q + \sum_{q,k,p} W_H(q)c_k^\dagger c_{k+q}c_p^\dagger c_{p-q}, \]

where the renormalized single particle dispersion $T_{\text{eff}}(q)$ after incorporating the self-energy effect and the effective interaction $W_H(q)$ screened by the H part constitute the model for the electrons in the L part represented by the creation (annihilation) operators for the electron, $c_k^\dagger(c_k)$ at momentum $k$. Here, for simplicity, spin and orbital indices are omitted.

Our task at this stage is thus to map the model with frequency dependent single- and two-particle terms onto a frequency-independent Hamiltonian in a controlled way. For this mapping, we propose a scheme that combines the merits of the works by Hirayama et al.$^{22}$ and Casula et al.$^{22}$. In a step-by-step procedure, we include the influence of the H-space into the L-space and eliminate the frequency dependence by taking into account its effect on the Hamiltonian in the form of an effective renormalization of the parameters.

We remark that, in practice, the derived effective low-energy Hamiltonian satisfies the following principle: If one solved the effective low-energy Hamiltonian within the GW-type perturbative treatment instead of the accurate low-energy solver, that would yield the same result as the solution obtained by the same perturbative scheme starting from the full space including the H and L parts. This is called the "chain rule", which justifies the effective Hamiltonian as that for the L part.

Renormalized single-particle Hamiltonian Our starting point for the single-particle part is the DFT band dispersion denoted by $\epsilon_{\text{DFT}}(q)$ and the corresponding Kohn-Sham Hamiltonian $H^{(0)} = \sum_q \epsilon_{\text{DFT}}(q)c_q^\dagger c_q$. Here, $c_q^\dagger(c_q)$, is the creation (annihilation) operator of an electron with wavevector $q$. We have suppressed the spin and band indices for simplicity. Then, the single particle Green's function $G_{\text{DFT}}(q,\omega)$ reads

\[ G_{\text{DFT}}(q,\omega) = \frac{1}{\omega - \epsilon_{\text{DFT}}}. \]

On the DFT level, electronic correlations are taken into account in the form of an effective exchange correlation potential $V_{\text{xc}}(q)$. As discussed above, treating the electron correlation effects in the L-space explicitly within the low-energy solver would lead to a double counting of electronic correlation in the L-space. To avoid the double counting, $V_{\text{xc}}(q)$ is subtracted and replaced by a corrective self-energy $\Delta \Sigma(q,\omega)$. By incorporating $\Delta \Sigma$, the effective single-particle part reads

\[ T_{\text{eff}}(q,\omega) = \epsilon_{\text{DFT}} - V_{\text{xc}}(q) + \Delta \Sigma(q,\omega). \]

B. H-space contribution to self-energy: constrained self-energy

$\Delta \Sigma$ comes from two contributions; $\Delta \Sigma = \Delta \Sigma_H + \Delta \Sigma_L$. $\Delta \Sigma_H$ is the contribution to the self-energy from the H space, while $\Delta \Sigma_L$ is from the frequency dependent part of the effective interaction incorporated into the self-energy, which is the constrained self-energy effect within the L space obtained by excluding the self-energy arising from...
the static effective interaction $W_H(q)$. Here, we sketch the idea for $\Delta \Sigma_H$ and discuss $\Delta \Sigma_L$ in the next subsection. A specific form for the correction $\Delta \Sigma_H$, dubbed “constrained self-energy”, was already derived in Ref. 78, based on a restricted GW calculation. The basic prescription is to add only the self-energy arising from the contribution of the H-space, by excluding the part stemming purely from the L-space. The reason why one should exclude the self-energy stemming from the L-space is that this part is more accurately calculated within the low-energy solver afterwards.

C. Renormalization to self-energy from frequency-dependent partially-screened interaction

The cRPA\textsuperscript{12} was proposed as a means to calculate the effective local Coulomb interactions to be used in the L-space from a systematic first-principles procedure. It can be understood as a way of tracing out the H-space for deriving the effective interaction, while keeping track of the resulting renormalization of the L-space degrees of freedom. The tracing out of the H-space by the standard cRPA results in an effective interaction for the two-particle part of the model in the L-space in the form

$$W_H(q, \omega) = \frac{v(q)}{1 - P_H(q, \omega)v(q)}; \quad (4)$$

where the wave-number ($q$) dependent bare Coulomb interaction $v$ is partially screened by the partial polarization $P_H$. Here, $P_H$ is defined in terms of the total polarization $P$ by excluding the intra-L-space polarization $P_L$: $P_H \equiv P - P_L$. $P_L$ involves only screening processes within the L-space.

Here, $W_H$ is frequency dependent as schematically illustrated in Fig. 1. However, most many-body calculations in the literature that use the effective interactions from the cRPA method or similar schemes neglect this frequency-dependence (exceptions are Refs. 71, 72, 74, 78, 79, 80, 81, 82, 83, 84, 85), and use only the zero-frequency value of the interaction $W_H(q, \omega = 0)$ for the construction of the low-energy effective Hamiltonian\textsuperscript{12, 78}.

We note that this static limit $W_H(q, \omega = 0)$ obtained by using Eq. 4 in fact satisfies the above mentioned chain rule: The whole dynamical interaction emerging when one solves the whole H- and L-space degrees of freedom by RPA is the usual fully screened interaction $W(q, \omega)$ given by

$$W(q, \omega) = \frac{v(q)}{1 - P(q, \omega)v(q)}; \quad (5)$$

as is depicted in Fig. 1.

On the other hand, if we calculate the screening by the RPA within the L-space by regarding as if $W_H(q, \omega = 0)$ would be the bare interaction, this leads to a screened interaction

$$W_L(q, \omega) = \frac{W_H(q, \omega = 0)}{1 - P_L(q, \omega)W_H(q, \omega = 0)}. \quad (6)$$

which is depicted schematically in Fig. 1. Here, $P_L$ is the RPA polarization in the low-energy subspace. Note that $W_L(q, \omega \to \infty) = W_H(q, \omega = 0)$. Then the chain rule $W_L(q, \omega) = W(q, \omega = 0)$ can be proven\textsuperscript{12}.

However, the static $W_H(q, \omega = 0)$ amounts to neglecting the frequency dependent part

$$W_{H}^{\text{dyn}}(q, \omega) \equiv W_H(q, \omega) - W_H(q, \omega = 0) \quad (7)$$

depicted by the vertical hatching in Fig. 1. In this paper, we will take into account the contribution of this dynamical part as the renormalization to the kinetic energy part, either as a perturbative self-energy or in a nonperturbative fashion. In the effective low-energy model, we then keep $W_H(q, \omega = 0)$ for the effective interaction. In the case of the perturbative treatment, for example, the contribution to the self-energy $\Delta \Sigma_L$ is

$$\Delta \Sigma^{\text{Pert}}_L = G_L W_{H}^{\text{dyn}}(q, \omega) \quad (8)$$

as was formulated in Ref. 78 and we review in detail in the next section.

![FIG. 1. (Color online) Schematic frequency dependence of effective interaction screened from bare interaction $v$, and obtained from full RPA (GW) ($W$), cRPA ($W_H$) and screened interaction by RPA ($W_L$) within low-energy effective model at the effective interaction $U = W_H(\omega = 0)$. This is only a qualitative feature and more realistic dependence is seen in Fig. 10.](image)

We also remark that the dynamical part to be considered can be improved from Eq. 7 in a more consistent manner: Since the screening on the RPA level within the L-space is $W_L$ in Eq. 6, one realizes that the dynamical part of the interaction ignored when we use the low-energy solver is

$$W_{GW}^{\text{dyn}}(q, \omega) \equiv W(q, \omega) - W_L(q, \omega) \quad (9)$$

as depicted as the horizontal hatching in Fig. 1.
Then we need to take into account the renormalization (namely, self-energy effect) originating from \( W_{\text{GW}}^{\text{dyn}}(q, \omega) \) instead of \( W_{\text{H}}^{\text{dyn}}(q, \omega) \). The perturbative contribution to the self-energy then replaces Eq. (5) with

\[
\Delta \Sigma_{\text{L}}^{\text{GW}} = G_{\text{L}} W_{\text{GW}}^{\text{dyn}}(q, \omega). \tag{10}
\]

Using \( W_{\text{GW}}^{\text{dyn}}(q, \omega) \) in Eq. (10) replacing \( W_{\text{H}}^{\text{dyn}}(q, \omega) \) is expected to improve the self-energy, because it takes into account the missing part of the L-space dynamics on the GW level and satisfies the chain rule even for the self-energy as we show in the following.

A conventional one-shot GW calculation in the full space gives full self-energy from the fully screened Coulomb interaction \( W \) (Eq. (5)) as

\[
\Sigma = G_{\text{L}} W \tag{11}
\]

(Note: we write here and in the following symbolically \( W_{\text{L}}^{\text{GW}} \).)

Then \( \Sigma = \Delta \Sigma_{\text{L}}^{\text{GW}} + \Sigma_{\text{L}} \) is obviously satisfied, which is the chain rule for the self-energy. In this article, we compare the results calculated from the two choices, Eq. (7) and Eq. (10) in examples to gain into physical insights.

The effective model is then given by

\[
H_{\text{eff}} = \sum_{q, \omega} T_{\text{eff}}(q, \omega) c_{q}^\dagger c_{q} + \sum_{q, k, p} W_{\text{H}}(q, 0) c_{k}^{\dagger} c_{k+q} c_{p} c_{p-q}, \tag{12}
\]

with \( T_{\text{eff}} \) given by Eq. (4) by employing either \( \Delta \Sigma_{\text{L}}^{\text{Pert}} \) or \( \Delta \Sigma_{\text{L}}^{\text{GW}} \) for \( \Delta \Sigma_{\text{L}} \) contained in \( \Delta \Sigma \) in Eq. (5).

The effective Hamiltonian of the DFT, even though other choices are possible. We assume that the block diagonality should be a good starting point, because in many typical correlated materials such as typical transition metal oxides, the bands that have dominantly the character of the localized orbitals are energetically separated from itinerant bands such as ligand bands. This fact helps the construction of effective models since it implicitly guarantees the existence of such a basis set. Indeed, vertex corrections that would mix the two spaces decrease with the energetic separation.

A consequence of the block diagonality is that the non-interacting Green’s function \( G_{i}^{(0)} \) is also block-diagonal and can be decomposed into

\[
G_{i}^{(0)} = G_{ii}^{(0)} |L \rangle \langle L| + G_{ih}^{(0)} |H \rangle \langle H| \tag{15}
\]

where the bra-kets are a shorthand for projectors onto the respective subspaces.

We stress that \( \Sigma \) in Eq. (11) is not in general block-diagonal. Rather, it has both off-diagonal and diagonal components, e.g.:

\[
\Sigma_{\text{ll}} = G_{ll}^{(0)} W_{\text{llll}} + G_{hh}^{(0)} W_{\text{hhhh}} - V_{\text{cell}} \tag{16}
\]

\[
\Sigma_{\text{lt}} = G_{ll}^{(0)} W_{\text{llrt}} + G_{hh}^{(0)} W_{\text{hhrh}} - V_{\text{cell}} \tag{17}
\]

Here, \( G_{ab}^{(0)} = -\langle T c_{a}(\tau) c_{b}^{\dagger}(0) \rangle \), where \( a, b \) denote elements of the H- or L-spaces, and \( W_{abcd} \) is the coefficient of the

\[
\Sigma_{\text{ll}} = G_{ll}^{(0)} W_{\text{llll}} + G_{hh}^{(0)} W_{\text{hhhh}} - V_{\text{cell}} \tag{16}
\]

\[
\Sigma_{\text{lt}} = G_{ll}^{(0)} W_{\text{llrt}} + G_{hh}^{(0)} W_{\text{hhrh}} - V_{\text{cell}} \tag{17}
\]

Here, \( G_{ab}^{(0)} = -\langle T c_{a}(\tau) c_{b}^{\dagger}(0) \rangle \), where \( a, b \) denote elements of the H- or L-spaces, and \( W_{abcd} \) is the coefficient of the
interaction term $c_i^e c_q c_i^e c_d$. In the following, we will use the convention that $l$ and $h$ represent degrees of freedom belonging to $L$ and $H$ degrees of freedom, respectively.

This matrix is used to calculate the interacting Green’s function

$$G(q, \omega) = \left[ G^{(0)}(\omega) - \Sigma \right]^{-1}.$$  

Straightforward matrix inversion gives for the $ll$-block (low-energy block) of this Green’s function:

$$G(q, \omega)_{ll} = \frac{1}{G^{(0)}_{ll} - \Sigma_{ll} - \Sigma_{lh} G_{hh} \Sigma_{hl}}.$$  

In the following, we will use this form to extract a corrective self-energy: The latter is given by those parts of $\Sigma_{ll} + \Sigma_{lh} G_{hh} \Sigma_{hl}$ that are generated by the presence of the H-space. This self-energy contribution should be taken into account at the level of the construction of the low-energy effective model, as an effective renormalization of the L-space by the H-space.

B. Interspace exchange term

The last term in the denominator of (19) is an “interspace exchange” self-energy contribution originating from the block-off-diagonal self-energy $\Sigma_{lh} (\Sigma_{hl})$ between L- and H-electrons. While it can in principle be treated by a direct calculation, we prefer to disregard it at this stage. The reason is that, within the low-energy subspace, it is in fact a higher (second) order contribution in the interspace interaction. The interspace exchange interaction is expected to be small if the H- and L-spaces are well separated. In addition, the interspace exchange may at least partially cancel with the first order vertex term.

C. Direct H-space contribution to constrained self-energy

The corrective self-energy that we are interested in here is thus contained in the second but last term in the denominator of (19), the block-diagonal self-energy $\Sigma_{ll}$ given by (17). This quantity includes some influence of the high-energy H-space through (a) the screened Coulomb interaction $W_{lll}$ in the first term and (b) the entire second term. Here, $W_{lll}$ is either $W_H(q, \omega)$ in Eq. (4) or $W(q, \omega)$ in Eq. (5) and the first term contains $\Delta \Sigma_L$. This former part will be discussed in the next subsection. The latter gives

$$\Delta \Sigma_H(q, \omega) = G^{(0)}_{hh} W_{llhl}.$$  

As we will see below its effect is a band narrowing with respect to the Hartree band structure, comparable to the effect of the exchange-correlation potential $V_{xc}$ of the DFT.

This correction can either be applied directly as a frequency-dependent additional self-energy term $\Delta \Sigma_H(q, \omega)$, in which case it leads to a dynamical low-energy model, or one can use a Taylor expanded approximate form. If the low-energy behavior is to a good approximation linear, that is, its frequency dependence is well approximated as

$$\Delta \Sigma_H(q, \omega) = \Delta \Sigma_H(q, \omega = 0) + \Delta \Sigma'_H |_{\omega = 0} \omega,$$  

where $\Delta \Sigma'_H = d \Delta \Sigma_H / d \omega$, then the renormalization factor resulting from this contribution is given by

$$Z_H = \frac{1}{1 - \frac{\partial \Delta \Sigma_H(q, \omega)}{\partial \omega} |_{\omega = 0}}.$$  

At this level the effective kinetic energy is renormalized to

$$T^{(1)}_{\text{eff}}(q) = [\epsilon_{\text{DFT}} - V_{xc} + \Delta \Sigma_H(q, \omega = 0)] Z_H.$$  

D. Frequency-dependence of interactions within low-energy space: non-local part

We finally analyze the remaining term $G^{(0)}_{ll} W_{lll}$, the first term in Eq. (17). The low-energy effective model has to be constructed in such a way that – at the GW level within the L-space – this self-energy would be reproduced. The influence of the H-space, contained in this term through the matrix element of the fully screened interaction $W$ or $W_H$ hereby has to enter in an effective way.

This can be naturally achieved when constructing a model with the dynamical interaction $W_H(q, \omega)$ as given in Eq. (1). One thus obtains at first a model with nonlocal and frequency-dependent interactions, and the task is to map this model onto a frequency-independent Hamiltonian form by effectively renormalizing the Hamiltonian parameters. For that purpose, we treat the nonlocal and local parts of the interaction (two-body) terms separately. We first eliminate the frequency dependence in the nonlocal part by treating it within the perturbative scheme proposed by Hirayama et al. 78. The perturbative treatment is justified, because the corresponding correction is small. On the other hand, the local and frequency-dependent part can be large and we will treat it nonperturbatively in the formalism proposed by Casula et al. 77. This procedure allows for a nonperturbative treatment but is only suitable for local interactions. An additional subtlety arises due to the fact that the nonperturbative treatment does not take on the form of a self-energy but rather a direct renormalization of the hopping. Therefore, no zero-frequency part appears in the procedure by Casula et al., and we therefore retain the local static part explicitly as an additional correction on equal footing as the nonlocal one.

In practice, we first reduce the problem to a low-energy many-body problem where only the local interactions are dynamical, but non-local ones are static. Following the strategy of Hirayama et al. 78, we treat the
non-local dynamical part of the interactions in a perturbative fashion. This amounts to (a) replacing the non-local dynamical interactions \([W_R^{\text{dyn}}(q, \omega)]_{\text{nonlocal}} \equiv W_R(q, \omega) - \sum_q W_R(q, \omega)\) by static non-local interactions \([W_R(q, \omega = 0)]_{\text{nonlocal}}\) and (b) treating the frequency-dependent correction \(W_R^{\text{dyn}}(q, \omega)\) perturbatively as an additional self-energy correction. \(W_R^{\text{dyn}}(q, \omega)\) takes on the form defined in Eq. (8) or Eq. (9) respectively depending on whether the Hartree-like treatment (denoted as \(R=\text{H}\)) or the GW-like treatment (denoted as \(R=\text{GW}\)) is chosen, and – depending on this choice – leads the to the correction Eq. (8) or Eq. (9) respectively.

Such a perturbative correction can be done in two different ways: The straightforward option is simple first order perturbation theory in the difference \([W_R^{\text{dyn}}(q, \omega)]_{\text{nonlocal}}\). This part contains the effects of the frequency-dependence of the interaction neglected in the effective Hamiltonian formalism with \(W_R(q, \omega = 0)\). Again \(R\) denotes either the Hartree-like or GW-like treatment (“\(H\)” or “\(\text{GW}\)”). We will discuss both options in the following paragraphs.

1. Direct perturbation theory

To first order, the simple perturbative option results in a correction term (for simplicity, we drop the frequency summation here)

\[
\Delta \Sigma_{\text{nonlocal}}^{(1)}(q) = \sum_{q'} G^{(1)}(q') [W_H^{\text{dyn}}(q + q')]_{\text{nonlocal}}
\]

\[
\equiv \sum_{q'} G^{(1)}(q') [W_H^{\text{dyn}}(q + q')] - \sum_q W_H^{\text{dyn}}(q + q')]
\]

\[
\simeq \sum_q G^{(1)}(q') W_H^{\text{dyn}}(q + q')_{\text{nonlocal}}.
\]

(24)

Here,

\[
G^{(1)}(q') \equiv G^{(0)}(q') + V_{xc} - \Delta \Sigma_{\text{H}},
\]

(25)

and \(W_H^{\text{dyn}}(q, \omega)\) is defined in Eq. (7). We stress that the last line of Eq. (24) is not strictly the same as the first line because of the nonzero overlap of the single- and two-particle Wannier bases, as discussed in the Appendix and in Ref. [83]. Nevertheless, as discussed in the Appendix, for sufficiently localized basis sets, the difference between the two previous lines of Eq. (24) is tiny and will be neglected hereafter. In later discussions, we describe this nonlocal part of the self-energy in a simplified notation as

\[
\Delta \Sigma_{\text{nonlocal}}^{(1)}(q) = G^{(1)}[W_H^{\text{dyn}}(q)]_{\text{nonlocal}} \text{ or equivalently }
\]

\[
= [G^{(1)}W_H^{\text{dyn}}(q)]_{\text{nonlocal}}
\]

(26)

2. GW-type perturbation theory

Alternatively, a more refined perturbation theory inspired by the GW approximation can be constructed for the nonlocal part of Eq. (10) as

\[
\Delta \Sigma_{\text{nonlocal}}^{(1)} = G^{(0)}_{\text{GW}} W^{\text{dyn}}_{\text{GW}} - G^{(0)}_{\text{GW}} W^{\text{dyn}}_{\text{GW}}_{\text{local}}.
\]

(27)

Here, \(W^{\text{dyn}}_{\text{GW}}\) as defined in Eq. (9) corresponds to the frequency-dependent part of the interaction that would be missing if the low-energy part were solved within the GW approximation. This justifies to employ the static effective interaction \(W_{\text{H}}(q, \omega = 0) = W_L(q, \omega \rightarrow \infty)\), because \(W_L(q, \omega)\) is the GW counterpart of what will be treated within the low-energy solver afterwards.

We note that without the subtraction of the local part, this correction would correspond to what has been constructed as \(\Delta \Sigma_{\text{L}}\) by Hirayama et al. in Ref. [78]. The local part is not touched here since it will be treated non-perturbatively below, following the work by Casula et al. [79].

Here, \(G^{(0)}(q)\) is used in the spirit of a (non-self-consistent) “one-shot GW” scheme. If one employs a (partially) self-consistent version of the GW scheme, \(G^{(0)}(q)\) may be replaced by \(G^{(2)}\) defined by

\[
G^{(2)}_{\text{GW}} = G^{(0)}_{\text{GW}} - V_{xc} - \Delta \Sigma_{\text{H}} - G^{(0)}_{\text{GW}} W_{\text{GW}}.
\]

(28)

At this level the effective dispersion is renormalized to

\[
T_{\text{eff}}^{(1)}(q) = [\mathcal{D}_{\text{FPT}} - V_{xc} + \Delta \Sigma_{\text{H}}(q, \omega = 0) + \Delta \Sigma_{\text{L}}(q, \omega = 0)]Z_{\text{HL}},
\]

(29)

where \(Z_{\text{HL}} = \frac{1}{1 - \frac{d\Delta \Sigma_{\text{H}}(q, \omega) + \Delta \Sigma_{\text{nonlocal}}^{(1)}(q, \omega, \omega = 0)}{d\omega}}\). Note that here we have included \(\Delta \Sigma_{\text{nonlocal}}^{(1)}(q, \omega = 0)\) as a direct correction, as discussed above. Together with the nonlocal part \(\Delta \Sigma_{\text{nonlocal}}^{(1)}(q, \omega = 0)\) it is thus the full \(\Delta \Sigma_{\text{L}}(q, \omega = 0)\) that enters.

E. Intra-d exchange

The resulting many-body problem with long-range interactions will have an intra-L-space exchange self-energy contribution of Fock form. Also this term takes different forms depending on whether one places oneself in the perspective of option (IIID1) or (IIID2) above.

1. Direct perturbation theory

In the first case, the exchange term is the simple Fock exchange calculated with the static interaction \(W_{\text{H}}(q, \omega = 0)\):

\[
\Delta \Sigma_{\text{L}}^{X} = G^{(1)}_{\text{GW}} W_{\text{H}}(q, \omega = 0).
\]

(30)
Once this term has been taken into account, only the correlation part of the self-energy will have to be calculated within the low-energy effective model.

However, in most practical many-body calculations, local exchange contributions will be kept within the low-energy description in the form of Hund’s coupling terms. We therefore prefer to incorporate only the nonlocal contribution in the one-shot GW as

$$\Delta \Sigma_L^{\text{nonlocal}} = G_{ll}^{(1)} W_L(q, \omega = 0) - \sum_q [G_{ll}^{(1)} W_L(q, \omega = 0)] \quad (31)$$

into the effective one-body Hamiltonian while keeping the local one as a many-body term.

An interesting cancellation is observed when the intra-L-space exchange is combined with the above correction $\Delta \Sigma_L^{\text{nonlocal}}$; the remaining correction

$$\Delta \Sigma_L^{\text{nonlocal}} + \Delta \Sigma_L^{\text{nonlocal}} = [G_{ll}^{(1)} (W_L(q, \omega) - W_L(q, \omega = 0))]_{\text{nonlocal}} + [G_{ll}^{(1)} W_L(q, \omega = 0)]_{\text{nonlocal}}$$

$$\Delta \Sigma_L^{\text{nonlocal}} = [G_{ll}^{(1)} W_L(q, \omega)]_{\text{nonlocal}} \quad (32)$$

reduces to the nonlocal part of a dynamical Fock term, calculated with the interaction $W_L(q, \omega)$, that is, the bare interaction within the low-energy space.

2. **GW-type perturbation theory**

If, however, the GW-like option is chosen for eliminating the frequency-dependence of the local interactions in the low-energy subspace (paragraph 2 above), the intra-L-space exchange should accordingly be interpreted as a screened exchange term. In practice, this means that again a GW-type expression has to be adopted:

$$\Delta \Sigma_L^{\text{nonlocal}} = [G_{ll}^{(0)} W_L(q, \omega)]_{\text{nonlocal}} \quad (33)$$

Combining this term with the above $\Delta \Sigma_L^{\text{nonlocal}}$, a similar cancellation as above is observed:

$$\Delta \Sigma_L^{\text{nonlocal}} + \Delta \Sigma_L^{\text{nonlocal}} = [G_{ll}^{(0)} (W(q, \omega) - W_L(q, \omega))]_{\text{nonlocal}} + [G_{ll}^{(0)} W_L(q, \omega)]_{\text{nonlocal}}$$

$$\Delta \Sigma_L^{\text{nonlocal}} = [G_{ll}^{(0)} W(q, \omega)]_{\text{nonlocal}} \quad (34)$$

The final correction is thus simply the nonlocal part of the usual GW self-energy.

At this stage, the effective dispersion is renormalized to

$$T_{\text{eff}}^{(1)}(q) = [\epsilon_{\text{DFT}} - V_{xc} + \Delta \Sigma_H(q, \omega = 0) + \Delta \Sigma_L^{\text{nonlocal}}(q, \omega = 0) + \Delta \Sigma_L^{\text{nonlocal}}(q, \omega = 0)] Z_{\text{HW}}. \quad (35)$$

where

$$Z_{\text{HW}} = (1 - d(\Delta \Sigma_H(q, \omega) + \Delta \Sigma_L^{\text{nonlocal}}(q, \omega) + \Delta \Sigma_L^{\text{nonlocal}}(q, \omega) / d\omega|_{\omega=0})^{-1} \quad (36)$$

F. **Frequency-dependence of interactions within low-energy space: local part**

The remaining problem is one with dynamical local interactions, for which the correlation part of the self-energy should be calculated. It can be reduced to a problem with purely static interactions following Casula et al. The recipe is to replace the local dynamical interactions by static local interactions while at the same time renormalizing the one-body part of the problem. A subtlety consists however in defining which dynamical interactions to take. We again differentiate the two options above. We also note that the self-energy from local dynamical interaction at zero frequency $\Delta \Sigma_L^{\text{nonlocal}}(\omega = 0)$ is already taken into account in Eq. (29).

1. **Direct perturbation theory**

In this case, the additional renormalization factor resulting from the frequency-dependence of the local interaction is the one derived in the original work by Casula et al.: Indeed, $W_{\text{loc}}^{\text{GW}}(\nu) \equiv \sum_q W(q, \nu)$, the effective dynamical interaction in the low-energy subspace corresponds to what is usually considered as local “Hubbard $U$”, and its frequency-dependence determines the renormalization factor according to

$$Z_B = \exp \left(1/\pi \int_0^\infty d\nu \text{Im} W_{\text{loc}}^{\text{GW}}(\nu)/\nu^2 \right). \quad (37)$$

2. **GW-type perturbation theory**

The GW-type strategy yields a more involved recipe: Defining the local part of Eq. (3), namely

$$[W_{\text{GW}}^{\text{dyn}}(\omega)]_{\text{local}} = \sum_q (W - W_L), \quad (38)$$

one can consider that the model to be treated as this stage is one with an interaction the static part of which is given by $W_L(q, \omega = 0)$ while its dynamical part reads $W_{\text{GW}}^{\text{loc}}$. (By construction $W_{\text{GW}}^{\text{loc}}$ vanishes at zero frequency.) The corresponding renormalization is given by:

$$Z_B = \exp \left(1/\pi \int_0^\infty d\nu \text{Im}[W_{\text{GW}}^{\text{dyn}}(\nu)]_{\text{loc}}/\nu^2 \right). \quad (39)$$
IV. SUMMARY OF THE SCHEME:

[1] Putting the above steps together, one obtains the total constrained self-energy

$$\Delta \Sigma = \Delta \Sigma_H + \Delta \Sigma_{L}^{\text{nonlocal}} + \Delta \Sigma_{L}^{\text{nonlocal}}$$

(40)

resulting in the following scheme:

- Calculate the LDA Hamiltonian in the localized basis. Block-diagonalize it.
- Calculate the sum of the correction self-energies above:

$$\Sigma_{\text{corr}}(q, \omega) = -V_{xc} + \Delta \Sigma.$$  

(41)

If the simple perturbative strategy is adopted, we employ \( \Sigma_{\text{corr}} = \Sigma_{\text{corr}}^{\text{pert}} \) (see II.D1 and II.E1):

$$\Sigma_{\text{corr}}^{\text{pert}}(q, \omega) = -V_{xc} + G_{\text{hh}}^{(0)} W_{\text{hh}} + [G_{\text{ll}}^{(1)} W_{\text{ll}}]_{\text{nonlocal}}$$

(42)

Following the GW-type perturbation theory, it becomes \( \Sigma_{\text{corr}} = \Sigma_{\text{corr}}^{\text{GW}} \) (see II.D2 and II.E2):

$$\Sigma_{\text{corr}}^{\text{GW}}(q, \omega) = -V_{xc} + G_{\text{hh}}^{(0)} W_{\text{hh}} + [G_{\text{ll}}^{(0)} W_{\text{ll}}]_{\text{nonlocal}}.$$  

(43)

This self-energy can be linearized, e.g. around the Fermi level, giving rise to a static correction \( \Sigma_{\text{corr}}(q, \omega = 0) \) and a Z-factor corresponding to its (linearized) frequency-dependence:

$$Z_{\text{corr}} = \frac{1}{1 - \frac{\partial \Sigma_{\text{corr}}(q, \omega)}{\partial \omega}|_{\omega = 0}}.$$  

(44)

[2] The effect of the local dynamical interaction is taken into account as follows:

- Calculate the renormalization factor \( Z_B \) arising from the local part of the frequency dependence in the screened interaction (see II.F1 and II.F2).
- The effective low-energy Hamiltonian is eventually given by

$$H_{\text{eff}}^{(1)} = \sum_q T_{\text{eff}}^{(1)}(q)c_q^\dagger c_q + \sum_{q, k, p} W_{\text{r}}(q, 0)c_k^\dagger c_{k+q}c_{p-q}^\dagger.$$  

(45)

with

$$T_{\text{eff}}^{(1)}(q) = [\xi_{\text{DFT}} + \Sigma_{\text{corr}}(q, \omega = 0)] Z_{\text{corr}} Z_B.$$  

(46)

[4] Solve the many-body problem with the one-body Hamiltonian from the preceding step and the static non-local interactions \( W_{\text{H}}(q, \omega = 0) \). Take care of removing the Hartree contribution from the solution of the many-body problem, in order to avoid double counting with the initial single-particle Hamiltonian where the Hartree potential was included in LDA. This can be done by following the procedure in Ref. [23] where the Hartree solution of the low-energy effective model is subtracted before solving by the low-energy solver. This can also be done as in LDA+U or LDA+DMFT techniques, by calculating the Hartree solution of the effective low-energy model.

V. VARIANTS OF THE LOW-ENERGY MODEL

The above discussion has focused on the construction of an effective low-energy many-body problem with static and local interactions, for which only the correlation part of the self-energy needs to be calculated from the many-body solver. Alternatively, if one uses a many-body solver that can fully handle long-range interactions, a variant of the above scheme can be envisioned. Another variant can be used if one wishes to construct a low-energy model with purely local interactions only. A different variant is useful if one wishes to update the single-particle part of the Hamiltonian, after an improved estimate for the electronic density is available after the many-body calculation. Those are the subject of the following paragraphs.

A. Low-energy model with long-range interactions

If the aim is the construction of a low-energy effective model with fully long-range Coulomb interactions, the treatment of the intra-L-space exchange term can be omitted at the level of the construction of the model. The remaining corrective self-energy reads:

$$\Sigma_{\text{corr}}(q, \omega) = \Delta \Sigma_H + \Delta \Sigma_{L}^{\text{nonlocal}} + \Delta \Sigma_{L}^{\text{nonlocal}}$$

$$= G_{\text{hh}}^{(0)} W_{\text{hh}} + G_{\text{ll}}^{(0)} W_{\text{ll}} + [G_{\text{ll}}^{(0)} W_{\text{ll}}]_{\text{nonlocal}}.$$  

(47)

where the option of direct perturbation theory \( W_{\text{H}}^{\text{dyn}} \) defined in Eq. (47) should be replaced by \( W_{\text{GW}}^{\text{dyn}} \) defined in Eq. (47) for the option of the GW-type perturbation theory.

We note however, that the reduction to a static model using the Casula procedure involves in this case an additional approximation: indeed, strictly speaking, the Casula procedure modifies the non-density-density terms of the interactions, by dressing the creation and annihilation operators with exponential weight factors. This can be seen as follows: the Casula procedure is based on a Lang-Firsov transformation, replacing the original fermionic operators \( c_{i\sigma} \), at \( i \)th site with spin \( \sigma (=\uparrow \text{ or } \downarrow) \), by polaronic operators \( a_{i\sigma} \), thus eliminating the explicit dependence on the bosonic operators \( b_i \) that describe the screening degrees of freedom: \( a_{i\sigma} = \exp(\lambda(b_i - \frac{1}{2}c^{\dagger}_{i\sigma}c_{i\sigma})). \)
B. Effective model with local Hubbard interactions only

The solution of the final many-body problem with nonlocal interactions may in principle be done within many-body solvers suitable for non-local interactions such as various Monte Carlo methods including the variational Monte Carlo methods. Alternatively, extended DMFT (EDMFT) can be viewed as a means to determine an effective local interaction that best represents the effects of the initial long-range interactions, and can be considered as a technique to “backfold” long-range interactions into effective local ones.

Very generally, from the above discussion it becomes obvious that the construction of the one-particle part of the Hamiltonian will depend on which interaction terms will be included in the many-body calculation, while physical properties obtained after solving the low-energy problem are expected to be insensitive to the choice. In the next section, we will see how the derived effective models behave in the case of the simple oxide SrVO$_3$.

C. Update of single-particle Hamiltonian

In some cases, many-body effects substantially change the charge distribution in the low-energy subspace as compared to the LDA one. Such redistributions of charge can for example happen between different orbitals in multi-orbital systems, and have actually been observed e.g. in titanium oxides, BaVS$_3$, or iron-based superconductors. If this happens, one might want to update the starting Hamiltonian and GW self-energies, based on the new charge density rather than the converged LDA one, analogously to what is done in the DFT+DMFT calculations. This effect can induce non-negligible corrections to the relative orbital levels.

Technically, the resulting self-consistency loop is analogous to what has been discussed in detail in the DMFT literature, in particular concerning the way the density is recalculated in the continuum after the solution of the effective model.

VI. RESULTS

The ternary 3d$^1$ transition metal oxide SrVO$_3$ has become one of the “drosophila compounds” of correlated systems. It is a correlated metal that has been characterized using various experimental and theoretical techniques, see e.g., and theoretical data has been given recently in Ref. SrVO$_3$ displays Fermi liquid behavior up to remarkably high temperatures of the order of 200 K, with a moderate mass enhancement of the order of 2. Detailed spectroscopic investigations have made it an ideal test compound for modern many-body calculations, and more and more refined dynamical mean field-based studies are available. The majority of studies so far have focused on the t$_{2g}$-manifold which forms the states close to the Fermi level, and those will also be the focus in the present investigations. Note however that this restriction quite severely limits the range of validity of the low-energy description. Indeed, as shown recently, at energies of about 2 to 3 eV above the Fermi level the spectral properties are largely determined by the e$_g$ states. This has in particular led to a reinterpretation of an inverse photoemission feature at about 2.5 eV that was frequently interpreted as an upper Hubbard band of t$_{2g}$ character in the earlier literature. Here, we use the compound only as an illustration of the principles of constructing effective low-energy models, without being concerned with a description of spectra beyond the pure t$_{2g}$ part.

The LDA band structure of SrVO$_3$ is shown in Fig. The LDA exchange-correlation potential has been subtracted, that is, the eigenvalues of $H_{LDA} - V_{xc}$ where these operators are evaluated for the self-consistent LDA density. The subtraction of $V_{xc}$ widens the band structure from the LDA bandwidth of 2.5 eV to more than twice this value: the new band width is 5.4 eV. This indicates that the exchange-correlation potential $V_{xc}$ of the LDA is responsible for the bandwidth.
possible for a substantial amount of the band-narrowing effect arising from electronic correlations, stressing the need to subtract the double counting in a consistent manner. Figure 4 is regarded as the starting point for the following considerations.

For simple materials (see e.g. the calculations on Li in Ref. 108) it has been noted in the literature that the Hartree band structure is close to the DFT one. This raises the question of the origin of the substantial band widening in the present case. Indeed, the present calculation shown in Fig. 4 differs from a Hartree calculation only by the fact that Fig. 4 is evaluated for the converged LDA density. We have performed a test calculation where we plot the Hartree band structure calculated for the converged Hartree density. The result is shown in Fig. 5. As seen from this plot, while the band is not fully as wide as in Fig. 4 a substantial widening is already present at this stage.

Starting from the Hamiltonian without $V_{xc}$ (see the dispersion in Fig. 1), we first take into account the static part of the corrective self-energy $\Delta \Sigma_H$: In Fig. 6 we plot the dispersion corresponding to $H_{LDA} - V_{xc} + \Delta \Sigma_H(\omega = 0)$. Compared to the dispersion of Fig. 4 the overall band structure is narrowed to 3.7 eV. This value is, however, still considerably larger than the LDA bandwidth (Fig. 2). Although the electronic correlations coupling the H- and the L space are included in Fig. 6 and narrow the band with respect to the case where $V_{xc}$ is taken out, correlations within the L space are not included. The LDA, on the other hand, at least partially includes correlations within the L space, and these are very effective in narrowing the band. Interestingly, the bottom of the occupied band is quite exactly at the LDA value, and the remaining widening is purely in the unoccupied part.

To go further and in particular to analyze the dynamic behavior of $\Delta \Sigma_H$ we plot in Fig. 7 the self-energy corrections $\Delta \Sigma_H$ (with $\Sigma$ (see Eq. (11)) for comparison) for the real and imaginary parts at several representative choices of momenta. The frequency dependence is smooth around the Fermi level. In particular, in contrast to the full self-energy, there are no poles in
\[ \Delta \Sigma_\text{H} \] in the low-energy region, thanks to the exclusion of fluctuations within the L-space. The frequency dependence of the real part indicates that the linearization \( \Delta \Sigma_\text{H}(\omega) \sim \Delta \Sigma_\text{H}(\omega = 0) + [d \Delta \Sigma_\text{H}(\omega)/d \omega]_{\omega=0} \omega \) offers a reasonably good approximation. In fact, the behavior of the constrained self-energy is much closer to linearity than that of the full GW self-energy \( \Sigma \). This is easily understood by the fact that the low-energy excitations are excluded in the present constrained self-energy \( \Delta \Sigma_\text{H} \) analogously to an insulator, thus eliminating the strong frequency dependence of the constrained self-energy near the Fermi level. This is one of the consequences of the controllability and an advantage of the present MACE scheme, as mentioned in the introduction. In the following discussion, we employ this linearized approximation. Then the renormalization factor \( Z_\text{H} \) defined by Eq. (22) is interpreted as that from the contribution of the H-space. After this renormalization factor is taken into account, the effective Hamiltonian is given by \( Z_\text{H}[H_{\text{LDA}} - V_\text{xc} + \Delta \Sigma_\text{H}(\omega = 0)] \) (see Fig. 8). Interestingly the renormalization factor \( Z_\text{H} \approx 0.92 \) stays close to one, so that the bandwidth is only slightly reduced (to 3.4 eV instead of the 3.7 eV above). We also note that \( Z_\text{H} \) has weak momentum dependence as we reveal in the following.

Figure 9 shows the local and nonlocal parts of \( \Delta \Sigma_\text{H} \). The frequency dependence of the local part (Figs. 9 (a)(b)) is quite similar to the frequency-dependent self-energies at various momenta in Fig. 4. One immediately reads off an interesting property, which is akin to what has been found for the full GW self-energy in Ref. 109; namely that the nonlocal part of \( \Delta \Sigma_\text{H} \) shows only weak frequency dependence as shown in Figs. 9 (c)(d). This explains why \( Z_\text{H} \) is only weakly momentum-dependent. On the other hand, \( \Delta \Sigma_\text{H}^{\text{nonlocal}}(0) \) at \( R \) is \( \sim 1 \) eV larger than at \( \Gamma \), which causes the band widening effect. \( \Delta \Sigma_\text{H} \) can thus to a good approximation be decomposed into a frequency-dependent local part and a static nonlocal one: \( \Delta \Sigma_\text{H}(k, \omega) = \Delta \Sigma_\text{H}^{\text{local}}(\omega) + \Delta \Sigma_\text{H}^{\text{nonlocal}}(k) \), with \( \Delta \Sigma_\text{H}^{\text{local}}(\omega) = \sum_q \Delta \Sigma_\text{H}(q, \omega) \).

Since in the simple case of SrVO\(_3\) where the t\(_{2g}\) states are degenerate, static local operators are scalar and are compensated by a chemical potential shift such that the correct particle number is obtained. The above band structure corresponding to \( H_{\text{LDA}} - V_\text{xc} + \Delta \Sigma_\text{H}(k, \omega = 0) \) is thus identical to that of \( H_{\text{LDA}} - V_\text{xc} + \Delta \Sigma_\text{H}^{\text{nonlocal}}(k) \). The local dynamical part of \( \Delta \Sigma_\text{H} \) then results in a narrowing of this band structure by a factor \( Z_\text{H} \approx 0.92 \).

Before turning to a discussion of the low-energy correction for the GW treatment \( \Delta \Sigma_\text{L} = G^{(0)}(W - W_\text{L}) \), we analyze the effective interaction \( W_\text{L} \) shown in Fig. 10 in comparison to \( W \) and \( W_\text{H} \). The fully screened Coulomb interaction \( W \) displays the familiar shape of an interaction that is strongly screened at low energies (with a value of 0.88 eV at \( \omega = 0 \)), while retrieving the value of the bare Coulomb interaction \( v \sim 16.0 \) eV at high energy. The crossover from the bare to the screened values takes place at the plasma energy of about 15 eV. This behavior has been discussed before\(^{23} \); we note in particular that the plasma frequency is known from electron energy loss spectroscopy measurements of the related SrTiO\(_3\) compound\(^{107,110} \). The partially screened interaction \( W_\text{H} \) constructed within cRPA converges to \( W \) at high energies, but displays weaker screening effects at low energies (with a value of 3.5 eV at \( \omega = 0 \)), while intra-t\(_{2g}\) screening channels are excluded. As was already anticipated in Sec. 11, \( W_\text{L} \) can be interpreted as the screened interaction of a low-energy model where a static interaction of value \( \Delta \Sigma_\text{H}(\omega = 0) \) has been imposed as the bare interaction. Since now only intra-t\(_{2g}\) screening channels are active, screening takes place only at low energies, where the scale is given by the t\(_{2g}\) bandwidth. Also plotted is the difference \( W_\text{GW}^{\text{dyn}} = W - W_\text{d} \); except at low energies where the t\(_{2g}\) screening channels come into play, its frequency dependence is essentially given by that of \( W \), while the high-energy limit is the bare Coulomb interaction \( v \) reduced by \( W_\text{H}(0) \).

The frequency dependence of the real and imaginary parts of the low-energy self-energy \( \Delta \Sigma_\text{L} = G^{(1)}W_\text{dyn} \) for the direct perturbative treatment is illustrated in Fig. 11. \( \Delta \Sigma_\text{L} = G^{(0)}W_\text{GW}^{\text{dyn}} \) used for the GW treatment is shown in Fig. 12 for several choices of momenta. The results for the perturbative and the GW treatment are nearly identical. The renormalization factor of \( \Delta \Sigma_\text{L}^{\text{nonlocal}} \) (and \( \Delta \Sigma_\text{L} \)) is \( \sim 0.77 \). The zero-frequency shift \( \text{Re}\Delta \Sigma_\text{L}^{\text{nonlocal}}(0) \) at \( R \) is \( \sim 3 \) eV larger than at \( \Gamma \). Again, one sees how \( \Sigma_\text{L} \) separates into local dynamical and nonlocal static parts: \( \Delta \Sigma_\text{L} = \Delta \Sigma_\text{L}^{\text{nonlocal}}(k) + \Delta \Sigma_\text{L}^{\text{local}}(\omega) \). This is expected since such a separation has been found within the full GW calculations, and is even more plausible for a GW treatment within the t\(_{2g}\) subspace.

The corresponding band structures are given by \( [\epsilon_\text{FFT} + \Delta \Sigma_\text{H} + \Delta \Sigma_\text{L}^{\text{nonlocal}}]Z_\text{HL} \) in Fig. 13 for the perturbative treatment (see Eq. (24)), and in Fig. 14 for the GW treatment, where \( \Delta \Sigma_\text{L}^{\text{nonlocal}} \) is defined in Eq. (27) and \( Z_\text{HL} \) is around 0.92. \( Z_\text{HL} \) is practically the same as \( Z_\text{H} \), meaning that the nonlocal dynamical correction...
FIG. 7. (Color online) Frequency dependence of \( -V_{xc} + \Delta \Sigma_H \) for SrVO\(_3\). (a) and (b) are the real and imaginary parts at the \( \Gamma \) point, respectively, and (c) and (d) ((e) and (f)) are those at \( X \) (\( R \)). For comparison, the full GW self-energies are also given (black dotted line).

in the H-space is small, which justifies the GW perturbative treatment for the nonlocal part. One finds that the nonlocal part \( \Delta \Sigma_L = G^{(0)}_L (W - W_L) \) narrows the empty states but widens the occupied ones, resulting in an overall bandwidth of 3.2 eV. The difference between the direct perturbation and the GW treatment is small.

After including the effect of the local self-energy by the nonperturbative Casula trick, we show the dispersion given by \([\epsilon_{DFT} - V_{xc} + \Delta \Sigma_H + \Delta \Sigma_L^{\text{nonlocal}}]Z_HLZ_B\) for the GW-type treatment in Fig. 14. The GW-like treatment gives a band dispersion close to the LDA one. The \( Z_B \) factor corresponding to the local dynamical part of \( \Delta \Sigma_L \) amounts to \( Z_B = 0.7 \). The nonperturbative treatment results in an LDA-like band dispersion for the empty states, but a slightly narrower bandwidth in the occupied part. The low-energy effective Hamiltonian at this level of treatment has a frequency independent effective interaction both with local and nonlocal interaction given.
by the Fourier transform of $W_H(q, \omega = 0)$, which contains both direct and exchange interactions.

We finally show the dispersion given by Eq. (16), namely $[\epsilon_{\text{DFT}} + \Sigma_{\text{GW}}]_{Z_{\text{corr}}}Z_B$ in Fig. (16). The result shows an LDA-like band dispersion for the occupied states, but a slightly wider bandwidth in the empty part, resulting in a bandwidth $14\%$ wider in total than the LDA bandwidth. The effective interaction of the low-energy effective Hamiltonian at this final level has frequency independent local and nonlocal interactions given by the Fourier transform of $W_{\gamma}(q, \omega = 0)$.

The resulting effective Hamiltonian in the L-space consists of single-particle and two-particle (interaction) parts. The effective interaction is the same as in previous estimates by the cRPA in the literature, while the single-particle dispersion is revised after removing the double counting and taking into account the frequency dependence of the effective interaction. The final effective bandwidth for SrVO$_3$ is, after partial cancellation, slightly (14%) larger than the LDA bandwidth. This is a reasonable result because the LDA takes into account all correlations though insufficiently, while the present scheme by the constrained self-energy excludes the correlation effects arising from the L-space. Although the bandwidth derived for the effective model is slightly larger than that of the LDA, it is clear that the correlation effects are stronger than in the LDA or standard GW when the ab initio model is solved by an accurate solver. In fact, if the effective interaction contained in the final effective model is treated by the GW scheme, one obtains the dispersion illustrated in Fig. (17), which is given from the self energy of the whole GW calculation $\Sigma$ by correcting the local dynamical part $W - W_L$ by $Z_B$. This indicates that even an insufficient treatment of the local static interaction by the GW scheme gives a dispersion with the bandwidth ($\sim 1.9$ eV) narrower than the LDA ($\sim 2.5$ eV, Fig. 2) and GW ($\sim 2.1$ eV, Fig. 3) dispersions. A slightly ($\sim 14\%$) wider dispersion than that of the LDA bands obtained for the effective Hamiltonian accompanied with frequency independent effective Coulomb interactions without the exchange part may account for the slight overestimate of correlation effects in the literature mentioned in the introduction. Our scheme offers an optimized way for the derivation of ab initio models for the L-space after eliminating the H-space in a systematic fashion.

Our findings of the band widening are consistent with studies based on the combined GW+DMFT method in the literature. There, it was argued that within GW+DMFT the best effective Hamiltonian that DMFT should be performed on, is a one-body Hamiltonian corrected by the nonlocal part of the GW self-energy. The corresponding spectral function (see e.g. Figure 5 of Ref. 85) displays a broadening similar to Fig. 14. Most interestingly, our present calculations confirm a pronounced asymmetry observed in Ref. 85, namely a stronger widening effect in the unoccupied part of the spectrum than in the occupied one.

VII. SUMMARY AND CONCLUSION

In this work, we have developed and elaborated a method for a truly first principles electronic description of correlated electron materials. Conceptually speaking, the scheme is based on renormalization group (RG) arguments, which guarantee the existence of an effective Hamiltonian valid at a given energy scale. The difficulty consists, however, in determining this Hamiltonian explicitly, since a direct quantitative RG treatment of the full Coulomb Hamiltonian is a very difficult task and has not been achieved so far. Indeed, performing RG calculations with long-range interactions in the continuum is an even more difficult task than for simplified models, and even for interacting lattice models explicit RG calculations remain a challenge.

Our scheme proposes an indirect way of constructing the low-energy Hamiltonian which can be considered a shortcut to a true RG treatment. The RG has to satisfy the chain rule, where the full trace summation denoted by $R$ can be decomposed into the subsequent two partial trace $R_H R_L$ as required for the semigroup. The first part $R_H$ can be replaced by a perturbative treatment in a controlled approximation because of the well separation of the L- and H- spaces. Then the idea can be understood as working one's way backwards, starting from the full solution obtained within some approximation (here, perturbation theory). The desired low-energy Hamiltonian is constructed such as to fulfill the following requirement: its solution within the same approximation applied to the low-energy subspace only should yield the same result as the projection of the full solution to that subspace. The motivation of this construction resides in the fact that instead of solving the resulting low-energy Hamiltonian within the approximation used for its construction, more accurate many-body solvers can be used for the final solution.
Strongly correlated electron systems provide a natural ground for such a treatment, due to their hierarchical structure in energy space, which facilitates the identification of appropriate low-energy windows. Nevertheless, in practice, the explicit construction of accurate low-energy effective Hamiltonians has remained a challenge due to the difficulties associated to bridging the description of the high-energy degrees of freedom usually treated in the DFT and the low-energy degrees of freedom described by the effective Hamiltonian in a consistent manner. The main obstacles are related to (1) the need of avoiding double counting of correlations and screening in the high- and low-energy treatments and (2) the frequency dependence of parameters in the low-energy effective models.

In this work, we have presented a way to overcome these bottlenecks: we propose a systematic recipe how a low-energy Hamiltonian can be constructed by starting from a perturbative treatment. We provide the best description under the constraint that the effective low-energy Hamiltonian contains only single-particle (kinetic energy term) and two-particle (interaction energy) terms with frequency independent parameters. Our construction relies on a controlled perturbative treatment, which is possible thanks to the hierarchical nature of correlated electron systems: even in cases, where perturbation theory would not provide a meaningful approximation to the full problem, a perturbative treatment of the high-energy degrees of freedom only can be justified thanks to the fact that quantum many-body fluctuations primarily live in the low-energy space only.

On the example of the ternary transition metal compound SrVO₃, we have explicitly demonstrated how this construction works: a low-energy Hamiltonian is built in such a way that a perturbative treatment would reproduce the result of a perturbative treatment in the full space as closely as possible. Solving the resulting many-body Hamiltonian within accurate nonperturbative many-body solvers then provides a description beyond the perturbative treatment, while still keeping the \textit{ab initio} nature of the calculation. We have tested our scheme in a step-by-step manner, identifying the effects of the different corrective terms. Most interestingly, our results confirm recent findings within GW+DMFT calculations on SrVO₃ which identified an intriguing asymmetry in the corrections to an LDA Hamiltonian. Our substantially improved MACE scheme should thus open...
new ways to accurate many-body calculations beyond current \textit{ab initio} methods.

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IX. APPENDIX

In this Appendix, we analyse the difference between the local GW self-energy

\[ \Sigma_{\text{loc}} = G_{\text{loc}}W_{\text{loc}} \tag{48} \]

and the GW self-energy obtained from a local $W$. We use the expansions

\[ G(r, r') = \sum_{RR'LL'} G_{RR'LL'} \chi_{RL}(r) \chi_{RL'}(r') \tag{49} \]

and

\[ W(r, r') = \sum_{RR'\alpha\beta} W_{RR'\alpha\beta} B_{R\alpha}(r) B_{R'\beta}(r') \tag{50} \]

on the one- and two-particle bases $\chi$ and $B$, respectively (following standard notations in the field). Then, the GW equation

\[ \Sigma(r, r') = G(r, r') W(r, r') \tag{51} \]

leads to

\[ \Sigma_{R_1 R_2 L_1 L_2} = \sum_{RR'LL'} \sum_{RR'\alpha\beta} G_{RR'LL'} W_{RR'\alpha\beta} \langle \chi_{R_1 L_1} \chi_{RL} | B_{R'\alpha}(r) \rangle \langle B_{R'\beta}(r) | \chi_{R_2 L_2} \chi_{RL'}(r') \rangle \tag{52} \]

For a local $W$, that is an interaction of the form $W_{RR'\alpha\beta} \sim \delta_{RR'}$ one has

\[ \Sigma_{R_1 R_2 L_1 L_2} = \sum_{RR'LL'} \sum_{RR'\alpha\beta} G_{RR'LL'} W_{RR'\alpha\beta} \langle \chi_{R_1 L_1} \chi_{RL} | B_{R'\alpha}(r) \rangle \langle B_{R'\beta}(r) | \chi_{R_2 L_2} \chi_{RL'}(r') \rangle \tag{53} \]

The structure of this equation is determined by the overlap matrices of two-particle and one-particle basis states. If the basis set is sufficiently localized that no overlaps between basis functions on different spheres need to be considered, these become local quantities themselves: $O_{L_1 L_2} = \langle \chi_{RL_1} \chi_{RL_2} | B_{R\alpha}(r) \rangle$ and the above expression equals the local self-energy

\[ \Sigma_{RRL_1 L_2} = \sum_{LL' \alpha \beta} G_{RRLL'} W_{RR\alpha\beta} \langle \chi_{RL_1} \chi_{RL} | B_{R\alpha}(r) \rangle \langle B_{R\beta}(r) | \chi_{RL_2} \chi_{RL'}(r') \rangle \tag{54} \]

This is used in order to write Eq. [20].

1. M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. \textbf{70}, 1039 (1998).
2. W. Kohn, Rev. Mod. Phys. \textbf{71}, 1253 (1999).
3. F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. \textbf{61}, 237 (1998).
4. M. Imada and T. Miyake, J. Phys. Soc. Jpn. \textbf{79}, 112001 (2010).
5. S. Biermann, “\textit{LDA+DMFT” - a Tool for Investigating the Electronic Structure of Materials with Strong Electronic Coulomb Correlations}, Encyclopedia of Materials:
FIG. 11. (Color online) Frequency dependence of $-V_{xc} + G^{(1)} W_{\text{H}}^{\text{dyn}}$ of SrVO$_3$. (a) and (b) are the real and imaginary local parts, respectively. (c) and (d) are the real and imaginary parts at several $k$ points.

Science and Technology (Elsevier, Amsterdam, 2005); S. Biermann, *Dynamical Mean Field-based Electronic Structure Calculations for Correlated Materials, First principles approaches to spectroscopic properties of complex materials, Topics in Current Chemistry* (Springer, Berlin, 2014).

6 G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, Rev. Mod. Phys. **78**, 865 (2006).

7 S. R. White and R. L. Martin, J. Chem. Phys. **110**, 4127 (1999).

8 Y. Kurashige and T. Yanai, J. Chem. Phys. **130**, 234114 (2009).

9 M. Casula, C. Attaccalite, and S. Sorella, J. Chem. Phys. **121**, 7110 (2004).

10 P. Navratil, S. Quagliani, I. Stetcu, and B. R. Barrett, J. Phys. G **36**, 083101 (2009).

11 G. Hagen, T. Papenbrock, D. J. Dean, and M. Hjorth-Jensen, Phys. Rev. C **82**, 034330 (2010).

12 F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B **70**, 195104 (2004).

13 T. Miyake and F. Aryasetiawan, Phys. Rev. B **77**, 085122 (2008).

14 T. Kashima and M. Imada, J. Phys. Soc. Jpn. **70**, 2287 (2001).

15 K.A. Hallberg, Adv. Phys. **55**, 477 (2006).

16 B. Edegger, V. N. Muthukumar, and C. Gros, Adv. Phys. **56**, 927 (2007).

17 D. Tahara and M. Imada, J. Phys. Soc. Jpn. **77**, 114701 (2008).

18 A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).

19 T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005).

20 K. Held, O. K. Andersen, M. Feldbacher, A. Yamasaki, and Y.-F. Yang, J. Phys.: Condens. Matter **20**, 064202 (2008).

21 V. I. Anisimov, A. I. Poteryaev, M. A. Korotin, A. O. Anokhin, and G. Kotliar, J. Phys.: Condens. Matter **9**, 7359 (1997).

22 A. I. Lichtenstein and M. I. Katsnelson, Phys. Rev. B **57**, 6884 (1998).

23 S. Biermann, J. Phys.: Condens. Matter **26**, 173202 (2014).

24 S. Biermann, A. Dallmeyer, C. Carbone, W. Eberhardt, C. Pampuch, O. Rader, M. I. Katsnelson, and A. I. Lichtenstein, JETP Letters **86**, 612 (2004); arXiv:0112430.

25 A. I. Lichtenstein, M. I. Katsnelson, and G. Kotliar, Phys. Rev. Lett. **87**, 067205 (2001).

26 I. V. Solovyev and M. Imada, Phys. Rev. B **71**, 045103 (2005).
FIG. 12. (Color online) Frequency dependence of $-V_{xc} + G^{(0)} W^{\text{dyn}}_{GW}$ of SrVO$_3$. (a) and (b) are the real and imaginary local parts, respectively. (c) and (d) are the real and imaginary parts at several $k$ points.

FIG. 13. (Color online) Band structure of $[\epsilon_{\text{DFT}} - V_{xc} + \Delta \Sigma_H + \Delta \Sigma_{\text{nonlocal}}]Z_{\text{HL}}$ of SrVO$_3$ in the direct perturbative treatment. For comparison, the LDA band structure is also given (black dotted line). The energy is measured from the Fermi level.

FIG. 14. (Color online) Band structure of $[\epsilon_{\text{DFT}} - V_{xc} + \Delta \Sigma_H + \Delta \Sigma_{\text{nonlocal}}]Z_{\text{HL}}$ of SrVO$_3$ in the GW treatment. For comparison, the LDA band structure is also given (black dotted line). The energy is measured from the Fermi level.

27 J. Braun, J. Minar, H. Ebert, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. Lett. 97, 227601 (2006).
28 J. Sanchez-Barriga, J. Braun, J. Minar, I. Di Marco, A. Varykhalov, O. Rader, V. Boni, V. Bellini, F. Manghi, H. Ebert, M. I. Katsnelson, A. I. Lichtenstein, O. Eriksson, W. Eberhardt, H. A. Durr, and J. Fink, Phys. Rev. B 85, 205109 (2012).
29 Y. Imai, I. Solovyev, and M. Imada, Phys. Rev. Lett. 95, 176405 (2005).
FIG. 15. (Color online) Band structure of \( [\varepsilon_{\text{DFT}}-V_{\text{xc}}+\Delta \Sigma+\Delta \Sigma_{\text{nonlocal}}] Z_{\text{HL}} Z_{\text{B}} \) of SrVO\(_3\) in the GW treatment. For comparison, the LDA band structure is also given (black dotted line). The energy is measured from the Fermi level.

FIG. 16. (Color online) Band structure of \( [\varepsilon_{\text{DFT}}-V_{\text{xc}}+\Sigma+\Delta \Sigma_{\text{nonlocal}}] Z_{\text{HL}} Z_{\text{B}} \) of SrVO\(_3\). For comparison, the LDA band structure is also given (black dotted line). The energy is measured from the Fermi level.

FIG. 17. (Color online) Band structure of \( [\varepsilon_{\text{DFT}}-V_{\text{xc}}+\Sigma-Z(0) W_{\text{GW}}^{\text{nonlocal}}] Z_{\text{HL}} Z_{\text{B}} \) of SrVO\(_3\) (Z is the renormalization factor of \( \Sigma-Z(0) W_{\text{GW}}^{\text{nonlocal}} \)). For comparison, the LDA band structure is also given (black dotted line). The energy is measured from the Fermi level.

30 Y. Imai and M. Imada, J. Phys. Soc. Jpn. 75, 094713 (2006).
31 Y. Otsuka and M. Imada, J. Phys. Soc. Jpn. 75, 124707 (2006).
32 S. Biermann, A. Poteryaev, A. I. Lichtenstein, and A. Georges, Phys. Rev. Lett. 94, 026404 (2005); J. M. Tomczak and S. Biermann, J. Phys.: Condens. Matter 19, 365206 (2007); Europhys. Lett. 86, 37004 (2009); Phys. Rev. B 80, 085117 (2009); J. M. Tomczak, F. Aryasetiawan, and S. Biermann, Phys. Rev. B 78, 115103 (2008).
33 F. Aryasetiawan, J. M. Tomczak, T. Miyake and R. Sakuma, Phys. Rev. Lett. 102, 176402 (2009).
34 P. Thunstrom, I. Di Marco, O. Eriksson, Phys. Rev. Lett. 109, 186401 (2012).
35 A. I. Poteryaev, J. M. Tomczak, S. Biermann, A. Georges, A. I. Lichtenstein, A. N. Rubtsov, T. Saha-Dasgupta, and O. K. Andersen, Phys. Rev. B 76, 085127 (2007); J. M. Tomczak and S. Biermann, J. Phys.: Condens. Matter 21, 064209 (2009).
36 F. Lechermann, S. Biermann, A. Georges, Phys. Rev. Lett. 94, 166402 (2005); Phys. Rev. B 76, 085101 (2007).

37 K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn. 77, 093711 (2008).
38 M. Aichhorn, L. Pourovskii, V. Vildosola, M. Ferrero, O. Parcollet, T. Miyake, A. Georges, and S. Biermann, Phys. Rev. B 80, 085101 (2009).
39 T. Miyake, K. Nakamura, R. Arita, and M. Imada, J. Phys. Soc. Jpn. 79, 044705 (2010).
40 M. Aichhorn, S. Biermann, T. Miyake, A. Georges, and M. Imada, Phys. Rev. B 82, 064504 (2010).
41 T. Misawa, K. Nakamura, and M. Imada, J. Phys. Soc. Jpn. 80, 023704 (2011).
42 Z. P. Yin, K. Haule, and G. Kotliar, Nat. Mat. 10, 932 (2011).
43 T. Misawa, K. Nakamura, and M. Imada, Phys. Rev. Lett. 108, 177007 (2012).
44 C. Platt, W. Hanke, and R. Thomale, Adv. Phys. 62, 453 (2013).
45 T. Misawa and M. Imada, Nat. Commun. 5, 5738 (2014).
46 B. Amadon, S. Biermann, A. Georges, and F. Aryasetiawan, Phys. Rev. Lett. 96, 066402 (2006).
47 J. Bieder and B. Amadon, Phys. Rev. B 89, 195134 (2014).
48 N. Devaux, M. Casula, F. Decremps, S. Sorella, Phys. Rev. B 91, 081101(R) (2015).
49 L. V. Pourovskii, B. Amadon, S. Biermann, and A. Georges, Phys. Rev. B 76, 235101 (2007).
50 L. Pourovskii, V. Vildosola, S. Biermann, and A. Georges, Europhys. Lett. 84, 37006 (2008).
51 T. Miyake, L. Pourovskii, V. Vildosola, S. Biermann, and A. Georges, J. Phys. Soc. Jpn. 77, (2008); Supplement C pp. 99-102.
52 J. M. Tomczak, L.V. Pourovskii, L. Vaugier, A. Georges, and S. Biermann, Proc. Nat. Ac. Sci. 110 904907 (2013).
53 H. C. Choi, B. I. Min, J. H. Shim, K. Haule, and G. Kotliar, Phys. Rev. Lett. 108, 016402 (2012).
54 L. V. Pourovskii, P. Hansmann, M. Ferrero, and A. Georges, Phys. Rev. Lett. 112, 106407 (2014).
55 S. Savrasov, G. Kotliar, and E. Abrahams, Nature 410, 793 (2001).
56 L. V. Pourovskii, G. Kotliar, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B 75, 235107 (2007).
