Frequency-dependent local interactions and low-energy effective models from electronic structure calculations

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Abstract

We propose a systematic procedure for constructing effective models of strongly correlated materials. The parameters, in particular the on-site screened Coulomb interaction $U$, are calculated from first principles, using the GW approximation. We derive an expression for the frequency-dependent $U(\omega)$ and show that its high frequency part has significant influence on the spectral functions. We propose a scheme for taking into account the energy dependence of $U(\omega)$, so that a model with an energy-independent local interaction can still be used for low-energy properties.
I. INTRODUCTION

Lattice fermion models such as the Hubbard model or the Anderson impurity model and their extensions have played a major role in studying electron correlations in systems with strong onsite correlations. Despite the widespread use of these models, little justification has been given in using them. The models are postulated on the basis of physical intuition. In particular, the models employ parameters, such as the famous Hubbard interaction $U$, which are normally adjusted to serve the given problem. Without judicious choice of parameters, the model may yield misleading results or in the worst case, the model itself is not sufficient to describe the real system. One can define rigorously these concepts in the path integral formulation of the many body problem by performing a partial trace over the degrees of freedom that one wants to eliminate, and ignoring the retardation in the interactions generated by this procedure. However, this elimination of the degrees of freedom is very hard to perform for real materials. It is therefore very desirable to figure out a systematic way of constructing low energy effective models with well defined parameters calculated from first principles such that the model can quantitatively reproduce and predict physical properties of interest of the corresponding real system, especially when the correlation effects are crucial.

Another important issue that has not received sufficient attention is the role of energy dependence of the screened local Coulomb interaction $U$. Model studies investigating the importance of high-energy states in the Hubbard model can be found in [1, 2, 3]. A dynamic Hubbard model has also been considered. [4]. In most cases however $U$ is assumed to be static, but on the other hand we know that at high energy the screening becomes weaker and eventually the interaction approaches the large bare Coulomb value, which is an order of magnitude larger than the static screened value. Of course the high-energy part of the Coulomb interaction has in some way been down-folded into the Hubbard $U$ but it is not clear how this downfolding is actually accomplished.

A number of authors have addressed the problem of determining the Hubbard $U$ from first principles. One of the earliest works is the constrained local density approximation (LDA) approach [1, 5] where the Hubbard $U$ is calculated from the total energy variation with respect to the occupation number of the localized orbitals. An approach based on the random-phase approximation (RPA) was later introduced [6], which allows for the calcula-
tions of the matrix elements of the Hubbard $U$ and its energy dependence. This was followed by a more refined approach for calculating $U$. A yet different approach, computes the matrix elements of the Coulomb interactions screened in real space and assumes a Yukawa form to extract the Hubbard $U$ and the other interactions which determine the multiplet splittings.

The purpose of the present work is to develop a precise formulation for a systematic construction of effective models where the parameters are obtained from realistic first-principles electronic structure calculations. In particular, we concentrate on the calculation of the Hubbard $U$ and demonstrate the importance of its energy dependence. We show that a static Hubbard Hamiltonian, obtained from a naive construction in which this energy dependence is simply neglected, fails even at low energy. This static model can be appropriately modified however, by taking into account the feedback of the high-energy part of $U$ into the one-particle propagator. We illustrate our scheme in transition metals, concentrating on Ni as an example, since it is a prototype system consisting of a narrow 3d band embedded in a wide band. Furthermore, Ni is one of the most problematic case from the viewpoint of the LDA.

II. THEORY

Let us suppose that the bandstructure of a given solid can be separated into a narrow band near the Fermi level and the rest, like, for example, in transition metals or 4f metals. Our aim is to construct an effective model which only includes the narrow 3d or 4f band. The effective interaction between the 3d electrons in the Hubbard model can be formally constructed as follows. We first divide the complete Hilbert space into the Hubbard space $\{\psi_d\}$, consisting of the 3d states or the localized states, and the rest. The bare Green’s function $G_d$, spanning the d-subspace is given by:

$$G_d(r, r'; \omega) = \sum_{\text{occ}} \frac{\psi_d(r)\psi_d^*(r')}{\omega - \varepsilon_d - i0^+} + \sum_{\text{unocc}} \frac{\psi_d(r)\psi_d^*(r')}{\omega - \varepsilon_d + i0^+}$$

(1)
Let $P$ be the total (bare) polarization, including the transitions between all bands:

$$
P(r, r'; \omega) = \sum_{i=\text{occ}} \sum_{j=\text{unocc}} \psi_i(r) \psi_i^*(r') \psi_j(r) \psi_j^*(r') \times \left\{ \frac{1}{\omega - \varepsilon_j + \varepsilon_i + i0^+} - \frac{1}{\omega + \varepsilon_j - \varepsilon_i - i0^+} \right\}
$$

(2)

$P$ can be divided into: $P = P_d + P_r$, in which $P_d$ includes only 3d to 3d transitions (i.e. limiting the summations in (2) to $i, j \in \{\psi_d\}$), and $P_r$ be the rest of the polarization. The screened interaction $W$ on the RPA level is given by

$$
W = [1 - vP]^{-1}v
= [1 - vP_r - vP_d]^{-1}v
= [(1 - vP_r)\{1 - (1 - vP_r)^{-1}vP_d]\}^{-1}v
= \{1 - (1 - vP_r)^{-1}vP_d\}^{-1}(1 - vP_r)^{-1}v
= [1 - W_rP_d]^{-1}W_r
$$

(3)

where we have defined a screened interaction $W_r$ that does not include the polarization from the 3d-3d transitions:

$$
W_r(\omega) = [1 - vP_r(\omega)]^{-1}v
$$

(4)

(we have not explicitly indicated spatial coordinates in this equation). The identity in (3) explicitly shows that the interaction between the 3d electrons is given by a frequency-dependent interaction $W_r$. It fits well with the usual physical argument that the remaining screening channels in the Hubbard model associated with the 3d electrons, represented by the 3d-3d polarization $P_d$, further screen $W_r$ to give the fully screened interaction $W$.

We now choose a basis of Wannier functions $\{\phi_{Rn}\}$, centered about atomic positions R, corresponding to the 3d Bloch functions $\{\psi_{kn}\}$, and consider the matrix elements of the (partially screened) frequency-dependent Coulomb interaction $W_r$:

$$
U_{R_1nR_2n',R_3mR_4m'}(\tau - \tau') \equiv \int d^3rd^3r'\phi_{R_1n}^*(r)\phi_{R_2n'}(r)W_r(r, r'; \tau - \tau')\phi_{R_3m}^*(r')\phi_{R_4m'}(r')
$$

(5)

We would like to obtain an effective model for the 3d degrees of freedom. Because of the frequency dependence of the U’s (corresponding to a retarded interaction), this effective theory will not take a hamiltonian form. We can however, write such a representation in the functional integral formalism by considering the effective action for the 3d degrees of freedom.
freedom given by:

\[
S = \int d\tau d\tau' \left[ -\sum d_{Rn}^\dagger(\tau)R_{n',R}\frac{1}{\tau - \tau'}d_{Rn'}(\tau') \right.
\]

\[+ \frac{1}{2} \sum : d_{R_1n}^\dagger(\tau)d_{R_2n'}(\tau) : U_{R_1nR_2n',R_3mR_4m'}(\tau - \tau') : d_{R_3m}^\dagger(\tau')d_{R_4m'}(\tau') \left. \right] \tag{6}
\]

where : \(d^\dagger d\) : denotes normal ordering, which accounts for the Hartree term, and the summation is over repeated indices. When using a Wannier transformation which does not mix the d-subspace with other bands, the Green’s function can be taken, to first approximation, to be the bare Green’s function \(G_{dd}^0\) constructed from the Bloch eigenvalues and eigenfunctions. If instead an LMTO formalism \[10\] is used, one should in principle obtain from a downfolding procedure onto the d-subspace, i.e perform a partial trace over s, p degrees of freedom (e.g to first order: 

\[-1 = [G_{dd}^0]^{-1} - [G_{ds}]^{-1}G_{ss}[G_{sd}]^{-1}.\]

In the following, we retain only the local components of the effective interaction on the same atomic site. This is expected to be a reasonable approximation because the 3d states are rather localized. The formalism may be easily extended to include intersite Coulomb interactions if necessary. Hence, we consider the frequency-dependent Hubbard interactions:

\[U_{nn',mm'}(\tau - \tau') \overset{\dagger}{=} \int d^3rd^3r'\phi_n^*(r)\phi_{n'}(r)W_r(r,r';\tau - \tau')\phi_m^*(r')\phi_{m'}(r') \tag{7}\]

with \(\phi_n\) being the Wannier orbital for \(R=0\). In order to illustrate the procedure within the linear muffin-tin orbital (LMTO) basis set, we use instead of the Wannier orbital the normalized function head of the LMTO \(\phi_H\) which is a solution to the radial Shrödinger equation matching to a Hankel function at zero energy at the atomic sphere boundary.

In this paper, we investigate the importance of the energy-dependence of \(U\). Therefore, we shall compare the results obtained from \[8\] with those of a Hamiltonian approach in which one would construct a Hubbard model with a static interaction \(U\):

\[H = \sum_{Rn,R'n'} c_{Rn}^\dagger h_{Rn,R'n'}c_{R'n'} + \frac{1}{2} \sum_{R,m',mm'} c_{Rn}^\dagger c_{Rn'}U_{nn',mm'}c_{Rm}^\dagger c_{Rm'} \tag{8}\]

It seems natural to identify the static Hubbard \(U\) with the (partially) screened local interaction in the low-frequency limit \(W_r(\omega = 0)\). Note that the Hubbard model \[8\] has been constructed in the most naive manner, by simply taking the quadratic part to be the d-block of the non-interacting hamiltonian.
In order to compare the results obtained from the full dynamical $U$ to those of the static Hubbard model, we need to solve (6) and (8) within some consistent approximation scheme. In the following, we adopt a “GW universe” where the exact self-energy for the solid is assumed to be given by the GW approximation (GWA) [11, 12], and where the GW approximation is also assumed to be a reliable tool in solving the effective models (6) and (8). This allows us to make a proper comparison between the “exact” self-energy and the Hubbard model self-energy. If the assumption of static $U$ is valid, the Hubbard self-energy and the true self-energy (both within the GWA) should be close to each other, at least for small energies. Or equivalently, the spectral function for small energies should resemble that of the full one.

III. RESULTS AND DISCUSSIONS

A. Comparing self-energies

The screened interaction with and without the 3d-3d transitions is shown in Fig. 1 in the case of Nickel. Here and in all the following, a spin-unpolarized (paramagnetic) solution is considered. At low energies, the (partially) screened interaction $W_r$ without the 3d-3d transitions is larger than the full one $W$, and at high energies they approach each other, as anticipated. Related calculations have also been performed by Kotani [1].

We first compare the self-energy obtained from a GW treatment of the full system, given
FIG. 2: The self-energy of the real system (nickel) and the Hubbard model with a frequency-dependent $U$.

by:

$$\Sigma(r, r'; \omega) = \frac{i}{2\pi} \int d\omega' e^{i\omega' \omega} G(r, r'; \omega + \omega') W(r, r'; \omega')$$ (9)

to the self-energy obtained from the effective model (6) with an energy-dependent interaction $U(\omega) = W_r(\omega)$. Because of (3), the screened interaction corresponding to this $U(\omega)$ is simply $W$, and the corresponding self-energy reads:

$$\Sigma_d(\omega) = \frac{i}{2\pi} \int d\omega' e^{i\omega' \omega} G_d(\omega + \omega') W(\omega')$$ (10)

The difference between this expression and the GWA for the full system (Eq.9) is that in (10) only the d-block of the Green’s function has been included (since the effective action was written for the d-band only). Hence, the two self-energies differ by a term $G_r W$, with $G_r = G - G_d$. We expect that the wavefunction overlap between two 3d states (one from $G_d$ and the other from the 3d state appearing in the matrix element of $\Sigma_d$) and other non-3d states is small so that $\Sigma_d$ should be close to the true $\Sigma$. In Fig. 2 the two self-energies are displayed (more precisely, in this figure and in all the following, we display the matrix element of the self-energy in the lowest 3d state (band number 2), at the $\Gamma$-point, corresponding to an LDA eigenenergy -1.79 eV). We observe that the two self-energies indeed almost coincide with each other, even at high energies. Hence, we conclude that the effective Hubbard model (6) for the d-subspace, with an energy-dependent interaction, provides a reliable description of the real system.
We now turn to the self-energy associated with the static Hubbard model with $U = W_r(0) \simeq 3.5$ eV. The local screened interaction for this model, within the GW approximation, is given by:

$$W_d(\omega) = [1 - UP_d(\omega)]^{-1}U$$

and the self-energy of the Hubbard model in the GWA thus reads:

$$\Sigma_d^H(r, r'; \omega) = \frac{i}{2\pi} \int d\omega' e^{i\omega'}G_d(r, r'; \omega + \omega')W_d(r, r'; \omega')$$

Note that the difference between this static Hubbard model self-energy and that of the effective model with a frequency-dependent interaction relies in the use of a different form of the screened interaction $W_d$ instead of the full $W$. In Fig. 3, the real part of this self-energy with that of the full GWA self-energy for nickel are shown. Since the energy scale of the self-energy of the real system is determined by the bare Coulomb interaction $v$ whereas the Hubbard self-energy is set by $U$, the latter has been shifted so that it is equal to the former at the LDA eigenvalue (-1.79 eV) of the band we have considered, at the $\Gamma$-point.

The difference in magnitude of the self-energies is not important since it simply shifts the spectrum (or, said differently, we have compared differences $\Sigma - \mu$ from the values of the chemical potential obtained in the various schemes). However, the difference in the variation of the self-energy with respect to energy matters, since it will give a different quasiparticle weight $Z = [1 - \partial \text{Re } \Sigma/\partial \omega]^{-1}$ and affect the spectral function. As can be deduced from the figure, the $Z$ factor of the Hubbard model taken at the energy of the quasiparticle band...
at the $\Gamma$-point ($\approx -1.79\text{eV}$) is much closer to unity as compared to the true (full GW) one because the former already contains the renormalization from the plasmon. Hence, neglecting frequency-dependence directly affects the physical results, even in the low-energy range. We shall see below, however, that it is possible to modify the static model in such a way that an accurate approximation is obtained at low energy.

In Fig. 4 the imaginary part of the self-energy is shown. Here we see that $\text{Im } \Sigma^{\text{Hub}}$ for the Hubbard model is peaked around 5 eV since there are no states above or below the 3d band. As a consequence, the real part of the self-energy exhibits the Kramers-Kronig behavior at around -5 eV. Within an energy region spanning about twice the 3d bandwidth, the imaginary part of the Hubbard model self-energy, in contrast to the real part, is not in bad agreement with the full one.

These findings can be understood qualitatively by considering more explicit expressions of the self-energy obtained within the GW approximation, for an effective model of the d-subspace defined on the periodic lattice. The imaginary part reads:

$$\text{Im}\Sigma_n(k,\omega) = \sum_{q,m} \text{Im}W_{nm}(q, \omega - \epsilon^m_{k-q}) [n_F(\epsilon^m_{k-q}) + n_B(\omega - \epsilon^m_{k-q})]$$  \hspace{1cm} (13)

In this expression, $n, m$ are band indices, $\epsilon^n_k$ corresponds to the n-th non-interacting band and $n_F$ (resp. $n_B$) is the Fermi (resp. Bose) function. $\text{Im}W$ is the spectral function associated with the effective interaction (to be taken as $W$ if the self-energy of the frequency-dependent effective model is considered, and as $W_d$ if that of the static Hubbard model is considered).

FIG. 4: The imaginary parts of the self-energy of the real systems (solid) and the Hubbard model (dash) in the GWA.
From this expression, one sees that if one considers an energy $\omega$, the bands contained in the energy interval $[0, |\omega|]$ are the only ones contributing significantly to $\text{Im}\Sigma$. This is the reason why the *imaginary part* of the self-energy at low-energy will be correctly reproduced by the effective low-energy model (provided of course that the spectral function $\text{Im}W$ is correctly approximated at low energy). In contrast, the real part of the self-energy is obtained from the Kramers-Kröening relation in the form:

$$\text{Re}\Sigma_n(k, \omega) = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} d\nu \sum_{q,m} \text{Im}W_{nm}(q, \nu) \frac{n_F(\epsilon_{k-q}^m) + n_B(\nu)}{\omega - \epsilon_{k-q}^m - \nu}$$

(14)

Because the principal-part integral extends over the whole frequency range, high-frequency contributions influence the self-energy even at low frequency. As a result, an accurate description of the real part of the self-energy cannot be obtained within the naive construction of the static Hubbard model because the effective interaction is not correctly approximated over the whole frequency range. This formula also suggests a way to appropriately modify the effective static model in order to obtain an accurate description at low energy, as discussed below.

**B. The puzzle of the satellite**

Fig. 5 compares the spectral function obtained for the full system within the GWA, and that of the static Hubbard model (8). A striking difference between these two results is the
absence of the 6 eV satellite in the GWA for the full system, while the static Hubbard model displays a satellite feature. This is to be expected from the structure of the self-energy. The GWA self-energy of the full system continues to grow and reaches a maximum around the plasmon excitation at around 25-30 eV, while the self-energy of the static Hubbard model has a maximum around the width of the 3d band (4 eV). In comparison with the true plasmon, the "plasmon" of the Hubbard model has a much lower energy, of the order of \(U\), which results in the "6 eV satellite". One could blame the appearance of a satellite in our static Hubbard model calculation on the fact that we have used a (non self-consistent) GW approximation. However, more accurate treatments of the static Hubbard model (such as DMFT) do preserve this feature, which has in this context a natural interpretation as a lower Hubbard band. On the other hand, it could be that the experimentally observed Nickel satellite has a somewhat different physical origin and that the satellite obtained in static Hubbard model calculations is spurious in the context of Nickel (e.g because it is not legitimate to use a low-energy effective model in this energy range). In our view, this issue is an open problem which deserves further work.

C. Improving the effective static model

The preceding discussion shows that an effective model for the d-band can be constructed, which accurately reproduces the full results over an extended energy range, provided the energy- dependence of \(U(\omega)\) is retained. However, performing calculations with an energy-dependent Hubbard interaction is exceedingly difficult. A more modest goal is to obtain an effective model which would apply to some low-energy range only (say, \(|\omega| < \Lambda\), with \(\Lambda\) a cutoff of the order of the d-bandwidth). In order to achieve this goal, we propose to adopt a renormalization group point of view, in which high energies are integrated out in a systematic way. Following this procedure, an appropriate low-energy model with a static \(U\) can be appropriately constructed. As we shall see, the bare Green’s function defining this low-energy model does not coincide with the non-interacting Green’s function in the d-subspace (we have seen that this does not lead to a satisfactory description, even at low energy).

Let us illustrate this idea within the GW approximation. The full Hilbert space is divided into the Hubbard space, comprising the 3d orbitals, and the downfolded space, comprising
the rest of the Hilbert space. This approach is complementary to the one in \[2, 13\], where the division is done in real space (onsite and off sites). Within the GWA we may write the full self-energy as follows:

\[
GW = G_d W_d + G_d (W - W_d) + G_r W. \tag{15}
\]

where \( G = G_d + G_r \). The term \( G_d (W - W_d) \) represents the high-energy contribution of the screened interaction. This is the main source of error in the naive static limit, as discussed in the previous sections. The term \( G_r W \) is not obtainable within the Hubbard model, even when a frequency-dependent \( U \) is employed since \( G_r \) resides in the downfolded space. This term was shown to be small. Its effect at low-energy can also be taken into account by appropriate modifications of the one-particle propagator, but we shall neglect it for simplicity.

We consider the following Hubbard model with a static \( U = W_r (0) \), but a modified one-particle propagator \( \tilde{G}_0 \), defined by the action:

\[
S_H = - \int d\tau d\tau' \sum \tilde{d}^\dagger_{R_n}(\tau) [\tilde{G}^0_{R_n, R_n'}]^{-1}(\tau - \tau') \tilde{d}_{R_n'}(\tau') + \frac{1}{2} \int d\tau \sum : d^\dagger_{R_1 n}(\tau) d_{R_2 n'}(\tau) : U_{R_1 n R_2 n', R_3 m R_4 m'} : d^\dagger_{R_3 m}(\tau) d_{R_4 m'}(\tau). \tag{16}
\]

The self-energy of this static Hubbard model in the GWA is:

\[
\tilde{\Sigma}^H d = \tilde{G}_d \tilde{W}_d \tag{17}
\]

where the new effective interaction is \( \tilde{W}_d = U [1 - U \tilde{P}_d]^{-1} \), with \( \tilde{P}_d \) constructed from the new Green’s functions \( \tilde{G}_d \) (schematically \( \tilde{P}_d = \tilde{G}_d \cdot \tilde{G}_d \)). We request that the interacting Green’s function of this modified static model coincides with that of the Green’s function calculated with the frequency-dependent interaction in the low energy range \(|\omega| < \Lambda\):), that is:

\[
\tilde{G}^{-1}_d - \tilde{\Sigma}^H_d \simeq G^{-1}_d - G_d W_d - G_d(W - W_d) \text{ for } |\omega| < \Lambda \tag{18}
\]

Using the identity \( G^{-1} - GW = [1 - UP]^{-1} G^{-1} \), this can be rewritten as:

\[
[1 - U \tilde{P}_d]^{-1} \tilde{G}^{-1}_d \simeq [1 - UP_d]^{-1} G^{-1}_d - G_d(W - W_d) \text{ for } |\omega| < \Lambda \tag{19}
\]

This is an integral equation which determines in principle the modified bare Green’s function \( \tilde{G}_d \) to be used in the ”downfolded” static action \[16\]. To first approximation, one can neglect the polarization terms in this equation, and obtain the first order modification of \( \tilde{G}_d \) as:

\[
\tilde{G}^{-1}_d = G^{-1}_d - G_d(W - W_d) + \cdots \tag{20}
\]
The first correction appearing in this equation is precisely the contribution coming from the high-energy part of the screened interaction. We have explained above that this correction is not small, which is the reason for the failure of the "naive" static Hubbard model using the non-interacting $G_d$. Dividing the screened interaction into a low-energy part for $|\omega| < \Lambda$ and a high-energy part for $|\omega| > \Lambda$, we can use the explicit forms (13,14) given in the previous section to obtain this first correction in the form:

$$\tilde{G}_d^{-1}(k,\omega)_n = G_d^{-1}(k,\omega)_n + \frac{1}{\pi} \int_{|\nu| > \Lambda} d\nu \sum_{q,m} \text{Im} W_{nm}(q,\nu) \frac{n_F(\epsilon_{k-q}^m) + n_B(\nu)}{\omega - \epsilon_{k-q}^m - \nu} + \cdots \quad (21)$$

In particular, we see by expanding this expression to first order in $\omega$, that the low frequency expansion of the modified one-particle propagator reads: $\tilde{G}_d^{-1}(k,\omega + i0^+)_n = (1 + \alpha_{k,n})\omega - \epsilon_k^n + \cdots$. The coefficient $\alpha_{k,n}$ is a partial contribution to the quasi-particle residue $\alpha_{k,n} = -\frac{1}{\pi} \sum_m \int_{|\nu| > \Lambda} d\nu \text{Im} W_{nm}(q,\nu) \frac{n_F(\epsilon_{k-q}^m) + n_B(\nu)}{(\nu - \epsilon_{k-q}^m)^2}$. In practice this integral can be easily evaluated using the well known plasmon pole approximation, which should contain most of the high energy contribution. This correction insures that the quasi-particle residue is obtained correctly from this "downfolded" static model. We do not, however, expect that this improvement solves the problem with the satellite discussed in the previous subsection.

**D. Beyond the GW approximation**

In strongly correlated systems, it is known that the GWA is not sufficient and improvement beyond the GWA is needed. Much of the short coming of the GWA probably originates from the improper treatment of short-range correlations within the random-phase approximation (RPA). Thus, one would like in the first instance attempt to improve these short-range correlations, which are essentially captured by the Hubbard model. The formula (15) suggests a natural way to do this, as follows. The contribution from the frequency-dependent $U$ as well as the contribution from the downfolded Hilbert space are treated within the GWA. The self-energy $G_d W_d$ corresponding to the $GW$ self-energy of the Hubbard model with a static $U$ can then be replaced by that obtained from more accurate theories such as dynamical mean-field theory (DMFT) [14] or from exact methods such as Lanczos diagonalization. Thus, if we use the LDA to construct $G_d$, the correction to the LDA exchange-correlation potential reads:

$$\Delta \Sigma = \Sigma_H + G_d(W - W_d) + G_r W - v_{xc}, \quad (22)$$
where $\Sigma_H$ is the Hubbard model self-energy obtained from more accurate methods, replacing $G_dW_d$. We note also that the scheme in [15] avoids the problem of double counting, inherent in LDA+U [15] or LDA+DMFT methods. In this way, it is possible to calculate the Hubbard $U$ using the response function constructed from the LDA bandstructure.

The application of DMFT requires the Hubbard $U$ for the impurity model. To calculate the Hubbard $U$ for an impurity model, it is necessary to downfold contributions to the polarization $P$ from the neighboring sites. Here, the identity in Eq. (3) shows its usefulness. Since the formulation in (3) is quite general, we merely need to redefine $P_d$ to be the onsite polarizations or equivalently, we redefine $P_r$ to also include polarizations from the neighboring sites. The computational result for Ni shows that the difference between the lattice and the impurity Hubbard $U$ is rather small, essentially negligible. Somewhat different but related calculations of the Hubbard $U$ for the impurity model has also been performed in [7] for Fe and Ni, which confirm the result obtained in our formulation.

Another feasible approach for calculating physical quantities of the derived Hubbard model is by using the path integral renormalization group (PIRG) method. [17] One advantage of this method is the possibility of using the lattice Hubbard model as opposed to the impurity model, thus including spatial fluctuations and possible symmetry breaking. The method is also suited for studying single-particle Green’s functions as well as thermodynamic quantities, in particular for accurate determination of the phase diagram, which often requires a determination of the possible symmetry breaking of the Hubbard Hamiltonian after taking account of spatial and temporal fluctuations on an equal footing. In calculating the self-energy, one may substitute $G_dW_d$ by the self-energy obtained within the correlator projection method [18] together with the PIRG. These form a future challenge in the field of strongly correlated materials.

**IV. SUMMARY AND CONCLUSION**

In conclusion, we have investigated the construction of effective models for the correlated orbitals in materials with a natural separation of bands. We have shown that, if one retains the full frequency dependence of the local components of the screened interaction, an accurate effective model can be obtained over an extended energy range. Simply neglecting this energy dependence and using the non-interacting hamiltonian into a static Hubbard model
does not provide an accurate description even at low energy. However, a proper modification of the bare propagator, obtained by integrating out high energies, allows for the construction of an effective Hubbard model which describes the low-energy physics in a satisfactory manner.

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