QS\textit{GW}+\textit{DMFT}: an electronic structure scheme for the iron pnictides and beyond

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Abstract. While in strongly correlated materials one often focuses on local electronic correlations, the influence of non-local exchange and correlation effects beyond band-theory can be pertinent in systems with more extended orbitals. Thus in many compounds an adequate theoretical description requires the joint treatment of local and non-local self-energies. Here, I will argue that this is the case for the iron pnictide and chalcogenide superconductors. As an approach to tackle their electronic structure, I will detail the implementation of the recently proposed scheme that combines the quasi-particle self-consistent GW approach with dynamical mean-field theory: QS\textit{GW}+\textit{DMFT}. I will showcase the possibilities of QS\textit{GW}+\textit{DMFT} with an application on BaFe$_2$As$_2$. Further, I will discuss the empirical finding that in pnictides dynamical and non-local correlation effects separate within the quasi-particle band-width.

1. Introduction
Many phenomena in correlated materials –the Kondo effect, the Mott insulator, etc.– can be described by local correlations. Such is the source of success of dynamical mean field theory (DMFT)[1, 2] for the quintessential physics in transition metals[3], their oxides[4, 5, 6, 7] and silicides[8], or rare-earth[9, 10, 11] and actinide[12, 13] compounds.

With experiments indicating sizable correlation effects in the newly discovered iron pnictides and chalcogenides[14], DMFT was swiftly called upon and delivered explanations for enhanced effective masses[15, 16, 17, 18, 19, 20, 21], lower-than-expected ordered moments[18, 22], as well as previously elusive structural aspects[23].

However, for these systems both experimental and theoretical evidence has emerged that non-local exchange and correlation effects are non-negligible, and at times even pivotal for a qualitative understanding. I will name two specific examples: (1) The Fermi surface of LiFeAs has been reported to have a distinctly different topology (number of sheets) in experiment[24] than in density functional theory (DFT) or DMFT[18, 19]. (2) The size of electron and hole pockets in BaFe$_2$As$_2$ are largely overestimated in DFT and DMFT[18, 25]. Thus quantities that are sensitive to excitations near the Fermi level, such as the thermopower, cannot be reproduced.

On the other hand, I have recently shown[26] that using quasi-particle self-consistent (QS) \textit{GW}[27, 28], a many-body perturbation theory[29] that excels at treating non-local exchange and also includes some non-local correlation effects, these problems are solved: (1) For LiFeAs QS\textit{GW} yields a Fermi surface in excellent in agreement with experiment, (2) a non-local self-energy shift shrinks both electron and hole pockets in BaFe$_2$As$_2$ to about half their size with respect to DFT, as shown in figure 1.
Many-body perturbation theory in its QSGW realization thus pinpoints non-local exchange and correlation effects to be crucial for the description of many aspects in the iron pnictides and chalcogenides. Nevertheless there are several properties that require the capturing of local dynamical renormalizations beyond the possibilities of a perturbative treatment[26]: Indeed quasi-particle weights come out too big in $GW$, electron lifetimes are overestimated, and incoherence effects at finite temperatures are out of reach.

For these reasons, combining the best of both methodologies, $GW$ and DMFT, is a promising route in electronic structure theory[30, 31]. Owing to the complexity of the $GW$+DMFT approach[30], however, applications are hitherto scarce: Fully dynamical and self-consistent implementations have been achieved for one-band systems only[32, 33, 34]. For other, realistic materials calculations, only lately an implementation that includes the pivotal dynamics of the Hubbard interaction has been pioneered and applied to SrVO$_3$[35, 36].

Recently, we proposed to merge QSGW with DMFT in a “QSGW+DMFT” approach[26] that retains most of the advantages of $GW$+DMFT[30] at a significantly reduced computational complexity. Here, after briefly reviewing QSGW, I will give practical details on how to implement the QSGW+DMFT scheme and showcase its potential for the case of BaFe$_2$As$_2$. Further, I will discuss the recent finding that in many systems, non-local and dynamical correlations can be separated for all practical purposes. This non-trivial result paves the way for the devising of physically motivated approximative electronic structure scheme, such as DMFT@non-local-$GW$[36] and SEX+DMFT[39] that I will comment on briefly.

![Figure 1. BaFe$_2$As$_2$: Comparison of the band-structures of DFT(LDA) with QSGW. Arrows indicate the shrinking of both the hole and electron pockets at Γ and X, respectively, in congruence with experiment (see e.g. Refs. [40, 25]) and not captured within DMFT.](image)

2. QSGW+DMFT – the formalism

2.1. QSGW: a self-consistent many-body perturbation theory

The central quantity for spectral properties of correlated materials is the one-particle Green’s function $G$, which can be expressed as

$$G^{-1}(k, \omega) = \omega - H^0(k) - \Sigma(k, \omega) \quad (1)$$

where we assume a matrix structure in the space of orbitals. Here, $H^0$ is a reference effective one-particle Hamiltonian, and $\Sigma$ a momentum and frequency dependent self-energy that is defined with respect to exchange and correlation effects already included in $H^0$.

For example, in DFT+DMFT[2], $H^0 = H^{\text{DFT}} = -\nabla^2 + v_{\text{crystal}} + v_{\text{Hartree}} + v_{\text{xc}}^\text{DFT}$ is the Kohn-Sham Hamiltonian, and $\Sigma^{\text{DFT+DMFT}}(\omega) = [\Sigma^{\text{DMFT}}(\omega) - E_{dc}]_L/LL^{\text{RR}} \langle RL'|RL\rangle$ is the DMFT self-energy that is local (momentum-independent) when expressed in a local basis set of correlated orbitals $\langle r|RL \rangle = \chi_{RL}(r)$, labelled by a lattice site or unit-cell $R$ and an orbital index $L$. From $\Sigma^{\text{DMFT}}$ the so-called “double counting” correction, $E_{dc}$, that mimics self-energy effects already

1 For calculations for SrVO$_3$ with static interactions and additional approximations, see Ref. [37]; and Ref. [38] for an ad hoc combination of $GW$ and DMFT self-energies.
contained in $H^0$ must be subtracted. Several proposals and rules of thumb for the choice of $E_{dc}$ exist. However, its exact form is unknown, introducing some arbitrariness to DFT+DMFT. Within the QS$GW$ approach[27, 28],

$$H^0 = H^{QS GW} = -\nabla^2 + v_{\text{crystal}} + v_{\text{Hartree}} + v^{QS GW}_{xc}.$$  \hspace{1cm} (2)

The $GW$ self-energy, $\Sigma_GW = G^{QS GW}_0 \cdot W$, where $G^{QS GW}_0 = \omega - H^{QS GW}$, enters with respect to the static, yet non-local and orbital-dependent QS$GW$ exchange-correlation potential, $v^{QS GW}_{xc}$:

$$\Sigma^{QS GW} = \Sigma^G - v^{QS GW}_{xc}.$$  \hspace{1cm} (3)

The potential $v^{QS GW}_{xc}$ is determined by the requirement that the quasi-particle energies $E_{kj}$, given by the poles of the interacting Greens-function (1),

$$\text{det} [E_{kj} - H^{QS GW}(k) - \Re \Sigma^{QS GW}_{V}(k, E_{kj})]^{1/2} = 0$$  \hspace{1cm} (4)

coincide with the eigenvalues of $H^{QS GW}$, i.e. $H^{QS GW}(k)|\Psi_{kj}\rangle = E_{kj}|\Psi_{kj}\rangle$. This means that at self-consistency $H^{QS GW}(k) + \Re \Sigma^{QS GW}_{V}(k, E_{kj}) = H^{QS GW}(k)$, or, equivalently, $\langle \Psi_{kj}|\Sigma^G V(k, E_{kj}) - v^{QS GW}_{xc}|\Psi_{kj}\rangle = 0$. The effective QS$GW$ potential thus in particular incorporates dynamical renormalizations of the band dispersions (e.g. the $Z$-factor in the Fermi liquid regime) through a state and momentum dependent static shift. It can be shown that self-consistency can be reached iteratively by hermitianizing the self-energy[41]:

$$v^{QS GW}_{xc} = \frac{1}{2} \sum_{ij} |\Psi_{ki}\rangle \Re \left[ \Sigma^{GW}_{ij}(k, E_{ki}) + \Sigma^{GW}_{ji}(k, E_{kj}) \right] \langle \Psi_{kj}|.$$ \hspace{1cm} (5)

The virtue of QS$GW$ is that in the end all remnants of the DFT starting point are gone, and the quasi-particle energies are unambiguously defined. Moreover, it was recently demonstrated that the above self-consistency procedure - irrespective of whether it is performed within the $GW$ approximation or any other many-body method - converges to the best possible effective one-particle theory accessible to the employed many-body technique[42].

### 2.2. QS$GW$+DMFT

The general strategy in QS$GW$+DMFT is to take out of the improved effective one-particle Hamiltonian, $H^{QS GW}$, all renormalizations that are propelled by local correlations. In the spirit of the above discussion, one is tempted to use $H^0 = H^{QS GW}$ and define the self-energy in a local basis $\{\chi_{RL}(r)\}$ as $\Sigma^{QS GW+DMFT}(\omega) = [\Sigma^{DMFT}(\omega) - \Re \Sigma^{GW}_{local}(\omega)]_{LL', RL} = \langle RL|\chi_{RL'}\rangle$, with the local projection $\Sigma^{GW}_{LL'}(\omega) = \sum_k \Sigma^{GW}_{LL'}(k, \omega)$. Indeed the quasi-particle Hamiltonian, $H^{QS GW}$, includes via (5) all hermitian self-energy effects, the local parts of which have to be taken out. However, in this naive ansatz the total self-energy $\Sigma^{DMFT} - \Re \Sigma^{GW}_{local}$ manifestly violates the Kramers-Kronig relations, i.e. causality.

Here, we propose two natural schemes to construct a quasi-particle Hamiltonian, $H^{QS GW}_{\text{non-local}}$, that is exactly double-counting free when combined with a local (DMFT) self-energy. As a first method, I shall detail an intuitive scheme that requires the hermitian part of the $GW$ self-energy to be linear in frequency over the quasi-particle band-width. In a second step, a general framework will be introduced.

While the effective one-particle Hamiltonian, $H^{QS GW}$, neglects life-time effects, $\Sigma^{QS GW}$ is included when computing spectra via the interacting Greens-function (1): $G^{QS GW-1}(k, \omega)\equiv \omega - H^{QS GW}(k) - \Sigma^{QS GW}(k, \omega)$.
2.2.1. unrenormalize $H^{QSGW}$ to linear order in the local self-energy. Suppose we already dispose of the Hamiltonian $H^{QSGW}_{\text{non-local}}$ in which only non-local correlations effects have been accounted for. Within QSGW, the latter is further renormalized by local correlations described by $\Sigma^{GW}_{\text{local}}(\omega)$. The interacting Greens-function then can be expressed with these two quantities:

$$G^{QSGW-1}(k,\omega) = \omega - H^{QSGW}_{\text{non-local}}(k) - \Sigma^{GW}_{\text{local}}(\omega)$$

(6)

Performing a low-energy expansion, $\Sigma^{GW}_{\text{local}}(\omega) \approx R \Sigma^{GW}_{\text{local}}(\omega=0) + (1 - Z^{-1}_{\text{loc}}) \omega$, in the local basis, and assuming this Fermi liquid-like self-energy to extend over the range of the quasi-particle dispersion, (6) becomes $\omega - Z_{\text{loc}} \left[ H^{QSGW}_{\text{non-local}}(k) + \Re \Sigma^{GW}_{\text{local}}(0) \right]$ from which we identify the full Hamiltonian $H^{QSGW}(k) = Z_{\text{loc}} \left[ H^{QSGW}_{\text{non-local}}(k) + \Re \Sigma^{GW}_{\text{local}}(0) \right]$, whence

$$H^{QSGW}_{\text{non-local}}(k) = Z^{-1}_{\text{loc}} H^{QSGW}(k) - \Re \Sigma^{GW}_{\text{local}}(\omega = 0)$$

(7)

This expression is very intuitive: The quasi-particle bandwidth, that has been narrowed by dynamical renormalizations, is widened by the inverse of the local component of the quasi-particle weight $Z_{\text{loc}}$. Additionally, local correlation-induced crystal-field splittings are subtracted. The local self-energy that will be provided by the DMFT will go these steps backwards and add the more reliable local shifts and quasi-particle renormalization factor $Z^{DMFT}$. While in many systems the hermitian part of the $GW$ self-energy will be linear order the bandwidth of low-energy orbitals, making the just described linear QSGW+DMFT prescription reliable for all practical purposes, a more general procedure is possible and will be described in the following.

2.2.2. non-local quasi-particleization. Again, instead of devising a separate double counting $E_{dc}$ à la DFT+DMFT, the idea is to construct a quasi-particle Hamiltonian, $H^{QSGW}_{\text{non-local}}$, that includes all non-local exchange and correlation effects beyond DFT, but is void of local correlations. In a local basis, $\{\chi_{RL}(r)\}$, we first determine local and non-local projections of the self-energy, $\Sigma^{GW}_{\text{local}} = \sum_k \Sigma^{GW}(k)$, $\Sigma^{GW}_{\text{non-local}} = \Sigma^{GW} - \Sigma^{GW}_{\text{local}}$, respectively. Then we transform these back into the band representation $\{\Psi_i(r)\}$, use (3), and identify the respective terms in equation (4):

$$\det [\omega - H^{QSGW}(k) - \Re \Sigma^{GW}_{\text{non-local}}(k,\omega) - \Re \Sigma^{GW}_{\text{local}}(\omega) + v^{QSGW}_{xc}(k)] = 0$$

(8)

Now we want to replace $\Re \Sigma^{GW}_{ij\text{non-local}}(k,\omega)$ by a static term that does not modify the energies $E_{ki}$ that are the solutions of (8). This is exactly the spirit the quasi-particle self-consistency[27, 28], but now we construct a potential that only includes non-local parts of the self-energy. Akin to (5) the natural choice is:

$$v^{QSGW}_{xc\text{non-local}} = \frac{1}{2} \sum_{ijkl} \langle \Psi_k | \Re \left[ \Sigma_{ij\text{non-local}}(k, E_{ki}) + \Sigma^{GW}_{j\text{non-local}}(k, E_{kj}) \right] | \Psi_j \rangle.$$

(9)

Transforming (9) into the local basis, $\{\chi_{RL}(r)\}$, the Hamiltonian for direct use in DMFT is:

$$H^{QSGW}_{\text{non-local}}(k) = H^{QSGW}(k) + v^{QSGW}_{xc\text{non-local}}(k) - v^{QSGW}_{xc}(k)$$

(10)

We stress that $v^{QSGW}_{xc\text{non-local}}$ is not the local projection of $v^{QSGW}_{xc}$, as the non-local projection of the self-energy was done at arbitrary frequency $\omega$, before evaluating it at the quasi-particle energies in (9). See Ref. [36] for a discussion of this intricacy. The term that takes out local correlation effects is therewith actually momentum-dependent –a clear necessity for $H^{QSGW}$ to have a wider band-width than $H^{QSGW}$.

3. We note that in the usual QSGW prescription, the operator $v^{QSGW}_{xc}$ of (5) does not always reproduce the quasiparticle energies exactly. This is owing to band-off-diagonal ($i \neq j$) elements of the self-energy. The resulting ambiguity in the self-consistent Hamiltonian was shown to be small[41, 43]. In particular, once self-consistency is achieved, $\Sigma^{GW}(k, E_{ki})$ should be diagonal in the band basis, and thus (9) reliable and unambiguous.
3. Application
In figure 2, I show a simplified realization of \(QSGW+DMFT\) for electron-doped \(\text{BaFe}_2\text{As}_2\). In comparison with angle resolved photoemission (ARPES) experiments\([40]\) there are two major discrepancies in the DFT(LDA) band-structure: (a) the size of hole pockets at the \(\Gamma\) point is drastically overestimated, and (b) the dispersion is too pronounced, i.e. effective masses are too small. DMFT does not correct problem (a) \([25]\), but it yields larger effective masses\([18]\). \(QSGW\) on the other hand, substantially improves on (b) the size of the hole pockets, which is interpreted as an effect of a non-local self-energy. The dispersion is however still too big with respect to experiment, owing to the perturbative treatment of the quasi-particle weight \(Z\)[26].

Mimicking \(QSGW+DMFT\) by substituting the local dynamical renormalizations (provided by the local quasi-particle weight \(Z_{\text{loc}}\) in \(QSGW\)[26] with published values from DMFT\([18]\), we see that \(QSGW+DMFT\) combines the best of both worlds: a good description of both, (a) the size of the pockets, and (b) the effective masses that renormalize the slope of the dispersion. We note that the dispersion of the non-local \(QSGW\), \(H_{QSGW}^{\text{non-local}}\) is larger than in DFT(LDA), as the non-local self-energy delocalizes charge carriers. The effective mass of \(QSGW+DMFT\) is thus lower than in DMFT\([26]\). This will have a notable effect also on the spin degrees of freedom: Besides the correction of the energy scale associated with the size of the charge pockets\([44]\), the carrier delocalization will push the onset of single-ion physics (Curie-like susceptibility) to higher temperatures. Indeed the magnetic susceptibility in the iron pnictides has a universal linear dependence up to high temperatures\([14]\).

Let me note in passing that also a second deficiency of DFT+DMFT methods is improved upon by \(QSGW+DMFT\): Indeed DMFT can only be applied to a low-energy subspace of orbitals (typically \(d\) or \(f\)-electron states). However, it is known that ligand states (e.g. the 2p-orbitals in transition metal oxides) are not well captured within DFT, owing to inter- and out-of-subspace exchange and correlation effects\([45, 46]\). As an all-electron method, \(QSGW\) includes these effects; for instance it corrects the position of the Se-4p states in the chalcogenide FeSe by almost 1 eV\([26]\) in excellent agreement with experiment\([47]\).

4. Relation of \(QSGW+DMFT\) to full \(GW+DMFT\)
The \(QSGW+DMFT\) approach, proposed in Ref. \([26]\) and detailed above, offers to retain salient features of the full \(GW+DMFT\) methodology\([30]\), and to remedy some of the pathologies of current \(GW+DMFT\) implementations: State-of-the-art \(GW\) codes rely on a non-interacting form of the Greens-function, complicating the feedback of the DMFT self-energy and susceptibility onto the \(GW\) part. Therefore, hitherto this has been achieved only in the one band case\([32, 33, 34]\). Indeed all other, realistic \(GW+DMFT\) calculations so far\([30, 35, 36]\) fix non-local correlations to the one-shot \(GW\) level and the screened interaction to constraint random phase
approximation (cRPA) results. These quantities thus depend on the effective one-particle Greens-function chosen as the starting point, most often provided by DFT. QSGW+DMFT circumvents global iterations by limiting the self-consistency of non-local correlation effects to the QSGW level. The pathology of a DFT starting point dependence is thus avoided.

In (QS)GW+DMFT the double counting, $E_{dc}$, is known exactly. Its static form in the QSGW+DMFT approach allows for a Hamiltonian description. Indeed, $F_{non-local}$ of equation (10) or (7), can be viewed as a vastly improved effective one-particle starting point for DMFT. Consequently, current DFT+DMFT implementations can be used with little or no modification. This also avoids handling the momentum and frequency dependent GW self-energy in the DMFT self-consistency, drastically reducing memory requirements.

The short-cuts introduced by QSGW+DMFT come with the cost of neglecting (a) the momentum variation of quasi-particle coherence, (b) local vertex corrections in the polarization beyond RPA, and (c) non-perturbative corrections to the GW one-particle propagator.

Figure 3. BaFe$_2$As$_2$ and FeSe: Real parts of the local QSGW self-energy ($xz$ Wannier component, upper panel) and the standard deviation $\Delta_k Z$ of the generalized quasi-particle weight $Z^k(\omega) = [1 - \partial_\omega \Re \Sigma^G(k,\omega)]^{-1}$ with respect to momentum (lower panel): The k-dependence of the dynamical self-energy is negligible in the (gray shaded) regime in which $\Re \Sigma$ is linear.

5. Separability of non-local and dynamical correlations

When not using the self-consistency prescription (5), for a Hamiltonian formalism to include non-local correlation effects necessitates that correlations are separable into non-local and dynamical contributions. Indeed, a self-energy can formally be split into $\Sigma^c(k) + \Sigma^\text{non-loc}(k,\omega) + \Sigma^\text{loc}(\omega)$, i.e. an exchange (“x”) and a correlation (“c”) part, in the latter of which we can isolate local (“loc”) and non-local (“non-loc”) components. Only if the non-local part of the correlation self-energy is static, i.e.

$$\Sigma^c(k,\omega) = \Re \Sigma^\text{non-loc}(k) + \Sigma^\text{loc}(\omega),$$

we can construct $H^{qp}_{\text{non-loc}}(k) = H^G(k) + \Sigma^x(k) + \Re \Sigma^c_{\text{non-loc}}(k)$ for use in DMFT. Requirement (11) is a non-trivial statement: it is known to fail in 1D & 2D systems. Recently, however, it was shown that correlation effects in 3D systems such as the iron pnictides and chalcogenides verify property (11) within GW for energies inside

\[ H^{qp}_{\text{non-loc}}(k) = H^G(k) + \Sigma^x(k) + \Re \Sigma^c_{\text{non-loc}}(k) \]
the $d$-electron bandwidth. This is exemplified in figure 3 for BaFe$_2$As$_2$ and FeSe. There, as a measure for the non-locality of dynamical renormalizations we plot the standard deviation 
\[
\Delta_k Z(\omega) = \sqrt{\sum_{kL} |Z_{kk}(\omega) - Z_{loc}^{LL}(\omega)|^2}
\]
of the momentum resolved quasi-particle weight $Z_k$ with respect to its local value $Z_{loc}$, both of which we formally extend to finite frequencies: 
\[
Z_k(\omega) = [1 - \partial_\omega \Re \Sigma(k, \omega)]^{-1}.
\]
Indeed the momentum dependence virtually vanishes at the Fermi level, $\Delta_k Z(\omega = 0) \approx 0$, and remains very low in the regime in which the hermitian parts of the self-energy are linear. This shows that in this energy range, non-local correlations are static, and dynamical correlations thus local.

This separability has two far-reaching consequences: (a) it provides a highly encouraging a posteriori justification for DMFT-based approaches that describe correlation effects with a dynamical, yet local, self-energy. (b) Identifying that the sizable non-local correlations are dominantly static in nature may pave the way for physically motivated approximate electronic structure schemes, such as the recently proposed DMFT@non-local-GW[36] and SEX+DMFT[39]. In DMFT@nonlocal GW, the separability (11) is used to construct a non-locally renormalized Hamiltonian $H_{\text{qp non-loc}}(k)$ from a one-shot $GW$ calculation. It was shown that this approach successfully reproduces for SrVO$_3$ the quasi-particle dispersion of full $GW$+DMFT calculations and, if a dynamic Hubbard interaction is used, even the position of satellite features such as the plasmons peak is captured[36]. SEX+DMFT[39] identifies exchange effects beyond DFT as crucial non-local self-energy contributions and computes a screened exchange (SEX) ingredient to supplement the one-particle Hamiltonian. Therewith (11) is fulfilled by construction. The approach has been shown to be very successful in the description of ARPES experiments for BaCo$_2$As$_2$[39].

Besides the exchange part, there potentially are, in correlated systems, momentum-dependent correlation effects. If these effects are important, a (QS) $GW$+DMFT calculation that includes both non-local exchange and correlation effects must be performed. We should however also note that $GW$ itself misses the important non-local correlations that derive from spin-fluctuations. Yet, interestingly, non-local spin fluctuations –e.g. those emerging in the vicinity of the Néel state of the 3D Hubbard model– do not introduce a momentum differentiation to the dynamics of the self-energy but rather yield a modulation of static contributions[49]. This reinforces the guidance that the separation (11) may give to future electronic structure theories.

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9 We note that this is true beyond the perturbative $GW$ methodology, as was shown for the 3D Hubbard model[49].

10 Indeed it was shown for the electron gas that corrections to the local approximation of the Coulomb hole are significant at large momentum transfer, yet mostly static in nature[51].
