The effects of k-dependent self-energy in the electronic structure of correlated materials

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I. INTRODUCTION

The electronic structure of a certain class of materials, commonly known as strongly correlated materials, is crucially determined by electron correlations. In these materials one-particle theory, predominantly the local density approximation (LDA) within density functional theory, is often far from sufficient in providing an accurate and reliable description of the electronic structure. The reason for the failure of one-particle theory may be traced back to the presence of many configurations close in energy arising from a partially filled narrow band characteristic of these materials, similar to the situation in atoms with partially filled shell. It is not surprising that description of the electronic structure in terms of a single Slater determinant is not satisfactory. One of the most fruitful approaches in treating the electronic structure of these materials is the Green function technique with a nonlocal and energy-dependent self-energy. Among the Green function approaches, the combination of the LDA and the dynamical mean-field theory (DMFT)$^2$, i.e., the LDA+DMFT method$^{3,4}$, is perhaps the most widely used technique in describing the electronic structure of strongly correlated materials.

In many calculations based on model Hamiltonians it is often assumed that the self-energy is local, meaning that it has no momentum or k dependence and the Hubbard U used in solving the impurity problem is assumed to be static. How these two approximations affect the resulting band structure remains to be investigated. Experience with the electron gas teaches us that there is a strong cancellation between the effects of k-dependent self-energy and frequency-dependent self-energy. This is revealed by the fact that effective mass of the electron gas with density relevant for most materials is quite close to unity. The effective mass in general depends on two factors: the derivative of the self-energy with respect to frequency, which tends to enhance the effective mass, and the derivative of the self-energy with respect to the k-vector, which tends to have the opposite effect. In the electron gas these two factors tend to cancel each other, hence the effective mass being close to unity$^{5,6}$. We have no apriori reason to believe that such an almost complete cancellation remains true in real materials, especially in the strongly correlated systems. Indeed, it is often claimed that for narrow-band materials the self-energy has little k-dependence so that a local but dynamic theory with frequency-dependent self-energy provides a good approximation to the full self-energy.

The k-dependent self-energy becomes even more relevant with the recent progress in solving the impurity problem with a frequency-dependent Hubbard U$^{7-9}$. This new algorithm makes it possible to perform LDA+DMFT calculations using a dynamic Hubbard U, instead of a static one as in conventional calculations. This raises an important issue concerning the role of nonlocal or k-dependent self-energy. The use of dynamic U might lead to an overestimation of band narrowing or mass enhancement because the dynamic U produces a self-energy that has a stronger frequency dependence or larger derivative at around the Fermi level. One might anticipate qualitatively that the use of a dynamic U ought to be counterbalanced by the inclusion of a k-dependent self-energy to restore the correct mass enhancement.

The purpose of this paper is to investigate the effects of momentum- and frequency-dependence of the self-energy on the electronic structure of materials with partially filled narrow bands. To address the aforementioned issues, instead of using a model Hamiltonian, we will employ the GW approximation (GWA)$^{10,11}$ which allows us to perform accurate calculations on real materials. As a test material we study specifically the electronic structure of SrVO$_3$ which has been widely studied in the literature both experimentally by means of photoemission...
spectroscopy and theoretically. We believe the results are general and will be directly relevant to realistic electronic structure calculations.

II. THEORY AND METHOD

The correlation part of the self-energy (excluding exchange) in the GWA is given by

\[ \Sigma^c(r, r'; \omega) = i \int \frac{d\omega'}{2\pi} G(r, r'; \omega + \omega') W^c(r, r'; \omega') \] (1)

where

\[ W^c = W - v. \] (2)

\( v \) is the bare Coulomb interaction and \( W \) is the fully screened interaction calculated within the random-phase approximation (RPA). Using the spectral representation of \( G \) and \( W \)

\[ G(r, r'; \omega) = \sum_{kn} \frac{\psi_{kn}(r)\psi_{kn}^*(r')}{\omega - \varepsilon_{kn} - i\delta} + \sum_{kn} \frac{\psi_{kn}(r)\psi_{kn}^*(r')}{\omega - \varepsilon_{kn} + i\delta}. \] (3)

\[ W^c(r, r'; \omega) = \int_0^\infty d\omega' \frac{B(r, r'; \omega')}{\omega - \omega' - i\delta} + \int_0^\infty d\omega' \frac{B(r, r'; \omega')}{\omega - \omega' + i\delta}, \] (4)

where

\[ B(\omega) = -\frac{1}{\pi} \text{Im} W^c(\omega)\text{sgn}(\omega), \] (5)

the spectral function of the correlation part of the self-energy can be expressed in terms of the imaginary part of the screened interaction as follows:

\[ \Gamma(r, r'; \omega \leq \mu) = \sum_{kn} \psi_{kn}(r)B(r, r'; \varepsilon_{kn} - \omega)\psi_{kn}^*(r')\theta(\varepsilon_{kn} - \omega), \] (6)

\[ \Gamma(r, r'; \omega > \mu) = \sum_{kn} \psi_{kn}(r)B(r, r'; \omega - \varepsilon_{kn})\psi_{kn}^*(r')\theta(\omega - \varepsilon_{kn}), \] (7)

where

\[ \Gamma(r, r'; \omega) = -\frac{1}{\pi} \text{Im} \Sigma^c(r, r'; \omega)\text{sgn}(\omega - \mu). \] (8)

The real part of the correlation self-energy (excluding exchange) is given by the Hilbert transform

\[ \text{Re} \Sigma^c(r, r'; \omega) = \int_{-\infty}^{\infty} d\omega' \frac{\Gamma(r, r'; \omega')}{\omega - \omega'}. \] (9)

In this work, the one-particle band structure \( \{ \psi_{kn}, \varepsilon_{kn} \} \) is taken to be the LDA one.

The full self-energy may be expanded in terms of Bloch states \( \psi_{kn} \):

\[ \Sigma(r, r'; \omega) = \sum_{kn} \psi_{kn}(r)\Sigma_{nn'}(k, \omega)\psi_{kn}^*(r'). \] (10)

The Bloch states may be expressed in terms of some Wannier orbitals \( \{ \varphi_R \} \)

\[ \psi_{kn}(r) = \sum_R \exp(-i\mathbf{k} \cdot \mathbf{R})\varphi_{Rn}(r) \] (11)

and the self-energy becomes

\[ \Sigma(r, r'; \omega) = \sum_{kn} \sum_{RR'} \exp(-i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}'))\varphi_{Rn}(r)\Sigma_{nn'}^{loc}(k, \omega)\varphi_{R'n'}^*(r'). \] (12)

The local self-energy centered at lattice site \( \mathbf{R} \) is defined according to

\[ \Sigma_{\mathbf{R}}^{loc}(r, r'; \omega) = \sum_{kn} \varphi_{Rn}(r)\Sigma^{loc}_{nn'}(k, \omega)\varphi_{R'n'}^*(r') \] (13)

where

\[ \Sigma^{loc}_{nn'}(k, \omega) = \sum_{k'} \Sigma_{nn'}(k, \omega) \] (14)

Since \( \Sigma^{loc}_{\mathbf{R}} \) is independent of \( \mathbf{R} \) we may choose \( \mathbf{R} = 0 \) and write

\[ \Sigma^{loc}(r, r'; \omega) = \sum_{nn'} \varphi_n(r)\Sigma^{loc}_{nn'}(\omega)\varphi_{n'}^*(r') \] (15)

\[ \varphi_n \equiv \varphi_{0n}. \] (16)

The above formulation is quite general and we now focus on SrVO₃ which has a narrow band, derived from the \( t_{2g} \) orbitals of the vanadium, crossing the Fermi level. The \( t_{2g} \) band is well separated from the rest of the bands so that we need only consider Wannier orbitals
constructed from Bloch states belonging to this band. Following the method of Marzari and Vanderbilt, 25,26, we construct the (maximally localized) Wannier orbitals \( \varphi_{Rn} \) according to

\[
|\varphi_{Rm}^w\rangle = \sum_k |\psi_{km}^w\rangle e^{i\mathbf{k} \cdot \mathbf{R}}, \quad |\psi_{km}^w\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} |\varphi_{Rm}^w\rangle e^{-i\mathbf{k} \cdot \mathbf{R}}
\]  

(17)

\[
|\psi_{km}^w\rangle = \sum_n |\psi_{kn}\rangle S_{nm}(\mathbf{k}), \quad m, n \in t_{2g}
\]  

(18)

where \( |\psi_{km}^w\rangle \) is a one-particle Bloch state which may be chosen to be that of the LDA. The matrix \( S \) is a square matrix when the subspace is well separated but for entangled bands, \( S \) is not necessarily a square matrix, the number of band index \( n \) may be larger than \( m \). The matrix \( S \) is chosen to make the Wannier orbitals as localized as possible according to a prescription by Marzari and Vanderbilt. 25,26

Using the expression in (15), the expectation value of the local self-energy in a Bloch state \( \psi_{kn} \), is given by

\[
\langle \psi_{kn} | \Sigma^{\text{loc}}(\omega) | \psi_{kn} \rangle = \sum_{mm',t_{2g}} \langle \psi_{kn} | \varphi_{m} \rangle \Sigma_{mm'}^{\text{loc}}(\omega) \langle \varphi_{m'} | \psi_{kn} \rangle
\]  

(19)

where \( \varphi_{m} \) is a maximally localized Wannier orbital defined in (17) for the central cell \( \mathbf{R} = 0 \) and the matrix elements \( \Sigma_{mm'}^{\text{loc}}(\omega) \) are taken in the Wannier gauge \( \psi_{km}^w \) defined in Eq. (18):

\[
\Sigma_{mm'}^{\text{loc}}(\omega) = \sum_{\mathbf{k}} \langle \psi_{kn} | \Sigma^{\text{loc}}(\omega) | \psi_{km'}^w \rangle.
\]  

(20)

The sum in Eq. (19) is restricted to the \( t_{2g} \) orbitals because the Bloch state \( \psi_{kn} \) belonging to the \( t_{2g} \) band has no component outside the \( t_{2g} \) subspace. In the case of SrVO\(_3\), due to cubic symmetry, the self-energy in Eq. (20) is diagonal and independent of the orbital index \( m \) so that the matrix element of the local self-energy in the Bloch state \( \psi_{kn} \) in Eq. (19) becomes independent of both \( \mathbf{k} \) and the band index \( n \).

The quasiparticle band structure is obtained from

\[
E_{kn} = \varepsilon_{kn} + \langle \psi_{kn} | \text{Re} \Sigma(E_{kn}) - v_{xc} | \psi_{kn} \rangle
\approx \varepsilon_{kn} + Z_{kn} \langle \psi_{kn} | \text{Re} \Sigma(\varepsilon_{kn}) - v_{xc} | \psi_{kn} \rangle,
\]  

(21)

where

\[
Z_{kn} = \left[ 1 - \frac{\partial \text{Re} \Sigma_{nn}(\mathbf{k}, \omega)}{\partial \omega} \right]^{-1}_{\omega = \varepsilon_{kn}}
\]  

(22)

is the quasiparticle weight. The angle-resolved spectral function is calculated as follows:

\[
A(\mathbf{k}, \omega) = \frac{1}{\pi} \sum_n \frac{|\text{Im} \Sigma_{nn}(\mathbf{k}, \omega)|}{[\omega - \varepsilon_{kn} - \text{Re} \Sigma_{nn}(\mathbf{k}, \omega)]^2 + |\text{Im} \Sigma_{nn}(\mathbf{k}, \omega)|^2},
\]  

(23)

where we have assumed that the self-energy is diagonal in the band index, and the total spectral function is given by

\[
A(\omega) = \sum_{\mathbf{k}} A(\mathbf{k}, \omega).
\]  

(24)

The band structure calculation is based on the full-potential LMTO implementation. 27 The exchange-correlation functional is the local density approximation of the Cepeley-Alder type. 28 The GW calculation uses mixed basis consisting of products of two atomic orbitals and interstitial plane waves. 29,30 The \( 8 \times 8 \times 8 \) mesh is used for Brillouin-zone integration. More technical details are found elsewhere. 31

### III. Results and Discussions

#### A. Local vs nonlocal self-energy

We first examine the results for the real and imaginary part of the self-energy at some representative \( \mathbf{k} \)-points \( \Gamma, X, \) and \( R \) shown in Fig. 2. \( \text{Im} \Sigma \) of the occupied states are distinctly different from those of the unoccupied states. The former have a peak structure below the Fermi level at around \(-3 \text{ eV}\) while such structure is essentially absent for the latter. The structure of \( \text{Im} \Sigma \) can be understood by taking the matrix element \( \text{Im} \Sigma \) in Eq. (16) and (17):

\[
\Gamma_m(\mathbf{q}, \omega \leq \mu) = \sum_{\mathbf{k}n} \langle \psi_{qnm} | B(\varepsilon_{kn} - \omega) | \psi_{kn} \rangle \times \theta(\varepsilon_{kn} - \omega),
\]  

(25)

\[
\Gamma_m(\mathbf{q}, \omega > \mu) = \sum_{\mathbf{k}n} \langle \psi_{qnm} | B(\omega - \varepsilon_{kn}) | \psi_{kn} \rangle \times \theta(\omega - \varepsilon_{kn}).
\]  

(26)

Since \( B \) is proportional to \( \text{Im} W \) the structure in \( \text{Im} \Sigma \) is essentially determined by the structure in \( \text{Im} W \) with intensity governed by the overlap between the state \( \psi_{qnm} \) and the occupied or unoccupied states \( \psi_{kn} \). Whether the structure in \( \text{Im} W \) is carried over to \( \text{Im} \Sigma \) depends on the character of the state \( \psi_{qnm} \). If the state \( \psi_{qnm} \) is occupied, there will be a strong overlap with occupied states \( \psi_{kn} \) so that the intensity of \( \Gamma(\omega \leq \mu) \) may be expected to be stronger than the intensity of \( \Gamma(\omega > \mu) \). Indeed, the peak structure in \( \text{Im} \Sigma \) for the unoccupied state at the \( X \) and \( R \) point is stronger above the Fermi level than below. This structure can be traced back to the peak structure in \( \text{Im} W \) at around \(-1 - 2 \text{ eV}\) as can be seen in Fig. 2.
Re $\Sigma$ of the occupied states have more structure around $-3 \text{ eV}$ than for the unoccupied states. This structure originates from the peak structure in Im $\Sigma$ at around the same energy. The straight lines represent $y = \omega - \epsilon_{kn}$ whose intersection with or proximity to the real part of the self-energy below or above the quasiparticle energy signals the formation of satellites, provided the imaginary part of the self-energy at the intersection energy is sufficiently small to produce a discernible feature. It is clear from the figures that the straight lines only cross Re $\Sigma$ at one point so that a well-defined satellite feature is not expected. However, for the unoccupied states at $X$ and $R$ the straight lines come close to the proximity of Re $\Sigma$ and we expect a formation of a weak satellite at around 4 $\text{eV}$ above the Fermi level.

To see the difference between the local self-energy and the $k$-dependent self-energy we plot in Fig. 1 the real part of the self-energy at some $k$-points and compare them with the local self-energy, which is the average of the self-energy over the Brillouin zone as defined in Eq. (20). The imaginary part of the local self-energy is also shown. It resembles the self-energy of the unoccupied states because the sum in Eq. (14) is dominated by the unoccupied states since the number of unoccupied states is much larger than that of the occupied states. The contribution from the small number of occupied states corresponding to one $t_{2g}$ electron is weighted down by the contribution from the rest of the $k$-points. The real part of the local self-energy is shown in Fig. 1 and similar to the imaginary part, it resembles that of the unoccupied states with little structure below the Fermi level. A local $GW$ self-energy would therefore not produce any distinct satellite below the Fermi level at around $-3 \text{ eV}$.

IV. QUASIPARTICLE BAND STRUCTURES

In Fig. 3 the quasiparticle band structures obtained within the LDA, the GWA and the local GWA are compared. The effect of the $k$-dependence of the self-energy is striking. The band width obtained from the full $GW$ calculation is reduced by almost a factor of two when the $k$-dependence is neglected. This result is consistent with the following consideration for the effective mass. The effective mass $m^*$ is given by

$$\frac{m}{m^*} = Z \left[ 1 + \frac{1}{d\epsilon/dk} \frac{\partial \text{Re } \Sigma(k, \omega)}{\partial k} \right]$$

where

$$Z = \left[ 1 - \frac{\partial \text{Re } \Sigma(k, \omega)}{\partial \omega} \right]^{-1}.$$
It is clear from the above expression that if the self-energy is assumed to be local or onsite then the effective mass or the quasiparticle band width is determined by the Z factor only since Re Σ is approximately linear within the band width. However, in the case of SrVO$_3$, the GW quasiparticle band width is narrowed from the LDA band by only 20% whereas the Z factor is about 0.5. The discrepancy between the band narrowing and the Z factor can be explained by the k-dependence of the self-energy. Indeed, when the quasiparticle band structure is calculated using a local GW self-energy it is found that the band width is reduced by one half from its LDA value as can be seen in the figure. Thus, the k-dependent self-energy widens the dispersion. This is in accordance with the electron gas result, in which the free-electron occupied band width is reduced by only 10% by the GW self-energy in the one-shot calculation whereas the Z factor is about 0.7. In the self-consistent calculation the free-electron occupied band width is widened, rather than narrowed. This would be contradictory to the fact that the Z factor is ~ 0.7 if the band width were determined by the Z factor only. Clearly, the k-dependent self-energy widens the band width.

To understand the origin of the band narrowing when a local self-energy is used, we plot in Fig. 4 the difference between the full and local self-energies, which represents the nonlocal contribution of the self-energy. For the occupied states at the Γ and X points the difference is negative whereas for the unoccupied states at the X and R points the difference is positive. This implies that the occupied states are pushed up whereas the unoccupied states are pushed down when a local self-energy is used, resulting in band narrowing. The effect of band narrowing is particularly revealing for the states at the X point as can be seen in Fig. 4 where the nonlocal self-energies for the occupied and unoccupied states have different signs.

Although in the present work we have only presented the results for SrVO$_3$ we have performed similar calculations on other materials such as iron and nickel with very similar results. This gives us sufficient confidence to believe that the results presented in this paper are quite general.

V. THE SPECTRAL FUNCTIONS

In Fig. 5 we compare the angle-resolved spectral functions at Γ, X, R and M points obtained from the LDA, the full GW self-energy and the local GW self-energy. As can be already expected from the plot of Re Σ in Fig. 1 no strong satellite structure is expected at the Γ point because the straight line $y = \omega - \varepsilon_{k_n}$ only crosses Re Σ at one point corresponding to the quasiparticle energy but away from this energy it does not come close enough to the proximity of Re Σ. Indeed the (total) spectral func-
tion shown in Fig. 6 only shows a very weak structure between −2 and −3 eV with no satellite feature above the Fermi level. Experimentally, a satellite at −1.5 eV is observed.

The spectral functions for the $X$ and $R$ points on the other hand show a broad but noticeable satellite feature at about 3.5 − 4.0 eV above the Fermi level but with no feature below the Fermi level. This is consistent with the results for Re $\Sigma$ shown in Fig. 1 where the straight line corresponding to the unoccupied states come close to a peak in Re $\Sigma$ around 4 eV. Since there is only one $d$ electron, we expect that the satellite above the Fermi level corresponding to configuration with two electrons is stronger than the one below corresponding to the removal of the electron.

It is known that the GWA tends to overestimate the position of the satellite peak arising from a plasmon excitation. The position of the plasmon peak in $W$ is well described by the RPA but the GW self-energy is first-order in $W$. It is this first-order approximation that places the plasmon peak satellite in the spectral function too high in energy. It is reasonable to expect a similar tendency in low-energy satellites that may be associated with the Hubbard bands. Indeed, the experimentally observed satellite structures have lower energies compared with the calculated ones.

VI. CONCLUSIONS

The present work reveals that even in materials with narrow bands, the nonlocal self-energy has a significant effect on the band structure. The band width obtained by neglecting the nonlocal self-energy is found to be too narrow compared to the result of a full calculation and consequently the effective mass is overestimated. Although the present investigation has been based on the GWA, it is feasible that the result is general. This result indicates that calculations based on DMFT using a dynamic $U$ where the self-energy is local may overestimate the effective mass but further investigations are needed before a definite conclusion can be reached because it is not clear how the local self-energy in the present work is related to the self-energy in DMFT. A promising approach for including the nonlocal self-energy on top of the DMFT self-energy is the combination of the GW method and DMFT34 where local correlations responsible for the formation of Hubbard bands not well described by the GWA is taken care of by the DMFT while the nonlocal self-energy responsible for modification of the quasiparticle energy is accounted for by the GWA.

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