Screening, RPA, GW and GW+EDMFT: an Introduction.

Lecture at the 2025 TRIQS summer school

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Disclaimer: Preliminary notes - some mistakes or misprints may remain.

I. MOTIVATIONS

We have seen that the DFT+DMFT approach to electronic structure, efficient as it is, has two *ad-hoc* aspects. Hence it is a theory that cannot be entirely derived from first principles. Namely:

- The many-body interactions acting in the correlated subspace are not computed from first-principles. They are either taken as empirical parameters (extracted from spectroscopy, or from fits to specific experiments) or obtained independently by other means - such as constrained DFT or constrained RPA (see below).
- In order to combine DFT and DMFT, a double-counting correction must be applied. This is because DFT functionals already take into account some of the effects of the Coulomb interaction. However, because DFT is not a Green's function based theory and is not diagrammatically controlled (i.e it is not possible to identify a class of diagrams which correspond to a specific functional used as an approximation to exact DFT), it is hard to derive an exact expression for the dc correction (some suggestions exist, see e.g. K.Haule's work). In practical terms, the dc correction directly influences the relative positioning of the correlated bands with respect to others (e.g. d-like bands vs O-p ones in transition-metal oxides).

These two limitations are inter-related. The evaluation of interaction parameters for the correlated subspace require that *screening* be taken into account. Screening effects are stronger and stronger as the target correlated space is built out of less localized orbitals. Hence, one is faced with the following conundrum:

- Either use a large energy window to construct correlated orbitals (hence more localized). In that case, there is better control (eg from spectroscopy experiments) on which interaction parameters to choose. But the dc correction plays an important role then.
- Or use a massively downfolded description on a small subset of isolated bands (when possible), hence working with more delocalized orbitals. In that case there may not be a double counting issue at all, but the screening effects are even more important in the determination of interaction parameters.

These features do not mean that DFT+DMFT has no predictive power (quite on the contrary!). But it certainly calls for a more ab-initio framework for computing the electronic structure of strongly correlated materials (and even weakly correlated ones, to overcome limitations of approximate DFT functionals).

The origin of the problem is that DFT and DMFT really come from very different points of views. The way to go forward is to ground electronic structure into a Green's function based, diagrammatically controlled, theory.

II. SCREENING AND RPA

A. Introduction

In an interacting electron system, the long-range Coulomb interaction

$$V(\mathbf{r}) = \frac{e^2}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}|}$$

is strongly modified by the collective response of the electron gas. This modification is known as **screening**.

More precisely: when introducing a test charge into the system, all other charged particles (electrons) react to that perturbation. Hence, the long-distance potential created by that test charge is not the usual Coulomb interaction in vacuum. This also implies that the effective interaction between two electrons is modified by the presence of the other electrons.

Units: In the following I will use mostly CGS units in which the vacuum permittivity is chosen to be $4\pi\varepsilon_0 = 1$. Furthermore I will use $e = 1$. In those units the charge density $\rho(r)$ and particle density $n(r)$ are related by:

$$\rho(r) = -n(r)$$

because the electron charge is, annoyingly (!) conventionally defined to be negative. In turn, the Coulomb potential and its Fourier transform reads:

$$V(\mathbf{r}) = \frac{1}{|\mathbf{r}|} \ , \ \text{Fourier transform}: \ V(\mathbf{q}) = \frac{4\pi}{q^2}$$

The Poisson equation reads:

$$\nabla^2\phi(r) = -4\pi\rho(r) = 4\pi n(r)$$

and $-V(r-r')/4\pi$ coincides with the inverse Laplacian (Green's function associated with the Poisson operator).

B. Linear Response Derivation

I now introduce the so-called Random Phase Approximation (RPA), which provides a microscopic, self-consistent theory of screening - although an *approximate* one.

The idea is to subject the system to an external potential ϕ_{ext} corresponding to an external test charge density:

$$\phi_{\text{ext}} = V(q)\,\rho_{\text{ext}}$$

This potential will induce an internal charge density ρ_{ind} and in turn an internal potential ϕ_{ind} so that the total potential is $\phi_{tot} = \phi_{ext} + \phi_{ind}$.

Using linear response theory, the induced density in momentum-frequency space is

$$\rho_{\text{ind}}(\mathbf{q},\omega) = -\chi^0(\mathbf{q},\omega)\,\phi_{\text{tot}}(\mathbf{q},\omega),$$

where $\chi^0(\mathbf{q},\omega)$ is the density-density correlation function (Lindhard function) of noninteracting electrons (note: the minus sign is because the charge density is minus the density).

The induced potential follows from Poisson's equation:

$$\phi_{\text{ind}}(\mathbf{q},\omega) = V(\mathbf{q})\,\rho_{\text{ind}}(\mathbf{q},\omega),$$

Self-consistency gives

$$\phi_{\text{tot}} = \phi_{\text{ext}} - V(\mathbf{q})\chi^0(\mathbf{q},\omega)\phi_{\text{tot}}.$$

Thus,

$$\phi_{\text{tot}}(\mathbf{q},\omega) = \frac{\phi_{\text{ext}}(\mathbf{q},\omega)}{1 + V(\mathbf{q})\chi^0(\mathbf{q},\omega)}.$$

Using the relation between the external potential and the test (external) charge density, we see that this amounts to an effective interaction given by:

$$\phi_{tot} = W\,\rho_{ext} \ , \ \boxed{W_{RPA}(q) = \frac{V(\mathbf{q})}{1 + V(\mathbf{q})\chi^0(\mathbf{q},\omega)}}$$

Expanding the denominator this reads:

$$W_{RPA} = V - V\chi_0 V + V\chi_0 V\chi_0 V + \cdots$$

which diagrammatically corresponds to a sum of bubble diagrams (note the $(-1)^n$ minus sign due to the Feynman rules associated with fermionic bubbles).

Note that this can be rewritten:

$$W_{RPA} = V - V\left[\frac{\chi^0}{1+V\chi^0}\right]V = W(q,\omega)_{RPA}$$

As shown below, if this expression in bracket was replaced by the *exact* charge response function, this expression would become exact.

C. Dielectric Function and Screened Potential

The (longitudinal) dielectric function (in units of ε_0) is defined as:

$$W(q,\omega) = \frac{1}{\varepsilon_L(q,\omega)}\,V(q)$$

so that at the RPA level:

$$\frac{\varepsilon_0}{\varepsilon_L(q,\omega)} = \frac{1}{1+V(q)\chi_0(q,\omega)}$$

D. Physical Meaning

The RPA neglects correlations between phases of electron oscillations beyond the mean-field level, keeping only bubble diagrams. Physically:

- Each bubble = polarization of the electron gas (screening cloud).
- Infinite resummation = self-consistent screening.

This theory explains both static screening (finite screening length) and dynamical effects such as plasmons.

III. GENERAL RELATION BETWEEN SCREENED INTERACTION, BARE INTERACTION, AND DENSITY–DENSITY CORRELATION FUNCTION

1) Definitions

- **Bare interaction:** $V(\mathbf{r},\mathbf{r}')$
- **Change of external test charge** $\delta\rho_{\text{ext}}$ produces a change of the external potential $\delta\phi_{\text{ext}} = V\,\delta\rho_{\text{ext}}$.
- The system responds with an induced density δn
- The total potential acting on electrons is

$$\delta\phi_{\text{tot}}(r) = \delta\phi_{\text{ext}} - V\,\delta n = \delta\phi_{\text{ext}}(r) - \int dr'\,V(r,r')\,\delta n(r')$$

- The **screened interaction** W is defined by

$$W(r,r') = \frac{\delta\phi_{\text{tot}}(r)}{\delta\rho_{\text{ext}}(r')}.$$

- The (reducible, or full, or physical) **density–density correlation function** is

$$\chi(r,r';t,t') = \frac{\delta n(r,t)}{\delta\phi_{\text{ext}}(r',t')} = \langle (n(r,t)-\overline{n})(n(r',t')-\overline{n})\rangle$$

2) Exact relation $W = V - V\chi V$

Starting from the above identities and varying with respect to ρ_{ext}:

$$\begin{aligned}\delta\phi_{\text{tot}} &= \delta\phi_{\text{ext}} - V\,\delta n \\ &= \delta\phi_{\text{ext}} - V\,\chi\,\delta\phi_{ext} \\ &= [V - V\chi V]\,\delta\rho_{ext}\end{aligned}$$

Therefore:

$$\boxed{W = V - V\,\chi\,V}.$$

Important remark: while the bare Coulomb interaction only depends on $r - r'$, the effective screened one W depends separately on r and r' since the crystal lattice breaks translational symmetry: $W = W(r, r', \omega)$. So that the above relation reads, more explicitly:

$$W(r, r; \omega) = V(r)\delta(r - r') - V(r)\chi(r, r'; \omega)V(r')$$

Remark - dimensions. Note that the previous equation is dimensionally correct. Indeed, $\chi(r, r'; \omega)$ has the dimension of the inverse of an energy. That is because the density correlation function $\chi(r, r'; t - t')$ is obviously dimensionless.

3) Dielectric function identities

4) Irreducible polarizability Π (Hedin's notation)

The irreducible polarisability is defined as the 2-particle "self-energy" associated with the screened interaction W, namely:

$$\boxed{W^{-1} = V^{-1} - \Pi \ , \ W = \frac{V}{1 - \Pi V}}$$

or equivalently as the solution of the Dyson equation:

$$W = V + V\,\Pi\,W,$$

One can also define a susceptibility χ_I which is irreducible with respect to cutting a single interaction line as:

$$\chi = \frac{\chi_I}{1 + V\chi_I} \ , \ \chi_I = \frac{\chi}{1 - V\chi}$$

Using $W = V - V\chi V$, we see that:

$$W = \frac{V}{1 + V\chi_I} \ , \ W^{-1} = V^{-1} + \chi_I$$

Hence the relation to the irreducible polarisability:

$$\Pi = -\chi_I$$

5) Relation to RPA

In RPA one approximates $\Pi \approx -\chi^0$, the Lindhard function, so that:

$$W_{\text{RPA}} = \frac{V}{1 + V\,\chi^0}.$$

From the expression in the previous section we see that the RPA description of screening indeed amounts to approximate the density-density correlation function χ by its RPA form:

$$\chi_{RPA} \simeq \frac{\chi^0}{1 + V\chi^0} \ , \ \chi_I^{RPA} \simeq \chi_0$$

But the boxed relations above are exact and hold beyond RPA. This expression also makes clear that χ is the physical response, and χ_0 the irreducible response at the bare (non-interacting) level.

IV. THE LINDHARD FUNCTION FOR THE 3D ELECTRON GAS

For noninteracting electrons with dispersion $\varepsilon_{\mathbf{k}} = \hbar^2 k^2/2m$ and spin degeneracy two, the finite-temperature Matsubara form is

$$\chi^0(\mathbf{q}, i\omega_n) = -2\int \frac{d^3k}{(2\pi)^3}\, \frac{f(\varepsilon_{\mathbf{k}}) - f(\varepsilon_{\mathbf{k}+\mathbf{q}})}{i\omega_n + \varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}. \tag{4.1}$$

After angular integration, analytic continuation $i\omega_n \to \omega + i0^+$ yields the retarded $\chi^0(\mathbf{q}, \omega)$. Define

$$x \equiv \frac{q}{2k_F}, \qquad u \equiv \frac{\omega}{v_F q}, \qquad D(0) \equiv \frac{mk_F}{\pi^2\hbar^2} \;\; \text{(total DOS at } E_F\text{, incl. spin)}. \tag{4.2}$$

Static limit ($\omega = 0$)

At $T = 0$ the classic closed form is

$$\boxed{\chi^0(q,0) = D(0)\left[1 + \frac{1-x^2}{2x}\ln\left|\frac{1+x}{1-x}\right|\right], \quad x = \frac{q}{2k_F}.} \tag{4.3}$$

Key consequences:

- **Long wavelength $q \to 0$:** $\chi^0(q,0) \to D(0)\,[2 - \frac{2}{3}x^2 + \cdots]$, hence $\chi^0(0,0) = D(0) \times 2$ equals minus the total DOS at E_F (two spins). In other words, if we take first $\omega \to 0$, then $q \to 0$ (in that order), χ_0 tends to the compressibility of the free electron gas, κ_0.
- **Kohn anomaly at $q = 2k_F$:** the derivative $\partial_q \chi^0$ is logarithmically singular at $2k_F$; in real space this produces Friedel oscillations $\delta n(r) \sim \cos(2k_F r)/r^3$.

Dynamics and the particle–hole continuum

The imaginary part $\mathrm{Im}\,\chi^0(q,\omega)$ is nonzero only inside the particle–hole continuum

$$\omega_-(q) \le \omega \le \omega_+(q), \qquad \omega_\pm(q) = \frac{\hbar q^2}{2m} \pm v_F q, \tag{4.4}$$

equivalently $u \in [x-1, x+1]$. Within this window, external fields decay into particle–hole pairs (*Landau damping*); outside it, χ^0 is purely real. The real part contains logarithms of $(u \pm x \pm 1)$ whose structure controls the dispersion and damping of collective modes.

A. Implications for RPA Screening

Hence at small q in the static limit:

$$W(q) \sim \frac{4\pi/q^2}{1 + \kappa_0 4\pi/q^2} = \frac{4\pi}{q^2 + q_{TF}^2}$$

with q_{TF} the Thomas Fermi wave-vector:

$$q_{TF}^2 = 4\pi\kappa_0$$

which by FT implies that the long distance potential is:

$$W(r) \sim \frac{1}{r} e^{-q_{TF} r}$$

By contrast in an insulator $\kappa = 0$ and hence the interaction remains $\sim 1/r$ at long distance

With $\chi \approx \chi^0$, the dielectric function and screened interaction are

$$\varepsilon(q,\omega) = 1 + V(q)\chi^0(q,\omega), \qquad W(q,\omega) = \frac{V(q)}{\varepsilon(q,\omega)}, \qquad V(q) = \frac{4\pi e^2}{q^2}. \tag{4.5}$$

(a) Static, long-wavelength limit: Thomas–Fermi screening

Using $\chi^0(0,0) = -D(0)$ gives

$$\varepsilon(q,0) = 1 + \frac{q_{TF}^2}{q^2}, \qquad q_{TF}^2 = 4\pi e^2 D(0), \tag{4.6}$$

so that

$$W(q,0) = \frac{4\pi e^2}{q^2 + q_{TF}^2} \iff V_{\rm scr}(r) \sim \frac{e^2}{r}\, e^{-q_{TF} r}. \tag{4.7}$$

(b) $2k_F$ structure: Friedel oscillations and Kohn anomalies

Because $\chi^0(q,0)$ is non-analytic at $2k_F$, $W(r,0)$ develops oscillatory power-law tails $\propto \cos(2k_F r)/r^3$. These features underlie RKKY interactions and Kohn anomalies in phonon dispersions near $2k_F$.

(c) Dynamics: plasmons and Landau damping

Plasmons appear as zeros of $\varepsilon(q,\omega)$ outside the particle–hole continuum. In 3D and for $q \to 0$,

$$\omega_p = \sqrt{\frac{4\pi n e^2}{m}}, \qquad \omega(q) \approx \omega_p \left[1 + \frac{3}{10}\left(\frac{q v_F}{\omega_p}\right)^2 + \cdots\right]. \tag{4.8}$$

When the plasmon dispersion enters the continuum, $\mathrm{Im}\,\chi^0 \neq 0$ and plasmons are Landau damped (finite lifetime).

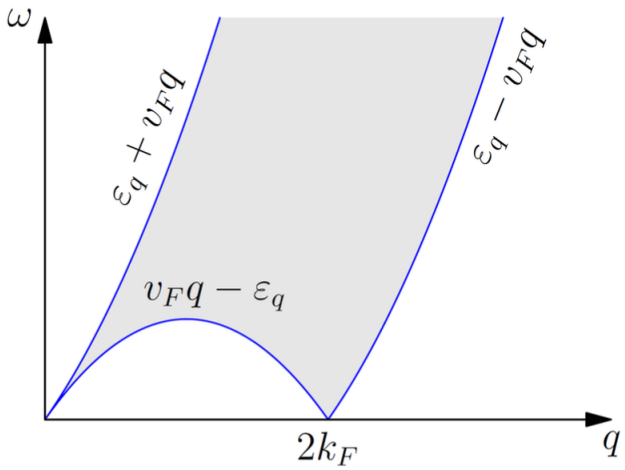

Figure 39-6 Schematic representation of the domain of frequency and wave vector where there is a particle-hole continuum.

FIG. 1 Figure courtesy of A.M. Tremblay (Many Body Lecture Notes)

These considerations also imply that in the high-frequency limit (in practice for $\omega \gg \omega_p$) there is no screening, and the dielectric constant goes to unity.

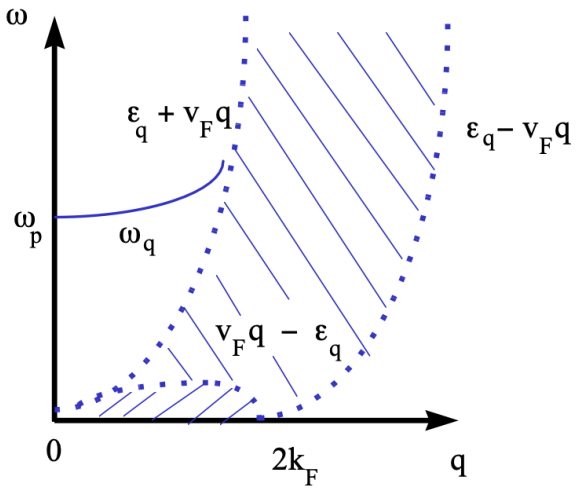

Figure 41-5 Schematic representation of the domain of frequency and wave vector where there are poles in the charge susceptibility, or zeros in the longitudinal dielectric function. In addition to the particle-hole continuum, there is a plasma pole.

FIG. 2 Figure courtesy of A.M. Tremblay (Many Body Lecture Notes)

V. WHAT IS U IN A SOLID? AN EMBEDDING VIEWPOINT.

Having defined the screened effective interaction W, we can now propose a (formal) answer to the question: what is the (Hubbard-Kanamori) interaction matrix in a solid? This answer follows the embedding philosophy. The resulting U-matrix will of course depend on the specific embedding under considerations, that is on the choice of the correlated orbitals χ_m.

We recall the *representability* idea at the heart of DMFT and embedding approaches. Given the *exact* Green's function $G(r,r';\omega)$ of the solid, one can define its local projection in the correlated subspace:

$$G_{m_1,m_2}(\omega) = \int dr dr'\, \chi^*_{m_1}(r) G(r,r';\omega) \chi_{m_2}(r')$$

One then constructs a local quantum impurity model, whose solution yields $G_{m_1m_2}$ $(= G_{loc})$. This QIM is parameterized by a local level position ε_d and a hybridization function $\Delta_{m_1m_2}$ (quantum weiss field) which is dual to $G_{m_1m_2}$. However, the interaction matrix $U_{m_1m_2m_3m_4}$ entering this QIM is specified externally.

If however we also know W, we can similarly consider its projection onto the correlated (embedded) subspace, $W_{m_1m_2m_3m_4}(\omega)$ $(=W_{loc})$. We can now introduce an extended QIM which involves not only the hybridisation function Δ but also a *retarded* interaction matrix $U_{m_1m_2m_3m_4}(\omega)$ such that the solution of this QIM reproduces simultaneously G_{loc} and W_{loc}.

In my view, this is the proper way of thinking of U in a solid. Note that:

- It depends on the choice of orbitals (on the specific embedding) - as it should be.
- The Hubbard-Kanamori interactions are frequency-dependent: screening is a dynamical effect which depends on energy scale.

Of course, for the moment, this is a formal definition because it assumes that we know G and W. It has a similar conceptual role than the Kohn-Sham representation of the local density in DFT. To make it practical, we need to introduce approximations to the solution of the many-body problem.

VI. EXTENDED DMFT (EDMFT)

References: A.Sengupta and A.Georges, PRB 52, 10295 (1995); J. Lleweilun Smith and Q.Si, PRB 61, 5184 (2000); R. Chitra and G.Kotliar PRB 63, 115110 (2001).

One such construction is the so-called extended DMFT approximation (EDMFT). in the same spirit than single-site DMFT, EDMFT makes a locality assumption: namely that *both* the self-energy and the polarisability are local *in the local orbital basis* and can be approximated by the corresponding QIM quantities.

Hence, given a bare lattice Green's function $G_0(k)$ and bare interaction $V(q)$, the EDMFT approximation introduces the following self-consistent closure equations:

$$G_{loc} = \sum_k \left[G_0^{-1}(k) - \Sigma_{imp}\right]^{-1} \quad , \quad W_{loc} = \sum_q \left[V(q)^{-1} - \Pi_{imp}\right]^{-1}$$

with:

$$\Sigma_{imp} \equiv \omega - \varepsilon_d - \Delta(\omega) - G^{-1}(\omega) \ , \ \Pi_{imp} \equiv U(\omega)^{-1} - W_{imp}^{-1}(\omega)$$

where W_{imp} can be calculated from the knowledge of the local (QIM) density-density response as:

$$W_{imp}(\omega) = U(\omega) - U(\omega)\chi_{imp}(\omega)U(\omega)$$

The EDMFT approximation has been used to study models with long-range interactions. It allows to take into account the dynamical effects of these interactions which, in standard static DMFT, are treated at the Hartree mean-field level only. In contrast to DMFT however, EDMFT does not become exact in any controlled. A notable exception to this remark is when the interactions in the models are quenched, random interactions as in the Edwards-Anderson model of a quantum spin-glass for example. Then, EDMFT becomes exact for a fully-connected lattice, as emphasized long ago by Bray and Moore and extensively used in the study of quantum spin glasses and SYK-like models.

For a real material, it would obviously be a very poor approximation to neglect the momentum dependence of the self-energy for *all* bands. Hence the GW+EDMFT formalism, which includes non-local contributions to both the self-energy and polarisability from states outside of the correlated subspace.

VII. CONSTRAINED RPA

Reference: F.Aryasetiawan, M.Imada, A.Georges, G.Kotliar, S.Biermann and A.Lichtenstein PRB 70, 195104 (2004)

The idea behind the cRPA method is to define a (frequency-dependent) matrix of interaction parameter $U(\omega)$ in the simplest possible way. Namely, by doing an RPA ($G_0W_)$) calculation in which screening processes internal to the target correlated manifold are removed from the screening process.

Hence, the irreducible polarisability calculated from the KS bare Green's function is decomposed as:

$$\Pi = G_0G_0 = \Pi_c + \Pi_r$$

In this expression, Π_c contains all the screening transitions internal to the correlated subspace, and Π_r those for which either the initial or final state (or both) are outside the correlated subspace. How that selection is done when bands are entangled is a fairly technical questions which doesnt have a unique answer and goes beyond the scope of these notes.

The full screened interaction is:

$$W^{-1} = V^{-1} - \Pi_r - \Pi_c$$

which can be rewritten:

$$W^{-1} = W_r^{-1} - \Pi_c \ , \ W_r^{-1} = V^{-1} - \Pi_r$$

The first formula is what we would obtain if we would solve the dynamical QIMP model using an RPA approximation, provided we take $U(\omega$ to be:

$$\boxed{U(\omega)_{cRPA} = W_r(\omega)}$$

This is the constrained RPA approximation to the determination of U. Usually, this approximation is a good first guess, but has a tendency to give values of $U(\omega = 0)$ which are somewhat too small as compared to what is needed to reproduce the physics from a static DMFT calculation. Indeed, recent fully self-consistent GW+EDMFT calculations usually give values of U that are higher than the cRPA estimate at low frequency (see Chia-Nan Yeh's lecture).

Below, I reproduce two figures which display the frequency dependence of the cRPA interaction for $SrVO_3$ (note the steep increase above the plasma frequency ~ 15 eV) and the dependence of $U_{cRPA}(\omega = 0)$ on the choice of target space.

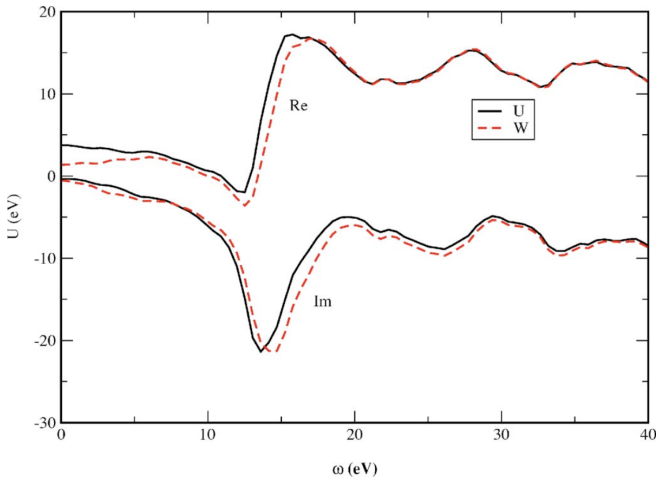

FIG. 3. (Color online) Frequency dependent U and W of $SrVO_3$.

FIG. 3 From F.Aryasetiawan et al. PRB 74, 125106 (2006)

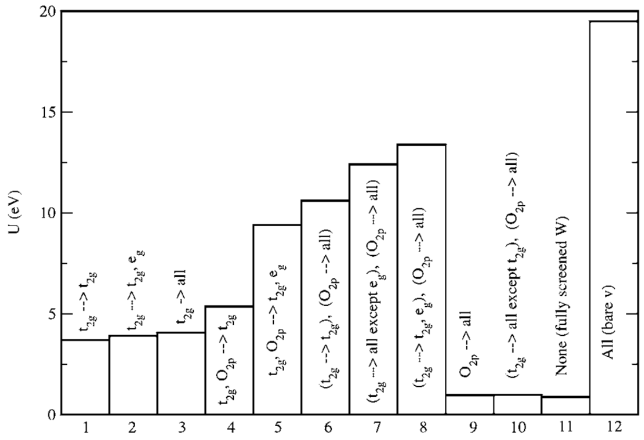

FIG. 2. The Hubbard U of $SrVO_3$ obtained by eliminating various transitions as indicated in the picture. For example, case 5 corresponds to eliminating transitions $t_{2g} \rightarrow t_{2g}$, $t_{2g} \rightarrow e_g$, $O_{2p} \rightarrow t_{2g}$, and $O_{2p} \rightarrow e_g$ and case 6 corresponds to eliminating $t_{2g} \rightarrow t_{2g}$ transition and all transitions from O_{2p}. Discussion of the result is described in the text.

FIG. 4 From F.Aryasetiawan et al. PRB 74, 125106 (2006)

VIII. HEDIN'S EQUATIONS AND THE GW APPROXIMATION

A. GW as self-consistent RPA

We have seen in previous sections that the RPA approximation amounts to approximate:

$$\Pi_{RPA} = -\chi_0 = G_0 G_0$$

As everywhere below, this expression is a shorthand for a product over space-time indices, or alternatively appropriate convolution over frequency and momentum. That is, introducing $x = (r, \tau)$:

$$\Pi_{RPA}(x_1, x_2) = G_0(x_1, x_2) G_0(x_2, x_1)$$

From this the RPA screened interaction is constructed as $W_0 = V/(1 - V\Pi_{RPA})$. The corresponding RPA approximation to the self-energy amounts to retain the lowest order diagram:

$$\Sigma_{RPA} = -G_0 W_0$$

The GW approximation amounts to promote these equations to self-consistent ones. The bare Green's function is replaced by the interacting one in the polarizability:

$$\Pi_{GW} = GG$$

and similarly:

$$\Sigma_{GW} = -GW$$

to be combined and solved self-consistently with the corresponding Dyson equations:

$$G^{-1} = G_0^{-1} - \Sigma \ , \ W^{-1} = V^{-1} - \Pi$$

Appealing and innocent as they look, these equations are:

- Highly non-trivial to solve since they demand the solution of these coupled integral equations over very large basis sets
- *Not* guaranteed to give better spectral properties than the bare RPA approximation - nothing tells us that self-consistency (neglecting vertex corrections, see below) is always a good thing to do! In fact there are cases where it's known not to be (e.g. the ~ 6 eV satellite 'problem' of nickel).

B. The Ψ functional

Reference: C.O. Almbladh et al. Int. J. Mod. Phys B 13, 535 (1999).

A more formal derivation of the GW approximation relies on the exact Hedin's equation, which are in turn conveniently derived by introducing a (free-)energy functonial of G and W, following Almbladh et al.

Let me recall the Baym-Kadanoff functional of G, which is defined as:

$$\Omega_{BK}[G] = tr \ln G - tr \left[(G_0^{-1} - G^{-1}) G \right] + \Phi[G]$$

It is obtained as a Legendre transform of the free-energy, constrained such that the value of the single-particle Green's function is set to be a specific function G. In constructing the functional, Σ can be viewed as the Lagrange multiplier constraining G. Φ is the Luttinger-Ward functional. Stationarity with respect to G yields:

$$0 = \frac{\delta \Omega}{\delta G} = G^{-1} - G_0^{-1} + \frac{\delta \Phi}{\delta G}$$

From which it follows that the self-energy can be viewed as a functional of the full G given by:

$$\Sigma[G] = \frac{\delta \Phi}{\delta G}$$

$\Phi[G]$ can be given a formal perturbative expression as a sum of all 1PI skeleton diagrams (ie without self-energy insertions). However, it is not guaranteed that the LW functional can be uniquely defined non-perturbatively, and in fact it is known to have multiple branches (i.e. the connection between G_0 and G is not necessarily bijective over all G_0's) – see E.Kozik, M.Ferrero and A.Georges. PRL 114, 156402 (2015).

The BK construction can be promoted to the 2-particle level, as a functional of both G and W. The construction involves two Lagrange multipliers, conjugate respectively to G and W, namely Σ and Π. This leads to:

$$\Omega[G,W] = tr\ln G - tr\left[(G_0^{-1} - G^{-1})G\right] - \frac{1}{2}tr\ln W + \frac{1}{2}tr\left[(V^{-1} - W^{-1})W\right] + \Psi[G,W]$$

Here, G_0 implicitly also contains the Hartree contribution. Stationarity yields:

$$\begin{aligned} 0 = \frac{\delta\Omega}{\delta G} = G^{-1} - G_0^{-1} + \frac{\delta\Psi}{\delta G} \Rightarrow \Sigma_{xc} = \frac{\delta\Psi}{\delta G} \\ 0 = \frac{\delta\Omega}{\delta W} = -\frac{1}{2}W^{-1} + \frac{1}{2}V^{-1} + \frac{\delta\Psi}{\delta W} \Rightarrow \Pi = -2\frac{\delta\Psi}{\delta W} \end{aligned} \tag{8.1}$$

C. Hedin's equations and the GW approximation

The GW approximation amounts to approximating the Ψ functional by the lowest order Fock-like diagram:

$$\Psi_{GW} = -\frac{1}{2}tr\left[GWG\right]$$

From which the above self-consistent GW equations follow.

More generally, it can be shown that the Ψ functional can be expressed *exactly* by introducing the 3-leg vertex $\Lambda(1,2,3)$ as:

$$\Psi = -\frac{1}{2}tr\left[GW\Lambda G\right] = -\sum_{x_1,x_2,x_3,x_4} G(1,3)W(1,2)\Lambda(3,4;2)G(4,1)$$

So that, from stationarity:

$$\Sigma_{xc}(1,2) = -tr_{3,4}\, G(1,4)W(1,3)\Lambda(3,4;2)\ \ ,\ \ \Pi(1,2) = tr_{3,4}\, G(1,3)G(4,1)\Lambda(3,4;2)$$

A last Hedin equation can be derived by relating the 3-point vertex to the 4-point one Γ (as introduced on Hugo Strand's lecture) and ultimately relating the latter to $\delta\Sigma/\delta G$, hence yielding a closed set of (intractable...) self-consistent equations. But I will not elaborate on this here.

The GW approximation amounts to approximating $\Lambda \simeq 1$. As mentioned above, neglecting vertex corrections while imposing self-consistency comes with no warranty...

IX. GW+EDMFT

References: S.Biermann, F.Aryasetiawan and A.G. PRL 90, 086402 (2003) - See also Chitra and Kotliar PRB 63, 115110 (2001); Sun and Kotliar PRB 66, 085120 (2002).

Combining all of the above, it should be now fairly clear how to combine GW and EDMFT within an embedding approach. Because both GW and EDMFT are formulated in terms of Green's functions and functionals and are diagrammatically controlled (ie we know precisely which contributions are and which ones are not), the two theoretical frameworks really speak the same language and can be naturally combined.

On the physics side, the reason for doing this is that the GW approximation by itself does a good job in describing the electronic structure of the more extended states (and hence of weaky correlated materials) but fails to handle strong correlations. On a more technical level, including the non-perturbative physics from DMFT is a way to reintroduce vertex corrections in the Hedin framework while keeping locality as a guiding principle.

Denoting as above (somewhat sloppily) by G_{loc} and W_{loc} the projections of G and W on the correlated subspace, the GW+EDMFT approach approximated the Ψ functional in the following way:

$$\Psi_{GW+EDMFT} = -\frac{1}{2}tr\left[GWG\right] - \Psi_{dc}[G_{loc},W_{loc}] + \Psi_{imp}[G_{loc},W_{loc}]$$

Here, the double-counting contribution removes the contributions of the GW theory which will be taken into account by solving the QIMP with appropriate algorithms, ie the contributions to the impurity model treated within the GW approximation applied to the embedded subspace. Hence:

$$\Psi_{dc} = -\frac{1}{2} tr\left[G_{loc} W_{loc} G_{loc}\right]$$

The impurity problem with retarded interactions can be viewed as a machine to generate the non-perturbative component of teh functional Ψ_{imp}, as emphasized above.

The full set of GW+EDMFT equations are now obtained as:

- Perform a GW calculation (either starting from a fully self-consistent one or partially self-consistent) and obtain G and W at the GW level ie using $\Pi_{GW} = G.G$ and $\Sigma_{GW} = -G.W$.
- Solve the QIMP specified by $\Delta(\omega)$ and $U(\omega)$ to obtain $G_{imp}(\omega)$ and $W_{imp}(\omega) = U - U\chi U$ - and correspondingly Σ_{imp} and Π_{imp}.
- Upfold Σ_{imp} and Π_{imp} to the whole system and construct the full polarization and self-energy: $\Sigma = \Sigma_{GW} - \Sigma_{dc} + \Sigma_{imp}$ and $\Pi = \Pi_{GW} - \Pi_{dc} + \Pi_{imp}$
- In the above expressions $\Sigma_{dc} = -G_{loc} W_{loc}$ and $\Pi_{dc} = G_{loc} G_{loc}$
- Construct the new local effective interaction W_{loc} and new local Green's function G_{loc} from these quantities as $W_{loc} = \sum_q P * [V_q^{-1} - \Pi]^{-1} P$ and $G_{loc} = \sum_k P^* [G_0^{-1} - \Sigma]^{-1} P$ with P appropriate projectors on the embedded subspace.
- Update $U(\omega)$ and $\Delta(\omega)$ as: $U^{-1} = W_{loc}^{-1} + \Pi_{imp}$ and $\Delta(\omega) = \omega - \varepsilon_d - \Sigma_{imp} - G_{loc}^{-1}$
- Iterate until convergence, and ideally iterate the outer GW loop to convergence as well

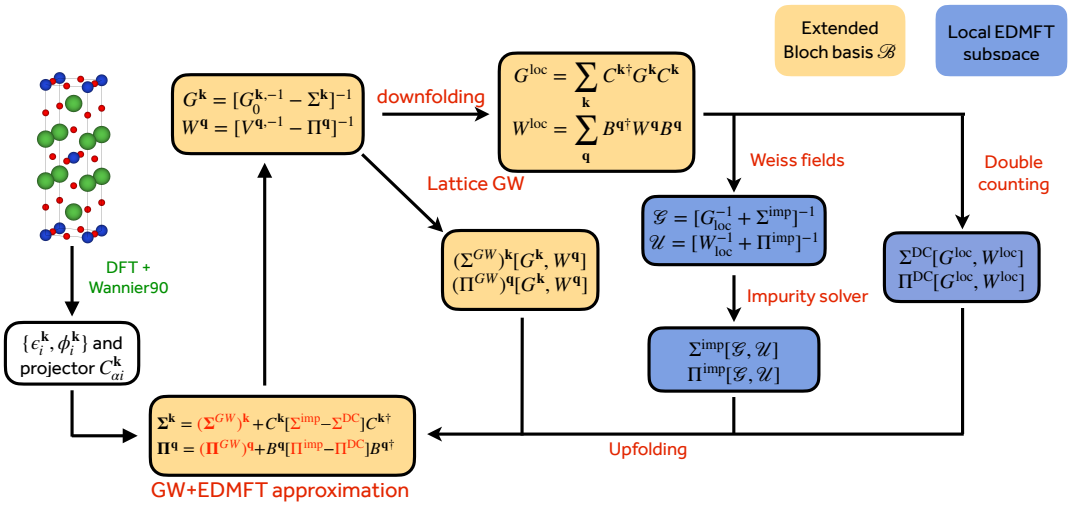

FIG. 5 Workflow of *ab initio* self-consistent GW+EDMFT (courtesy Chia-Nan Yeh)