Self-consistency in *GW* calculations

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Our "Cast of Players"

- *G* – Green's function
- Σ_{xc} – Self-energy (related to *G* as discussed)
- *W* – Dynamically screened Coulomb interaction
- *P* – Irreducible polarisation propagator
- Γ – Vertex function

Hedin's Equations

$$
\begin{aligned}
\Sigma(1,2) &= \mathrm{i}\int W\left(1^{+},3\right) G(1,4)\,\Gamma(4,2,3)\,\mathrm{d}(3,4) \\
P(1,2) &= -\mathrm{i}\int G(2,3)\,G(4,2)\,\Gamma(3,4,1)\,\mathrm{d}(3,4) \\
W(1,2) &= v(1,2)+\int W(1,3)\,P(3,4)\,v(4,2)\,\mathrm{d}(3,4) \\
\Gamma(1,2,3) &= \delta(1,2)\,\delta(1,3) \\
&+ \int \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)\,G(7,5)\,\Gamma(6,7,3)\,\mathrm{d}(4,5,6,7)
\end{aligned}
$$

With Σ/G relation, exact closed equations for G, Σ etc.

The *GW* Approximation

Iterate Hedin's equations once starting with $\Sigma = 0$

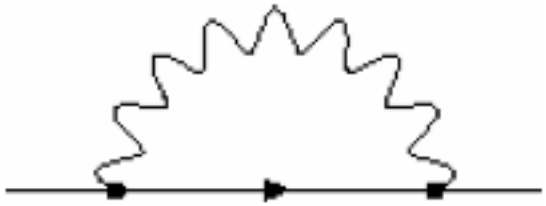
$$\Sigma(1,2) = \mathrm{i}\int W\left(1^{+},3\right) G(1,4)\,\Gamma(4,2,3)\,\mathrm{d}(3,4)$$

$$P(1,2) = -\mathrm{i}\int G(2,3)\,G(4,2)\,\Gamma(3,4,1)\,\mathrm{d}(3,4)$$

$$W(1,2) = v(1,2) + \int W(1,3)\,P(3,4)\,v(4,2)\,\mathrm{d}(3,4)$$

$$\Gamma(1,2,3) = \delta(1,2)\,\delta(1,3) + \int \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)\,G(7,5)\,\Gamma(6,7,3)\,\mathrm{d}(4,5,6,7)$$

The *GW* Approximation



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

where $\mathbf{x} \equiv (\mathbf{r},\xi)$ is space+spin

In the time domain

$$\Sigma(\mathbf{x},\mathbf{x}';t-t') = iW(\mathbf{x},\mathbf{x}';t-t')G(\mathbf{x},\mathbf{x}';t-t')$$

W is the dynamically screened Coulomb interaction between electrons

G_0W_0 Band Structures of Insulators

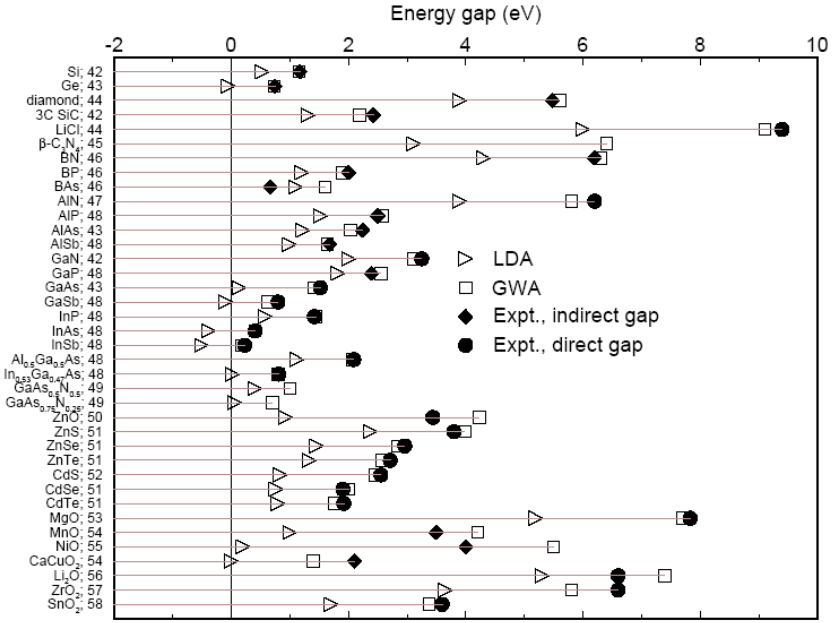
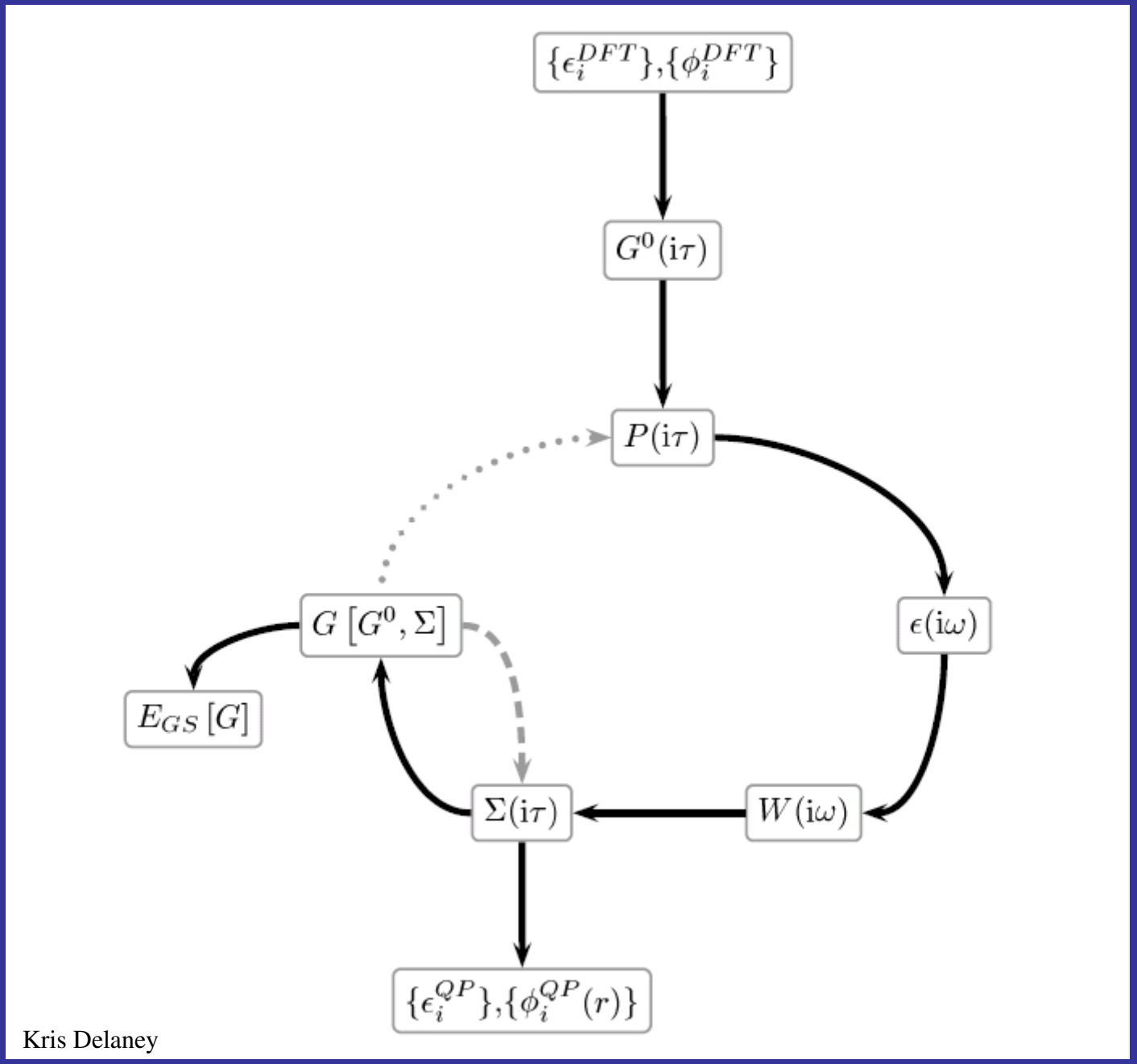


Figure 3: Comparison of characteristic direct and indirect LDA, GWA, and experimental energy gaps for all semiconductors and insulators for which first-principles GWA calculations have been reported. GWA corrects most of the LDA band gap underestimation over more than one order of magnitude in the experimental band gap. The values for MnO, ZnO, and $CaCuO_2$ are from model-GWA calculations, which are accurate to within 0.4 eV. The discrepancy between GWA and experiment for LiO_2 results from the neglect of excitonic effects. The experimental value for BAs is tentative. The references for the LDA, GWA, and experimental values are listed after the element symbols.

From "Quasiparticle calculations in solids", W.G. Aulbur, L. Jönsson and J.W. Wilkins, Solid State Physics **54** 1 (2000)

[also available in preprint form at http://www.physics.ohio-state.edu/~wilkins/vita/publications.html#reviews]

Self-Consistency



Arno Schin

Kris Delaney

Tests for Be atom (QP energies)

TABLE I. Ionization energy (in eV) of an isolated Be atom from the *GW* approximation. Experimental = 9.33 eV.

Method	All-electron	Pseudopotential
DFT-LDA	5.43	5.43
G_0W_0	9.25 ± 0.01	9.24 ± 0.01
GW_0	8.75 ± 0.01	8.75 ± 0.01
GW	8.47 ± 0.01	8.64 ± 0.01

K.T. Delaney, P. García-González, Angel Rubio, Patrick Rinke and RWG, Phys. Rev. Lett. 2004

Quasiparticle Self-Consistency

- A **partial** kind of self-consistency as far as *G* and *W* are concerned
- Most complete implementation: Kotani and van Schilfgaarde
- Iterate *G* and *W*, but restricting *G* to come from static Hermitian hamiltonian
- Criterion for self-consistency: quasiparticle energies and quasiparticle wavefunctions match as far as possible

The Consensus on Self-Consistency in *GW*

- G_0W_0 gives generally good spectral properties, provided starting point (e.g. LDA) is physically reasonable
- "Quasiparticle self-consistency" essentially "automates" the choice of starting point
- Full self-consistency destroys spectral properties but improves total energies
- Resolution: improved vertex