Performance of the GW approximation at reproducing key features in exact Kohn-Sham potentials

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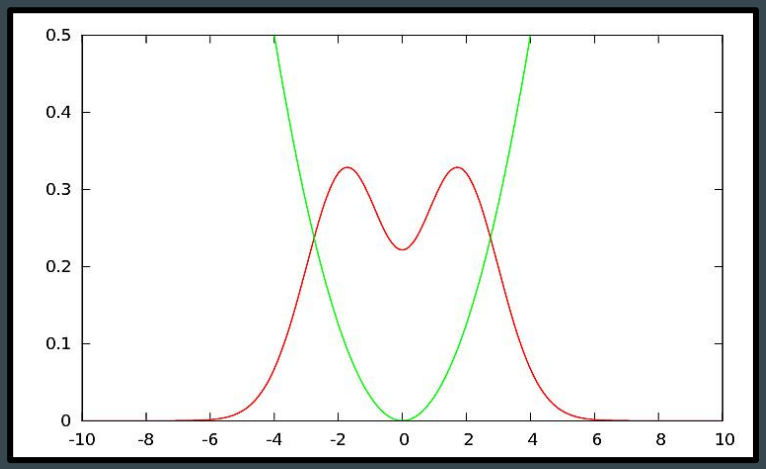
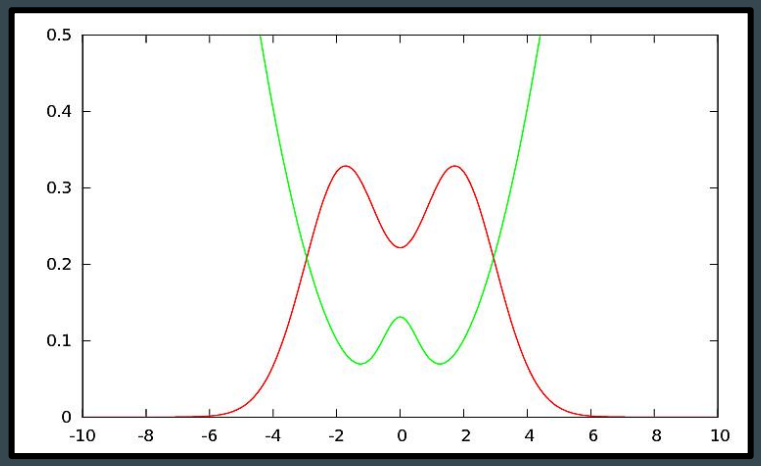
Theory

Density Functional Theory

We can imagine a fictitious system of non-interacting electrons that has the **same density** as the real system



Real

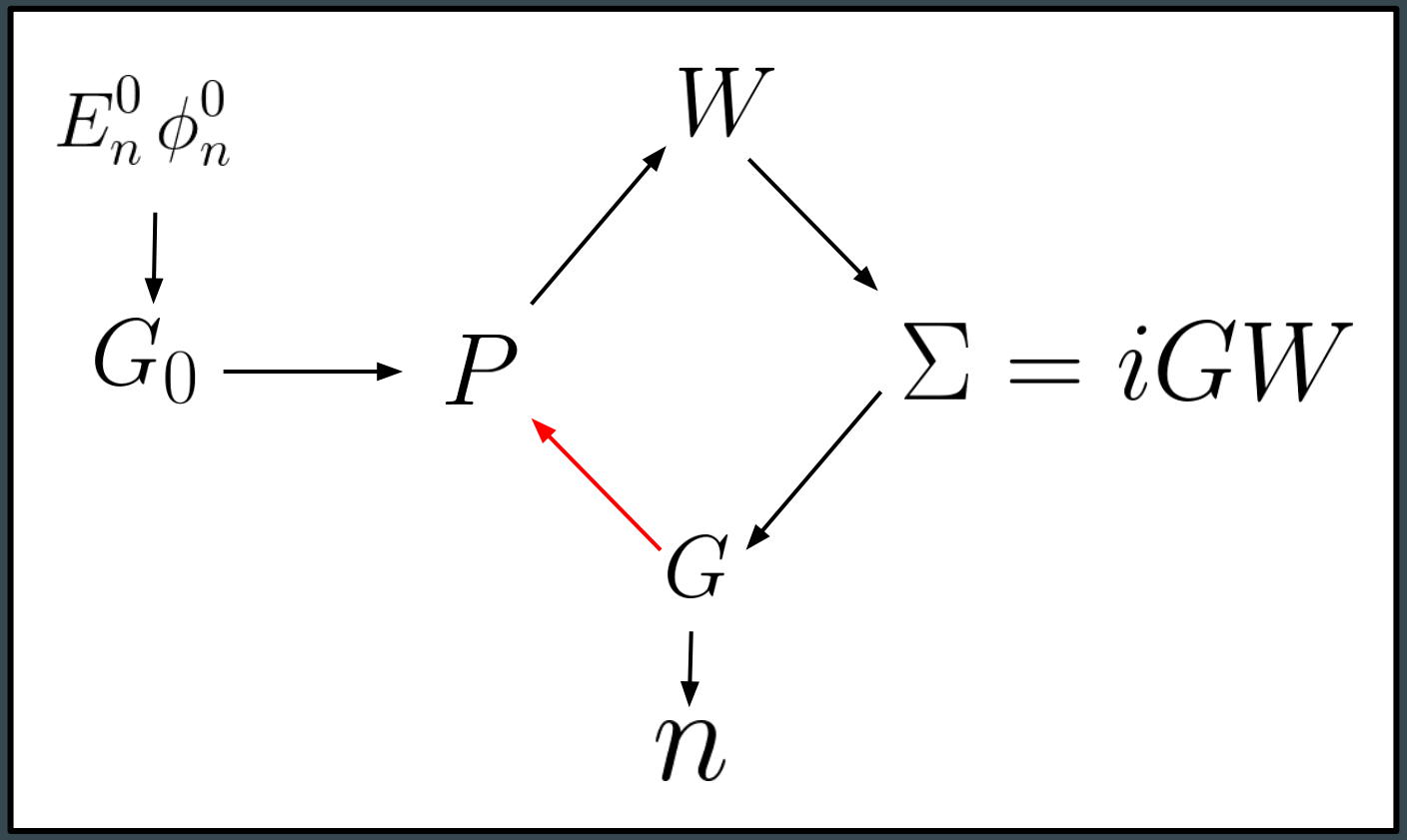


Fictitious

$$V_{ks}[n] = V_{ext} + V_H[n] + V_{XC}[n]$$

Many-Body Perturbation Theory

How does a system respond when an **added electron** propagates through the system?



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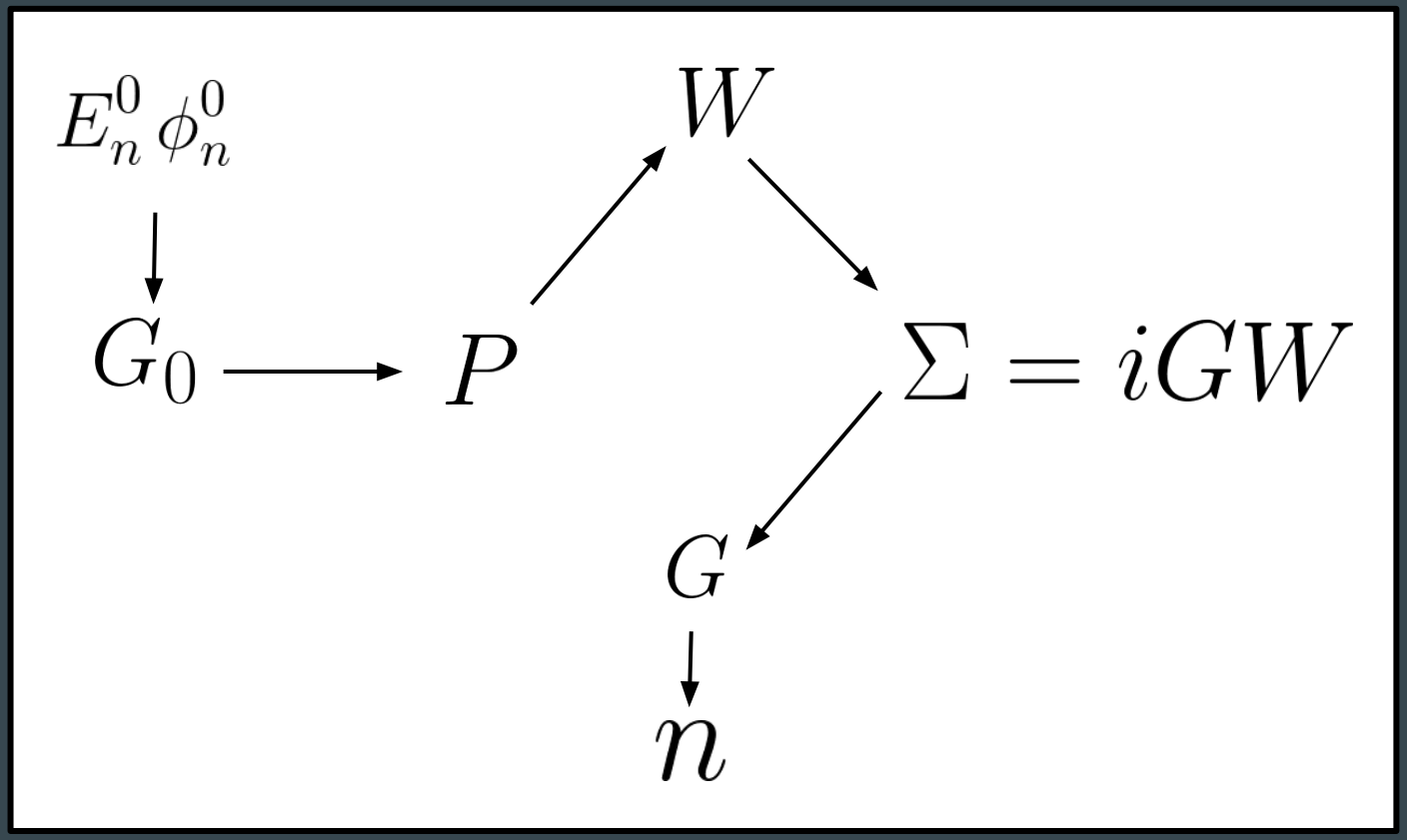
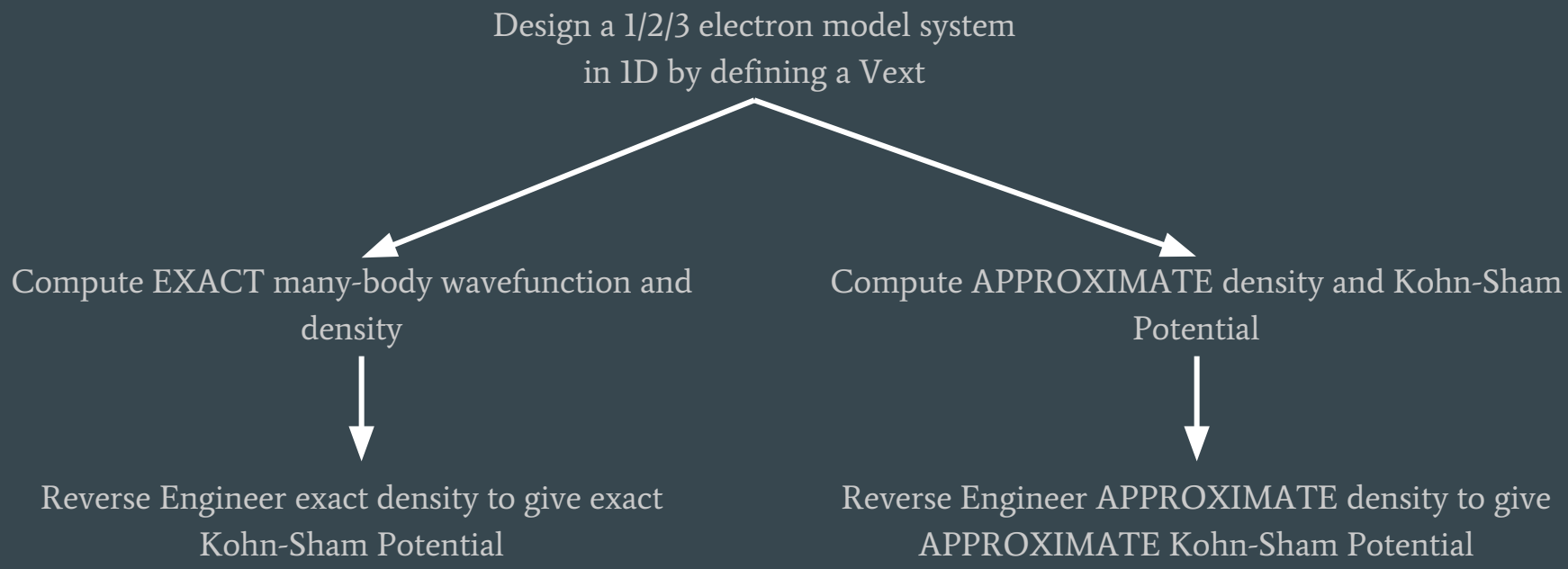


iDEA

iDEA



Approximations Available:

Non-Interacting

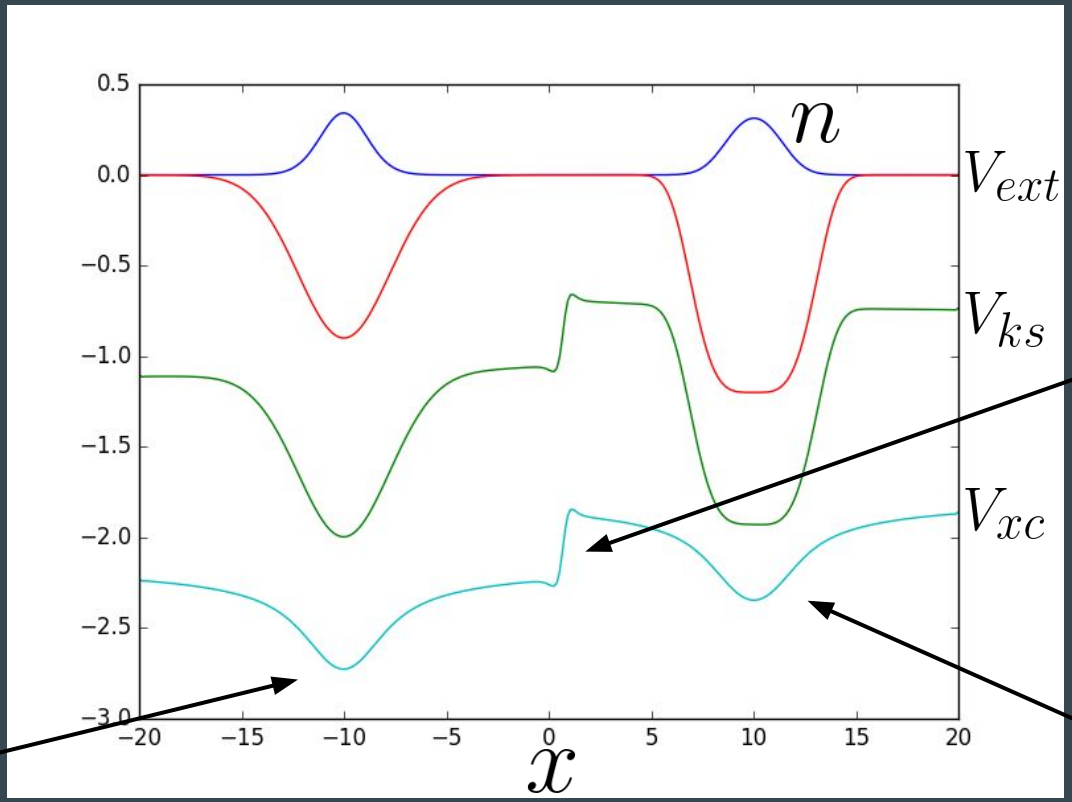
DFT (LDA)

Hartree-Fock

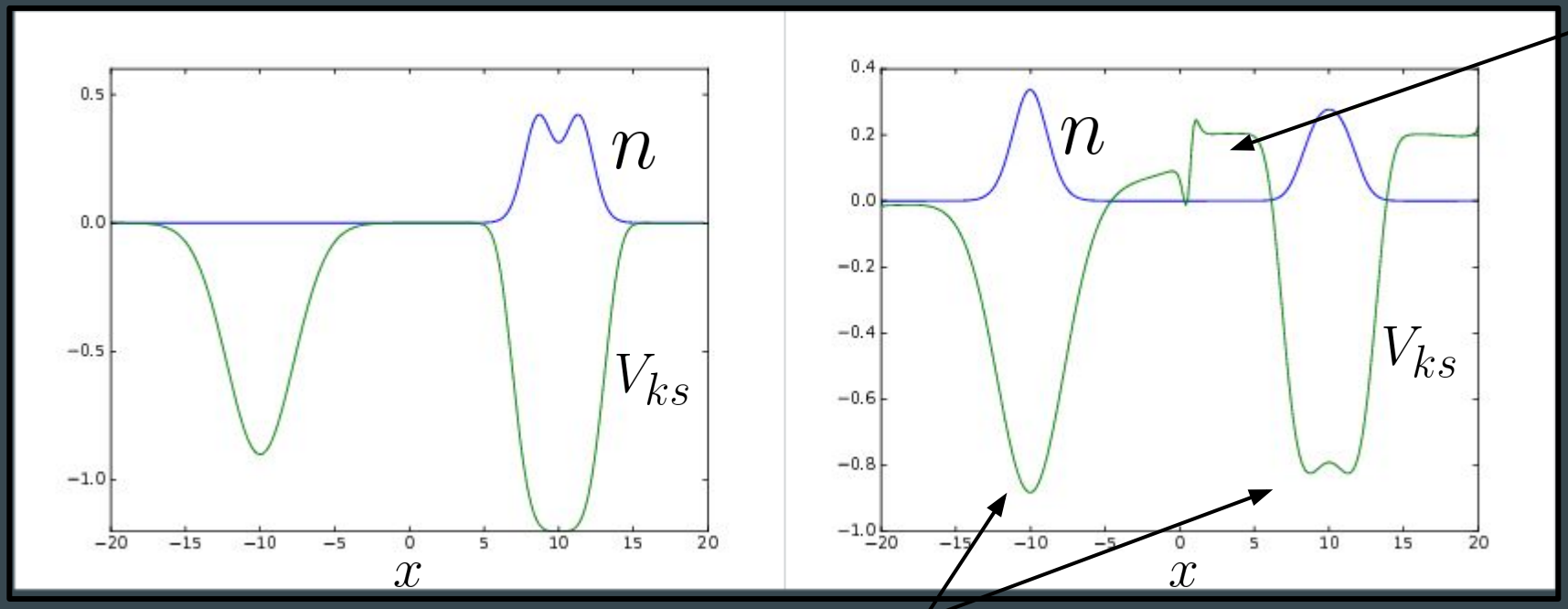
Many-Body Perturbation Theory (GW)

The Exact Kohn-Sham Potential

Exchange Dominated: Asymmetric Double Well

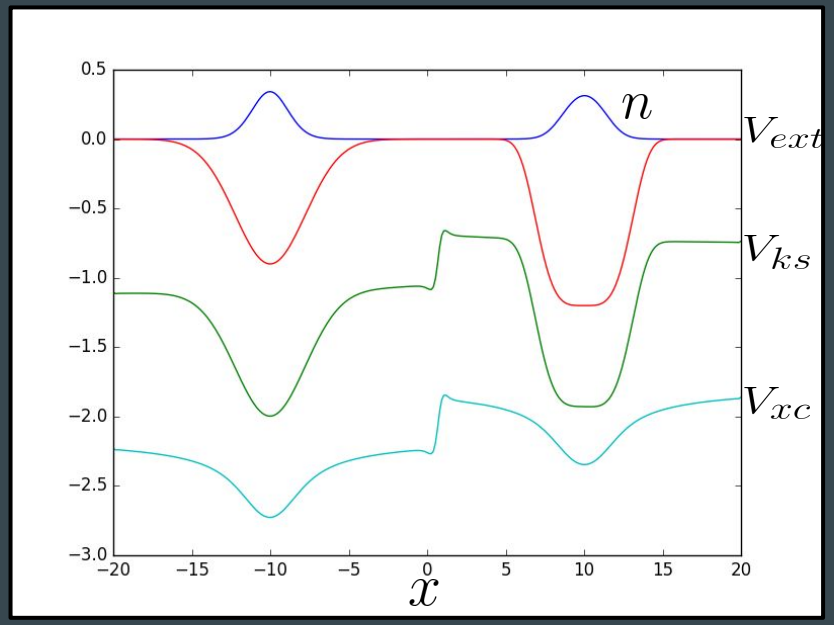


Note: Curves are shifted for clarity

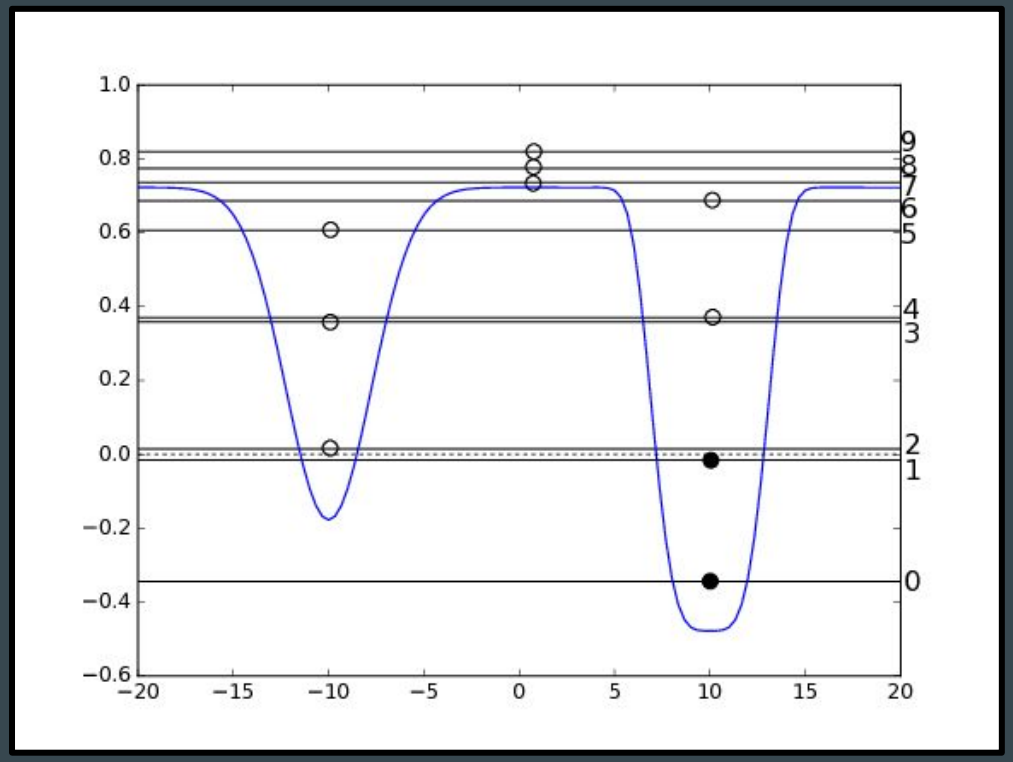


GOWO@NON-INTERACTING

EXACT

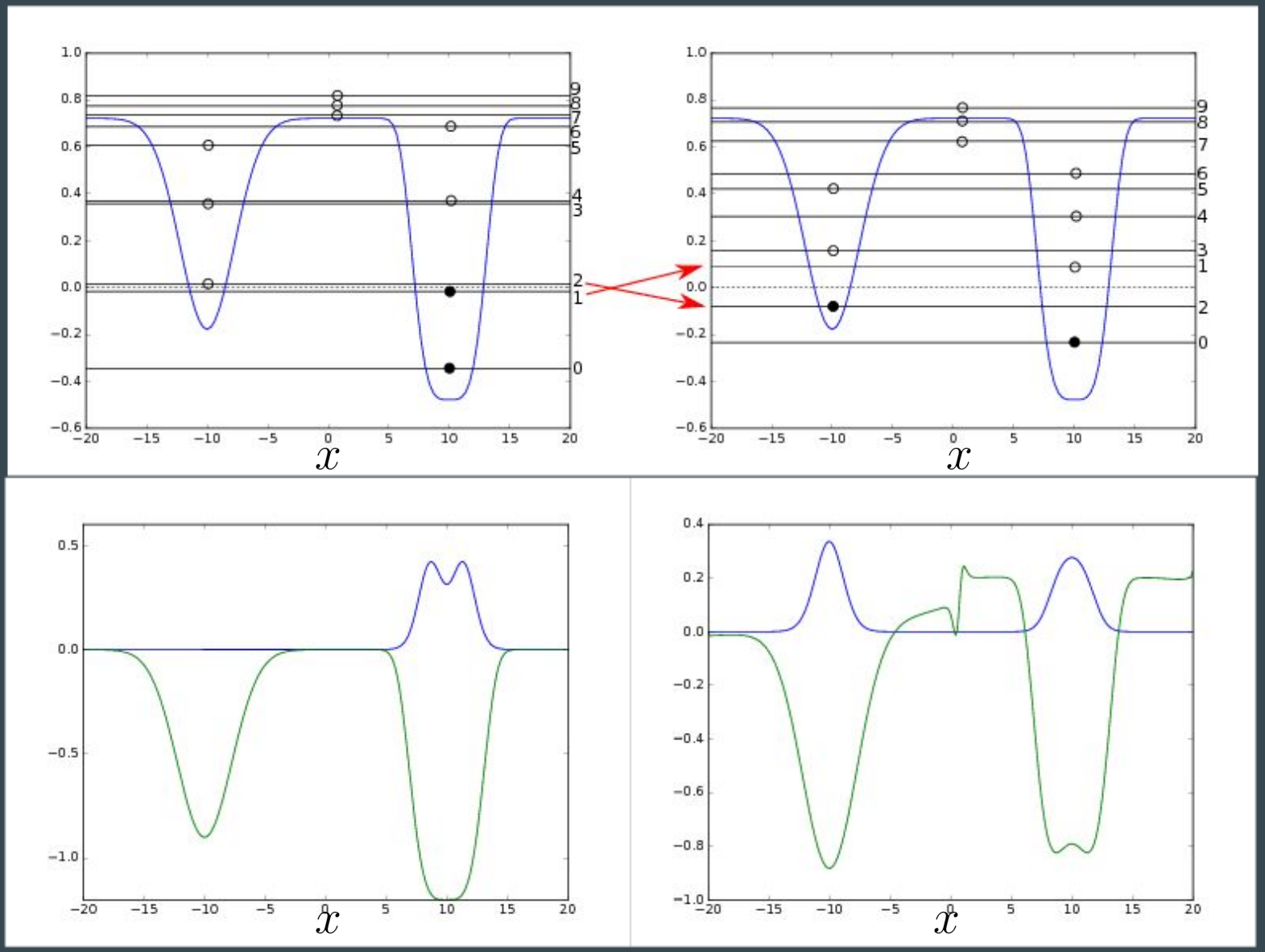


Orbital Reordering: Starting Orbitals



$$\phi^{QP} \approx \phi^{0}$$

$$E_i^{QP} \approx E_i^0 + < \phi_i^0 | \Sigma | \phi_i^0 >$$



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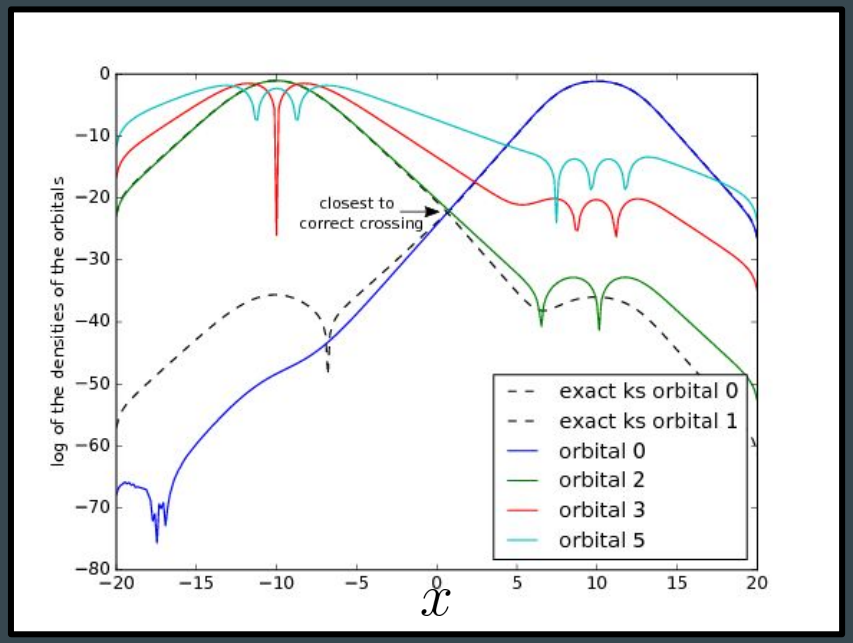
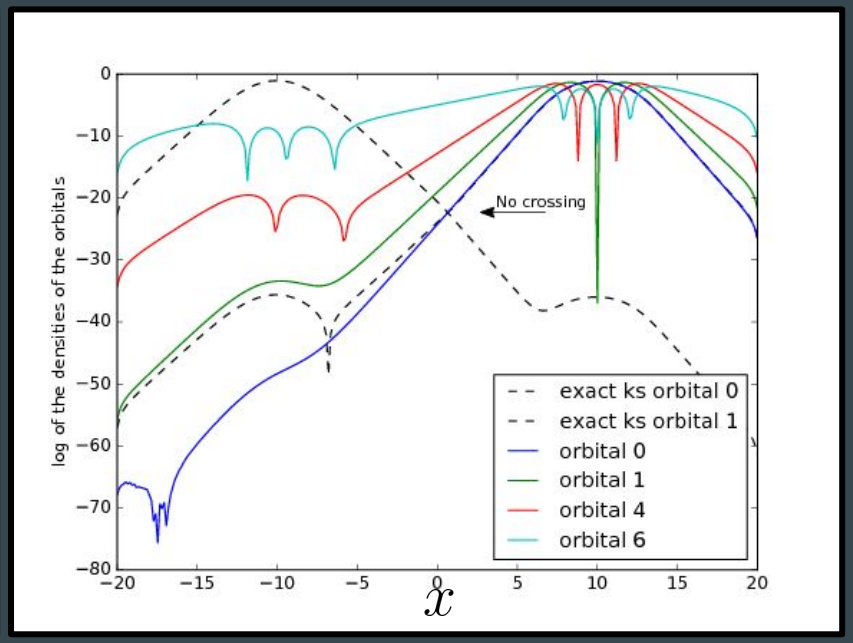
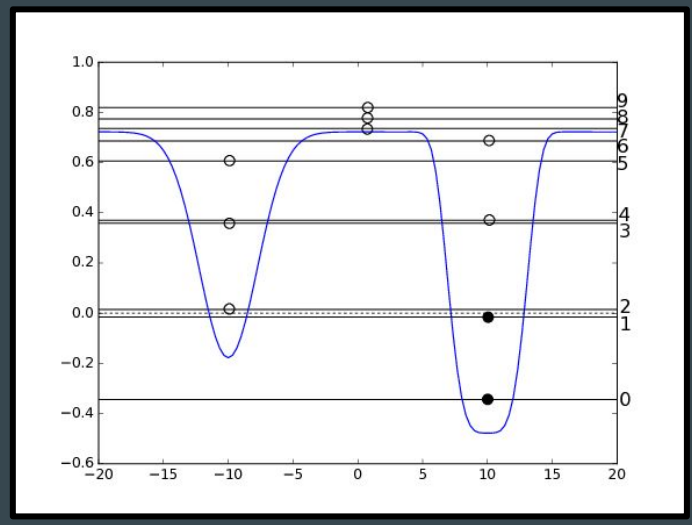
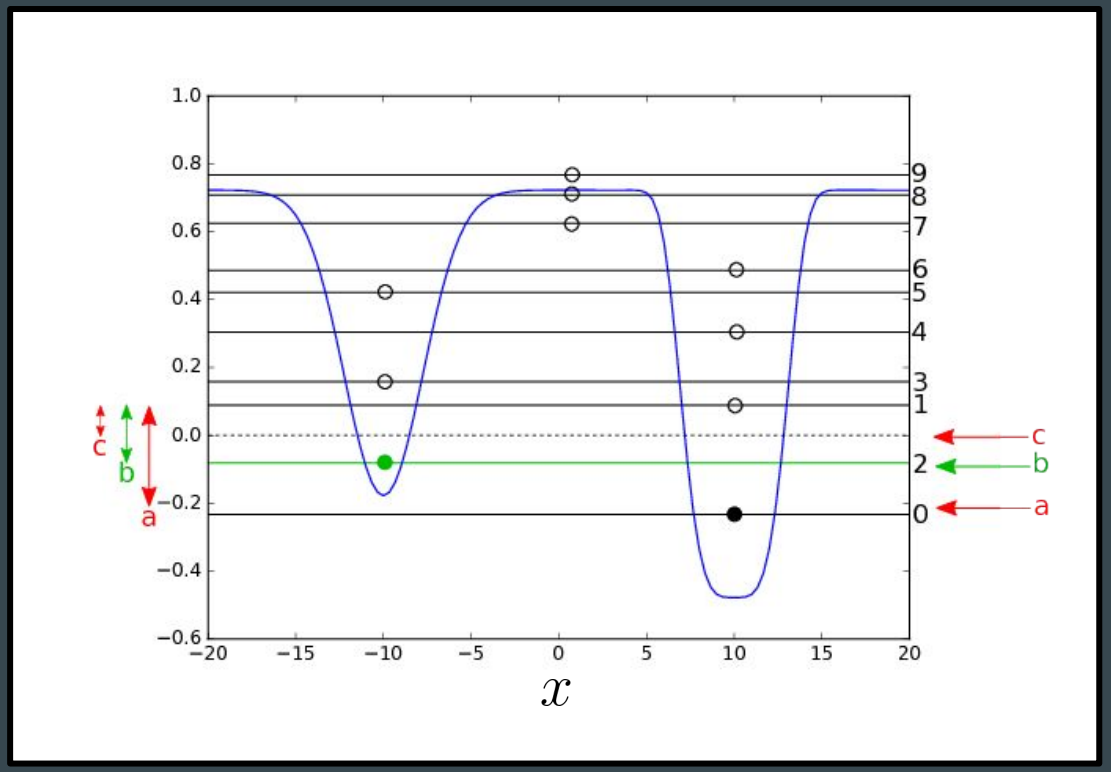


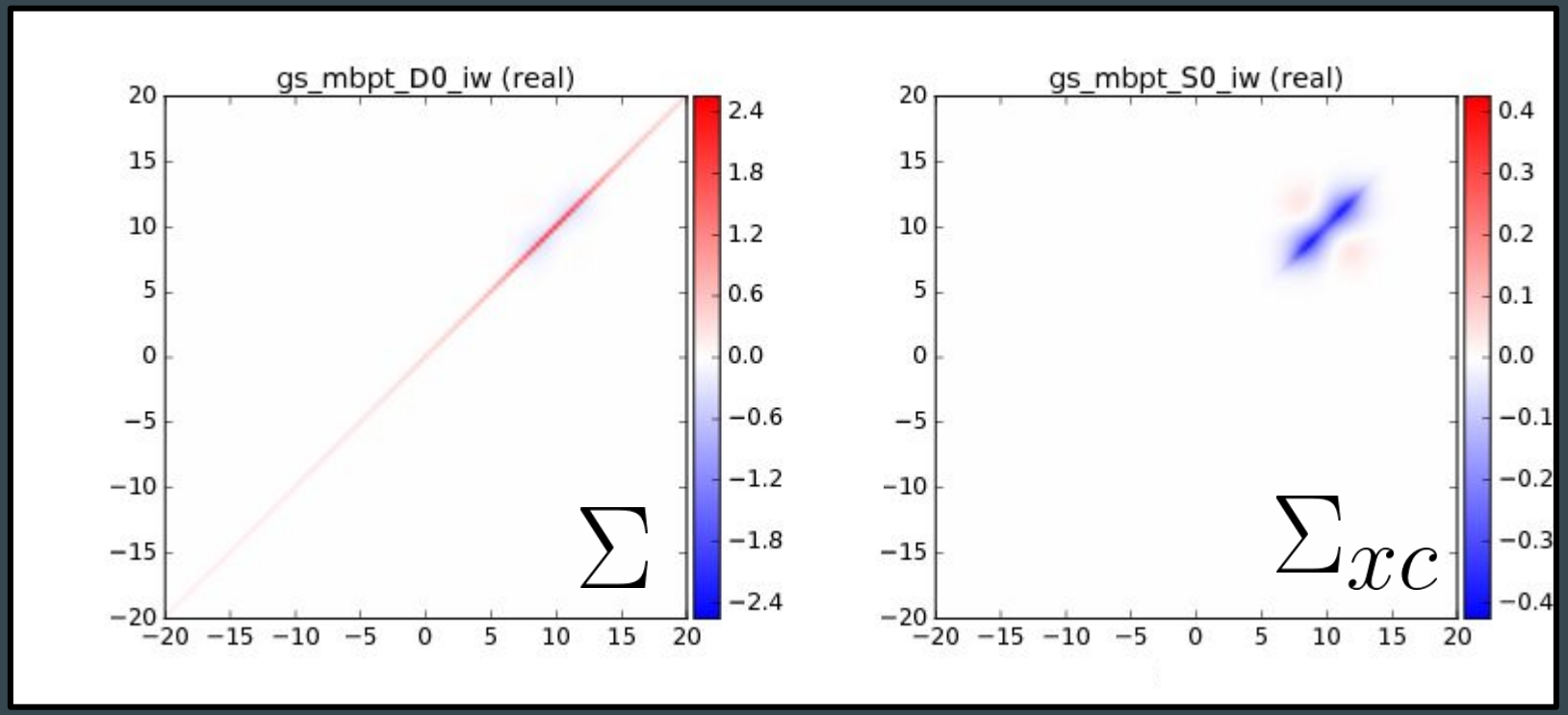




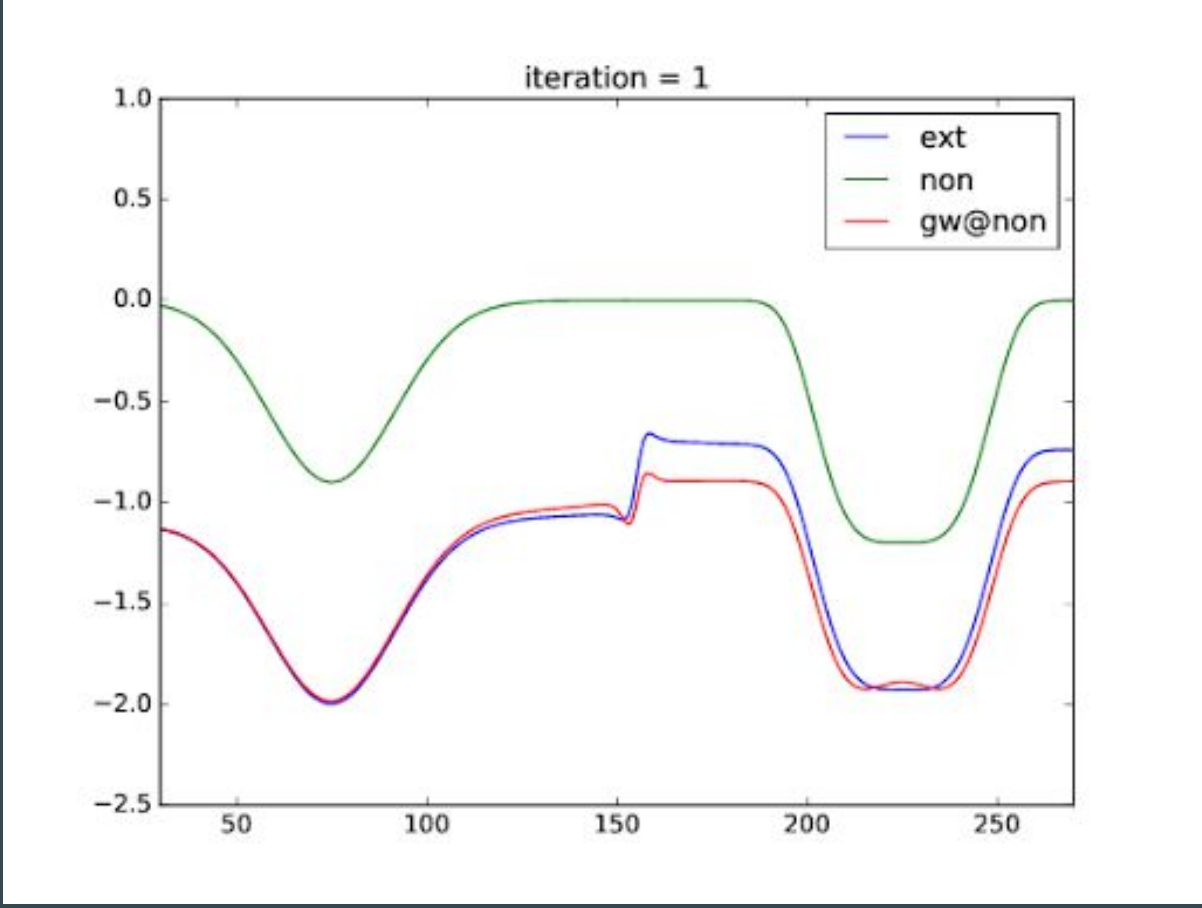
Orbital Reordering: Determining the step position



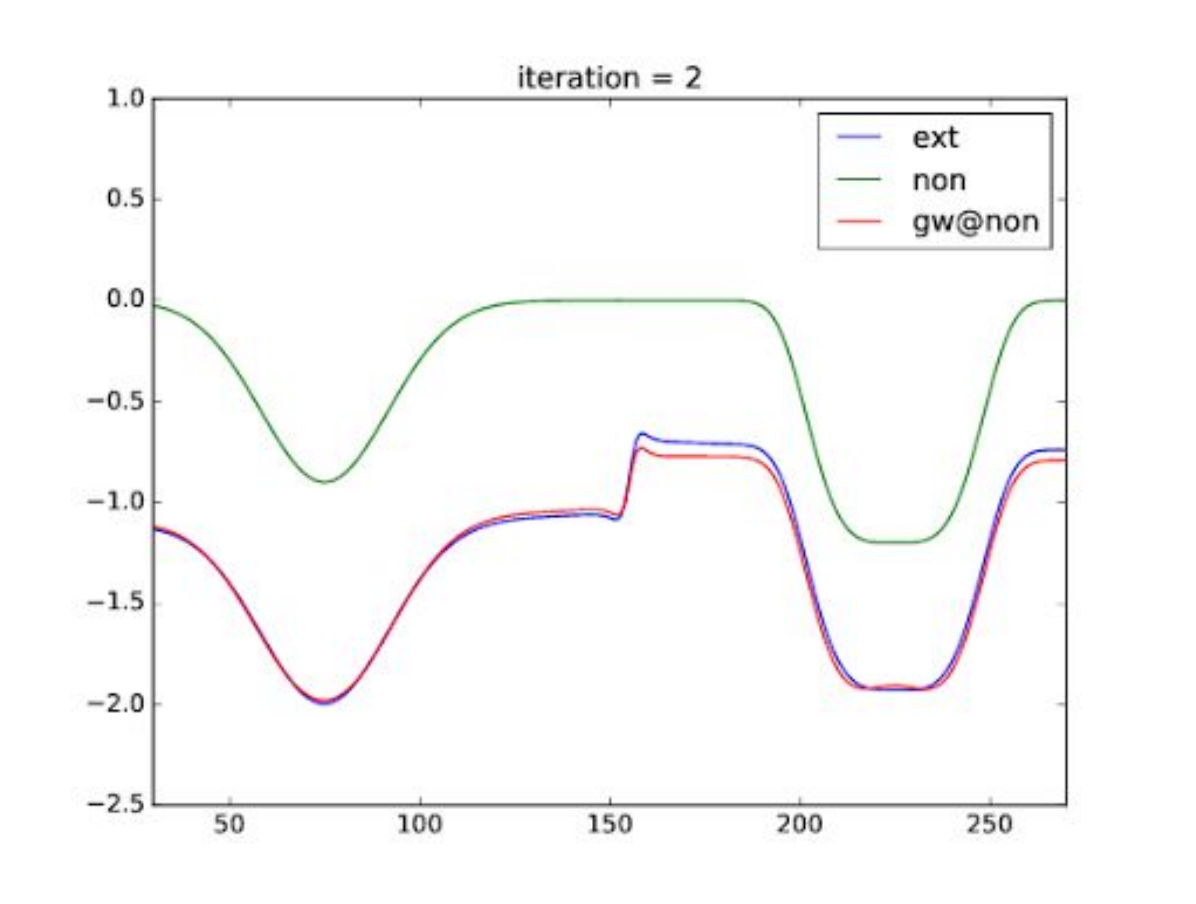
Orbital Reordering: Determining the step height



Orbital Reordering: What feature in the Self-Energy adds the step?



How does the step change in self-consistency?



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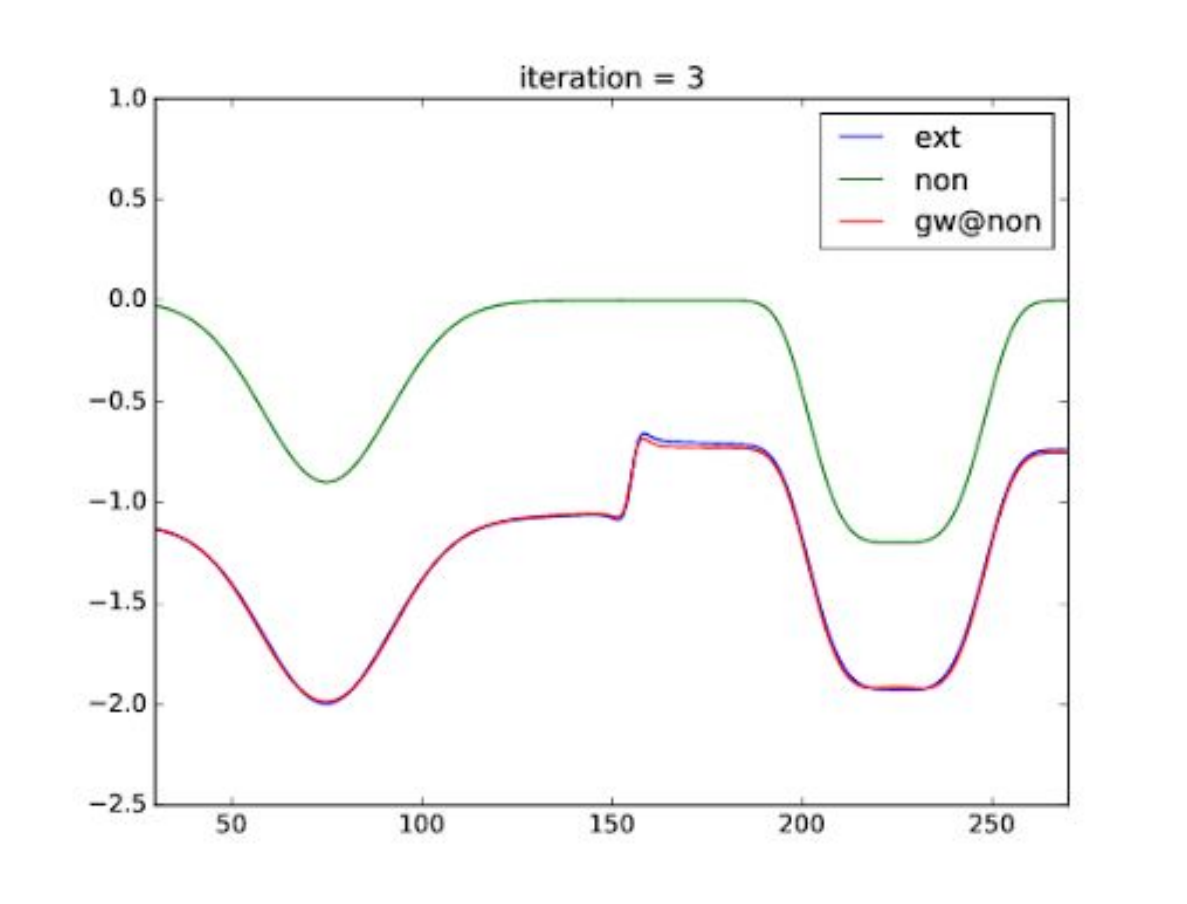

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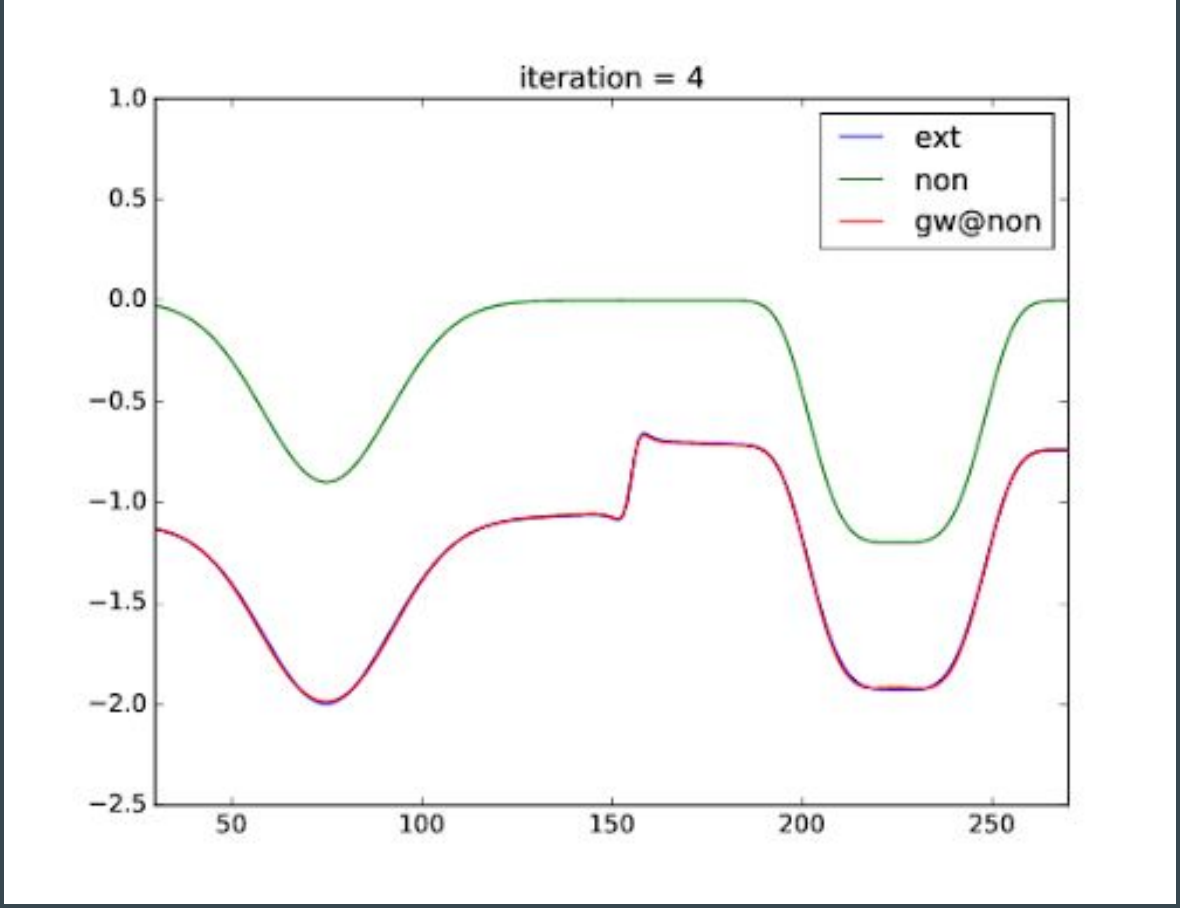
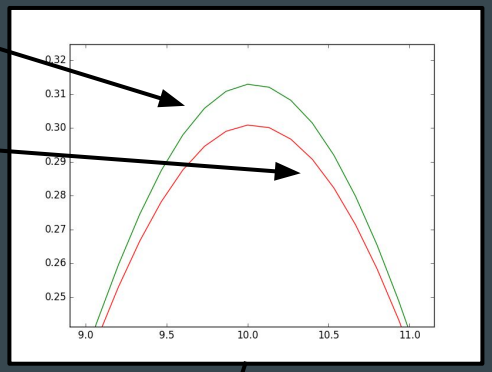
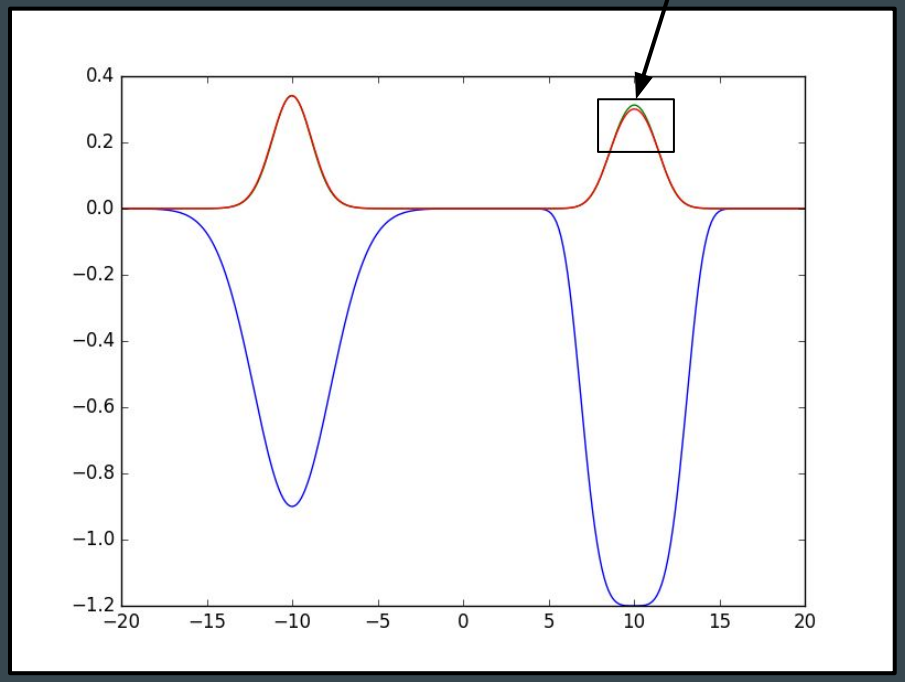


How does the step change in self-consistency?

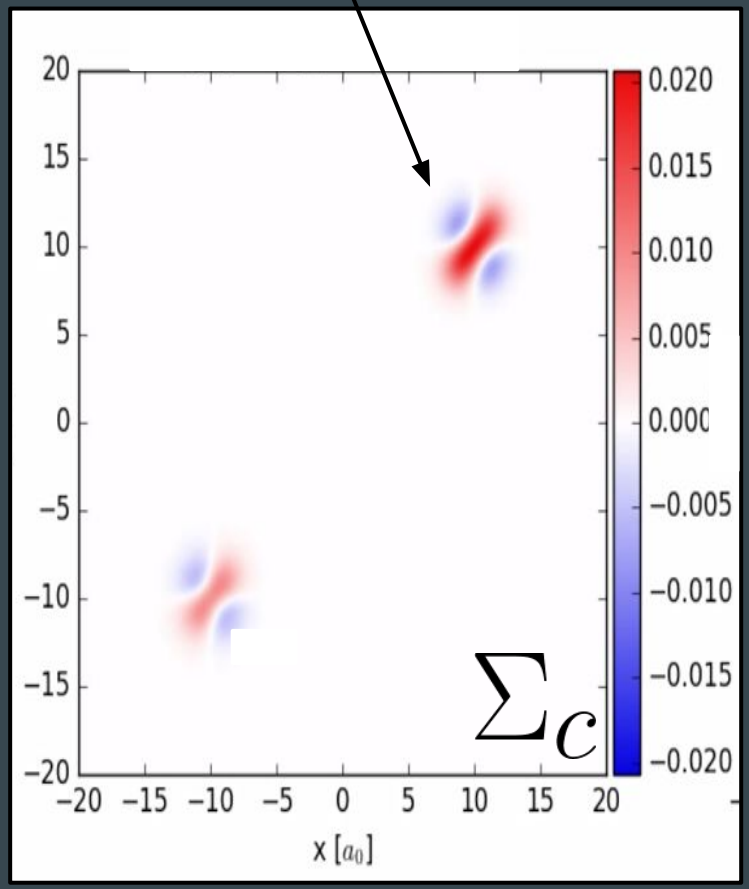
GW@NON

Exact





One-electron correlation



How good is the fully self-consistent density?

Key Points

1. Using iDEA we can compare the exact density and Vks with that produced by by GW
2. In exchange-dominated systems G0W0 can describe steps (correct position, incorrect height) and fails to completely remove SI
3. Fully self-consistent GW corrects the step height and removes almost all of the SI
4. Small amount of SI remaining due to one-electron correlation

Thanks for Listening!

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