The GW self-screening error and its correction using a local density functional

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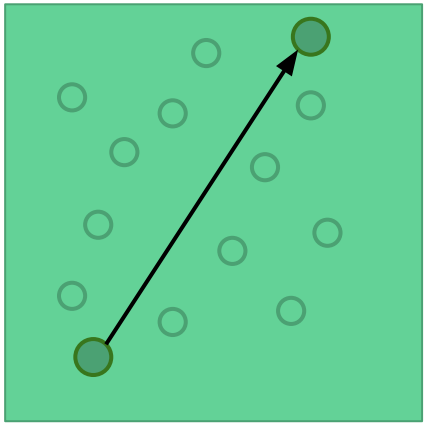
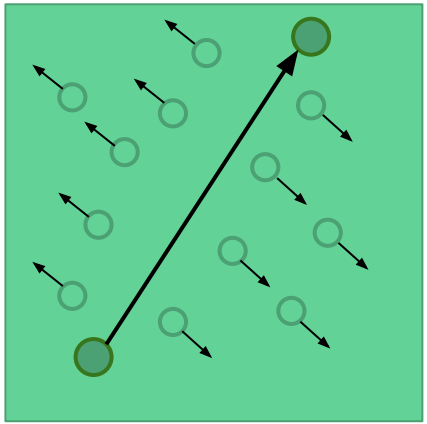
What is the GW Approximation?



No Screening: Hartree-Fock (HF)



Screening: GW

$$\Sigma_{xc} = Gv$$

$$P = 0$$

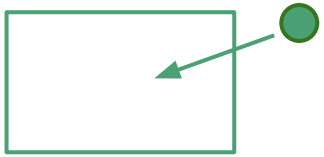
$$\Sigma_{xc} = GW$$

$$P = GG$$

What is the Self-Screening Error?

What is the energy required to add an electron to an empty box?

The LUMO of the zero-electron system:



$$\hat{H}\phi_0 = \varepsilon_0\phi_0$$

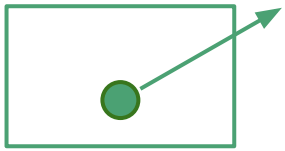
$$\hat{H} = K + V_{\text{ext}} + V_{\text{H}} + V_{\text{xc}}$$

$V_{\text{H}} = 0$, $V_{\text{xc}} = 0$

What is the Self-Screening Error?

What is the energy required to remove the electron?

The HOMO of the one-electron system:



$$\hat{H}\phi_0 = \varepsilon_0\phi_0$$

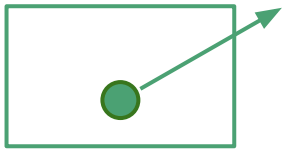
$$\hat{H} = K + V_{\text{ext}} + V_{\text{H}} + V_{\text{xc}}$$

$$= V_H \qquad = -V_H$$

What is the Self-Screening Error?

What is the energy required to remove the electron?

The HOMO of the one-electron system:



$$\hat{H}\phi_0 = \varepsilon_0\phi_0$$

$$\hat{H} = K + V_{\text{ext}} + V_{\text{H}} + V_{\text{xc}}$$

$$= V_H \qquad \neq -V_H$$

If we use the correct P, we screen the exchange and so the potentials now no longer cancel!

So with screening the electron screens its own removal!

What is the Self-Screening Error?

When we screen the exchange operator we add correlation, but also reduce the self-interaction correction.

If the exchange operator were to be screened exactly within the GW approximation, this self-interaction error would remain.

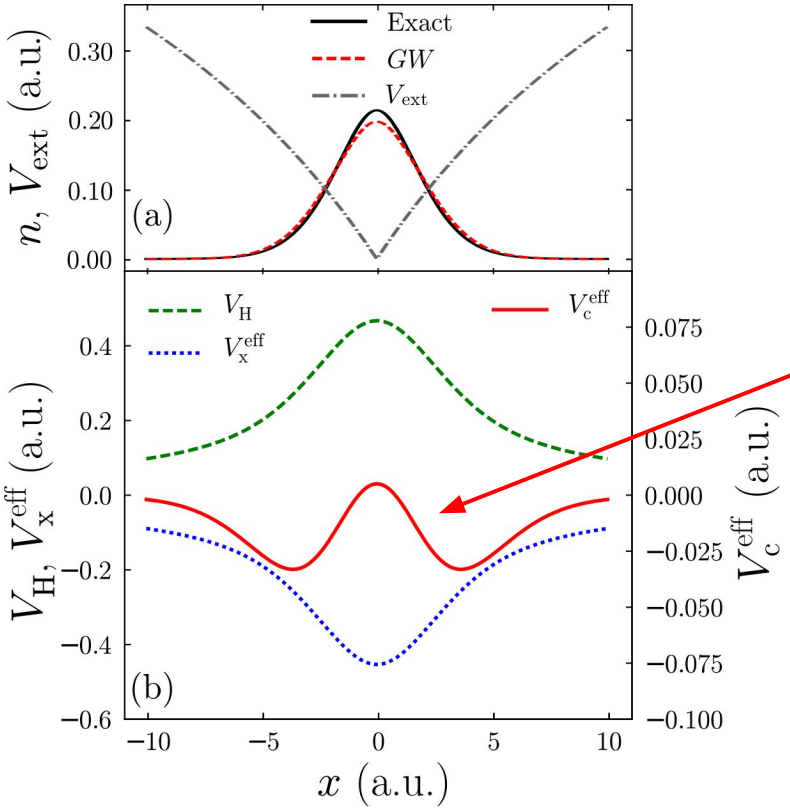
This remaining error is termed the **self-screening error** as it can be thought of each electron screening it's own presence.

P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys. 131, 154111 (2009).

F. Aryasetiawan, R. Sakuma, and K. Karlsson, Phys. Rev. B 85, 035106 (2012).

W. Nelson, P. Bokes, P. Rinke, and R. W. Godby, Phys. Rev. A. 75, 032505 (2007).

What is the Self-Screening Error?

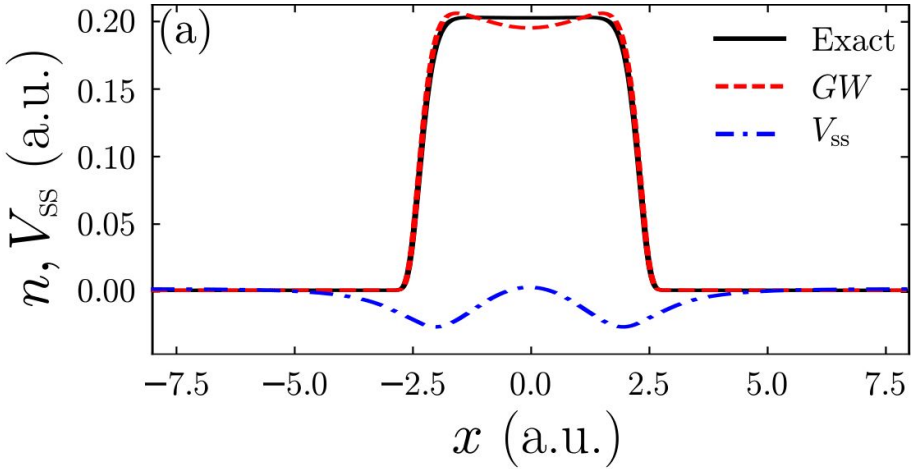


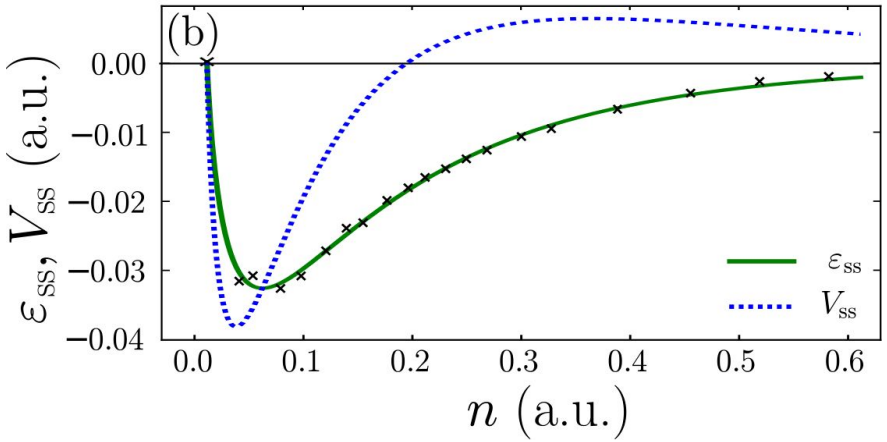
$$V^{\text{eff}}(x) = \frac{1}{\phi(x)} \int \Sigma(x, x', \varepsilon)\phi(x')dx'$$

Self-screening potential!

- Finite systems of electrons in 1D where the SE can be solved exactly.
- Electrons treated as spinless to maximise correlation for given computation effort.
- Can be performed with any given external potential.

Our Local Density Self-Screening Correction

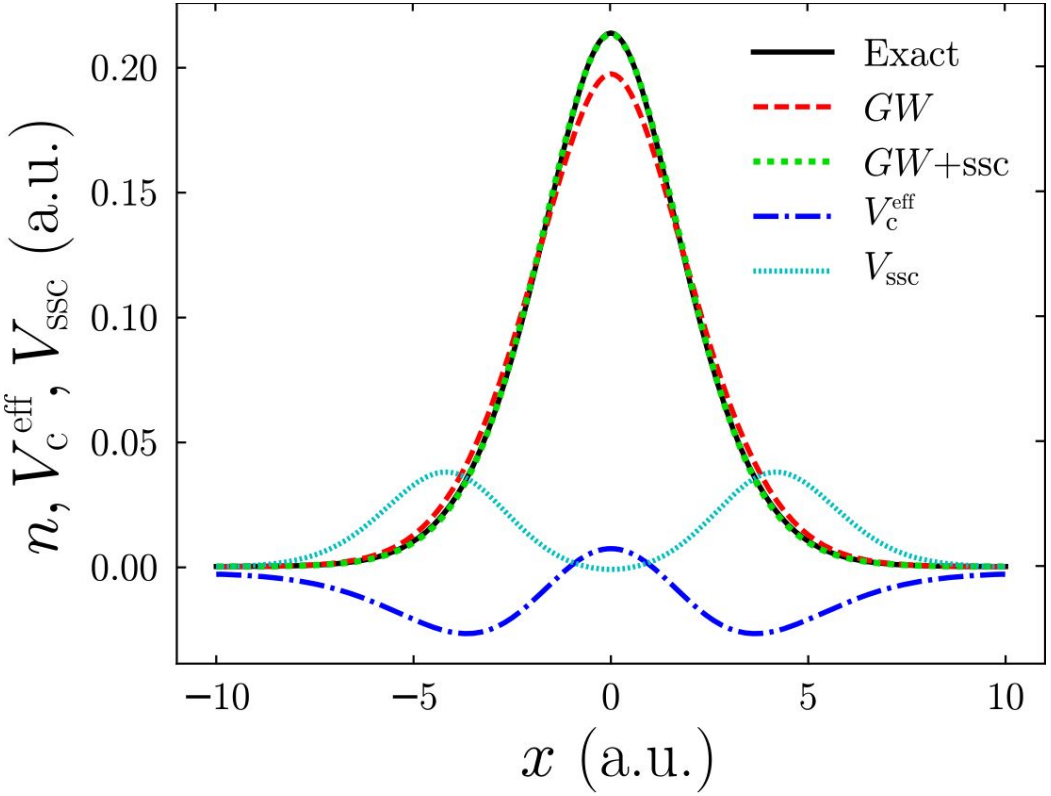




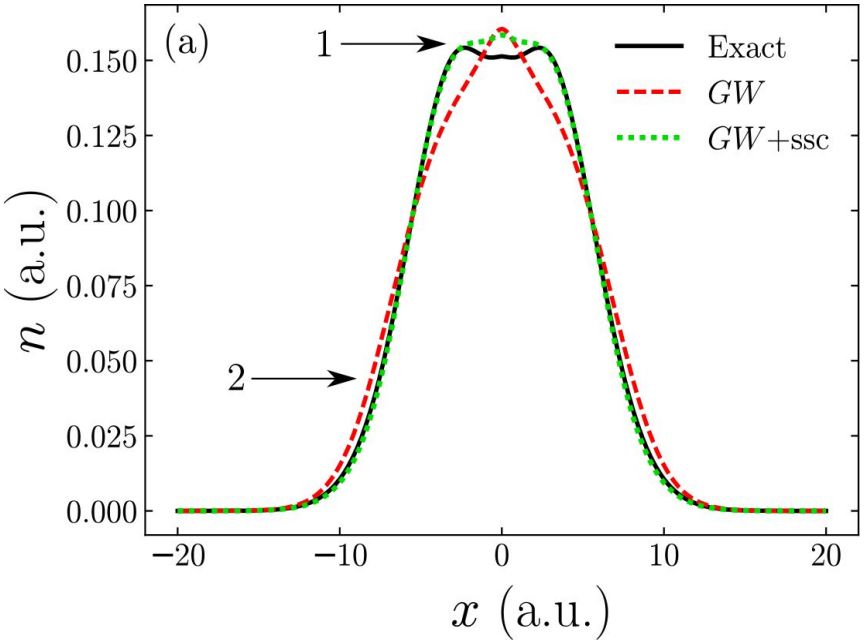
$$V_{\mathrm{ssc}}[n(x)] = ane^{-bn^c}(2 - bcn^c)$$

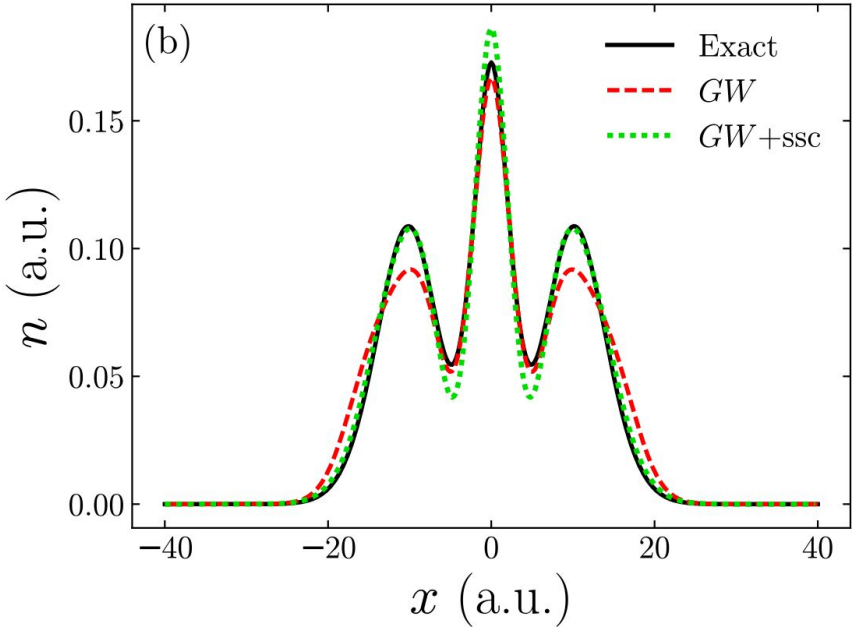
$$a = 4.09268, b = 9.20609, c = 0.53652$$

Performance for Model Systems



Performance for Model Systems





Performance for Model Systems

Ionisation Potentials (Hartrees):

System	GW	Exact
1	0.908	0.900
2	0.624	0.611
3	0.662	0.642

Performance for Model Systems

Ionisation Potentials (Hartrees):

System	GW	GW+ssc	Exact
1	0.908	0.900	0.900
2	0.624	0.610	0.611
3	0.662	0.641	0.642

Key Points

1. The GW approximation suffers from the self-screening error
2. We construct a local density functional to correct this error
3. The density and ionisation energies from our GW+ssc is a significant improvement as from GW

Thanks for Listening!

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ArXiv: 1802.06826

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