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

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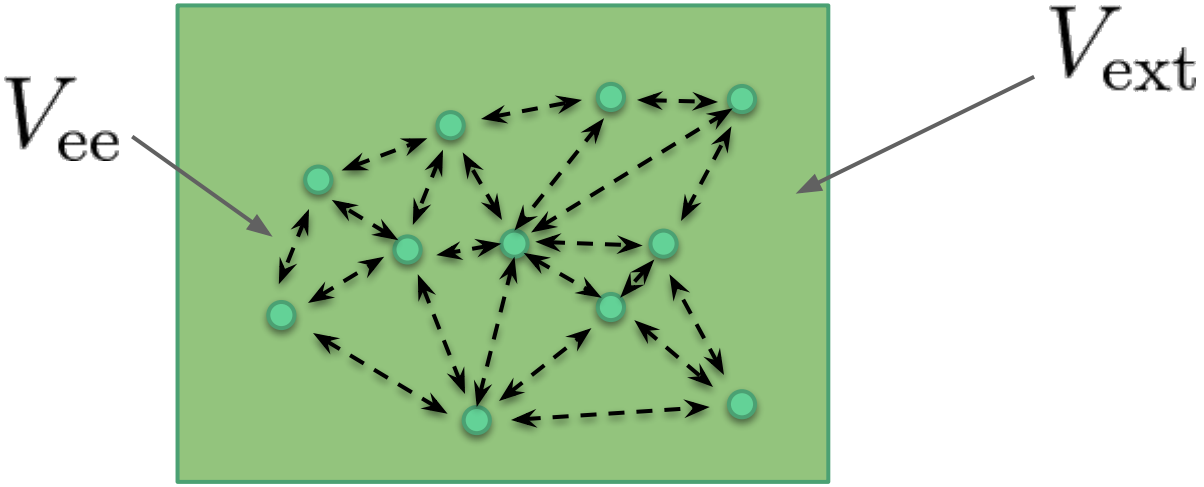
Overview

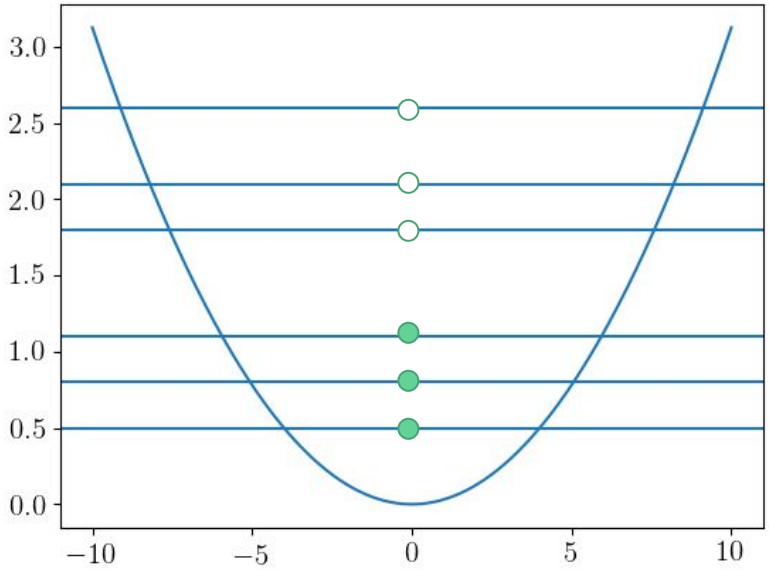
1. What is the *GW* approximation?
2. What is the self-screening error?
3. Our correction
4. Performance for model systems
5. Conclusion

The system of interacting electrons



$$\Psi\left(x_1, x_2, x_3, \ldots\right)$$

The Green's function

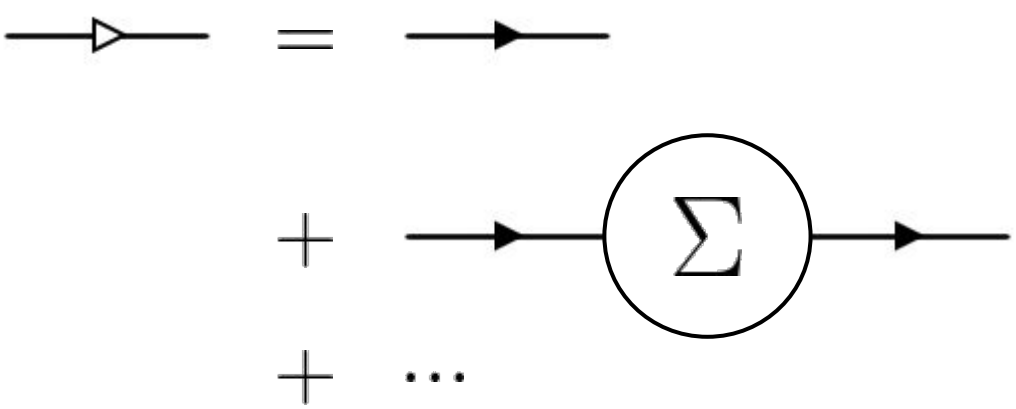


t_1

$$G(x_1, x_2, t_2 - t_1)$$

t_2

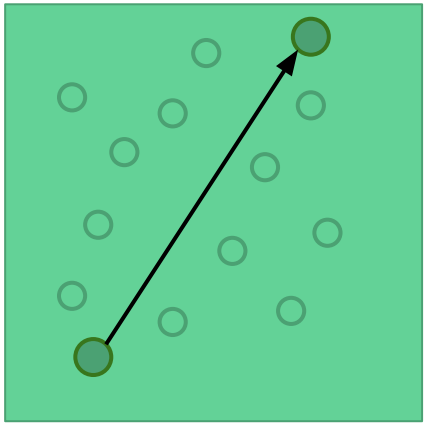
The many-body Green's function



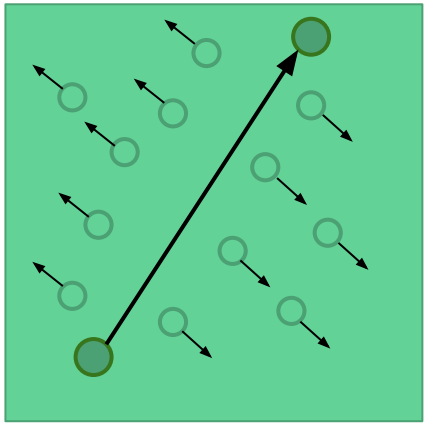
$$G = G_0 + G_0\Sigma G_0 + G_0\Sigma G_0\Sigma G_0 + \ldots$$

$$G = G_0 + G_0\Sigma G$$

What is the *GW* Approximation?



No Screening: Hartree-Fock (HF)



Screening: *GW*

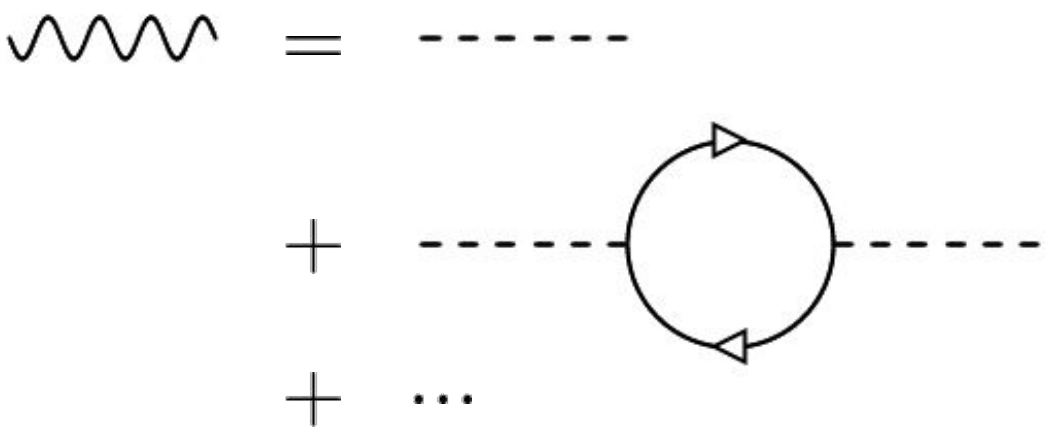
$$\Sigma_{xc} = Gv$$

$$P = 0$$

$$\Sigma_{xc} = GW$$

$$P = GG$$

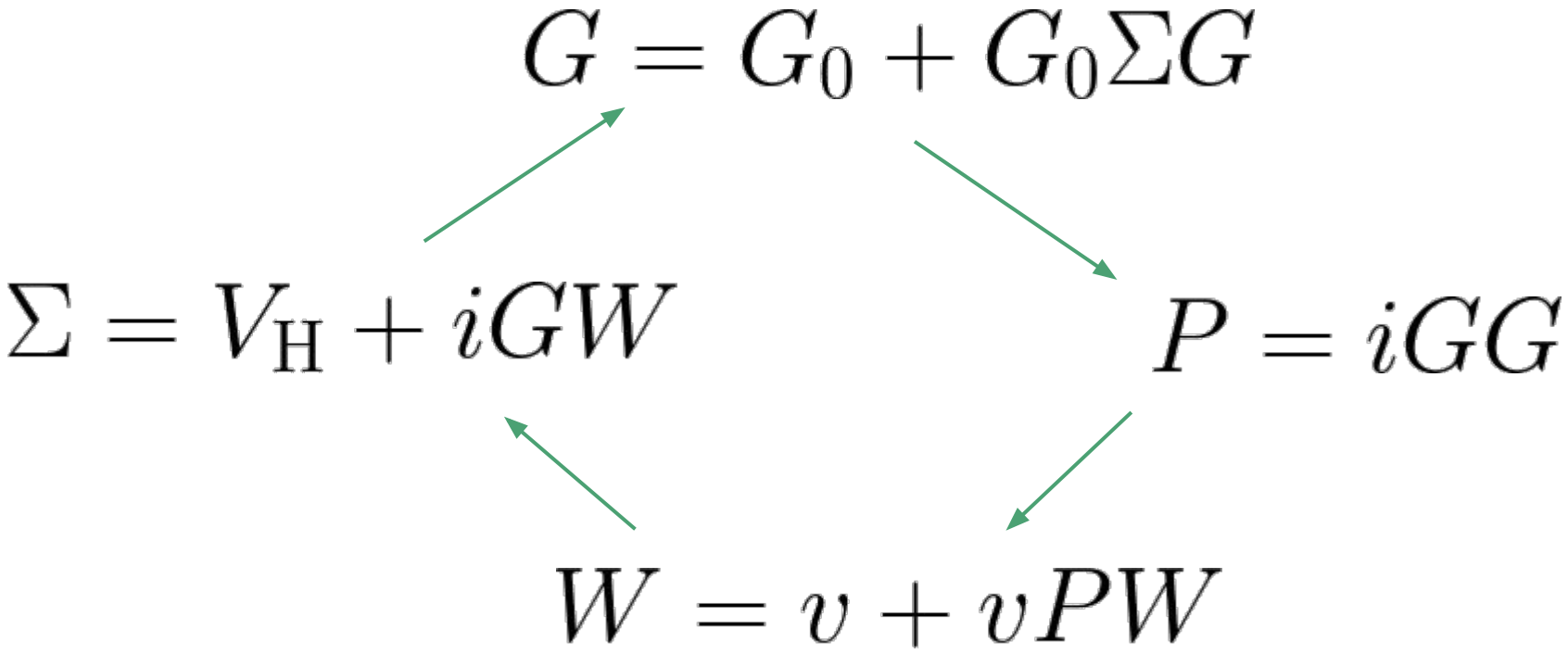
The Screened Coulomb Interaction



$$W = v + vPv + vPvPv + \ldots$$

$$W = v + vPW$$

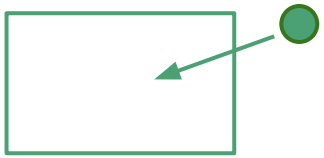
The *GW* equations



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:



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

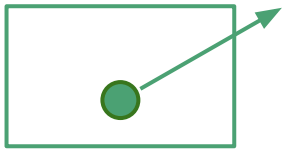
$$\hat{H} = K + V_{\text{ext}} + V_{\text{H}} + V_{\text{xc}}$$

$$= 0 \qquad = 0$$

What is the self-screening error?

What is the energy required to remove the electron?

The HOMO of the one-electron system:



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

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$$= V_H \qquad = -V_H$$

What is the self-screening error?

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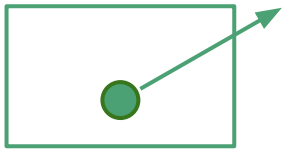


$$\hat{H}\phi_0 = \varepsilon_0\phi_0$$

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

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

If we use the correct *P*, we screen the exchange and so the potentials 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 effectively 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.

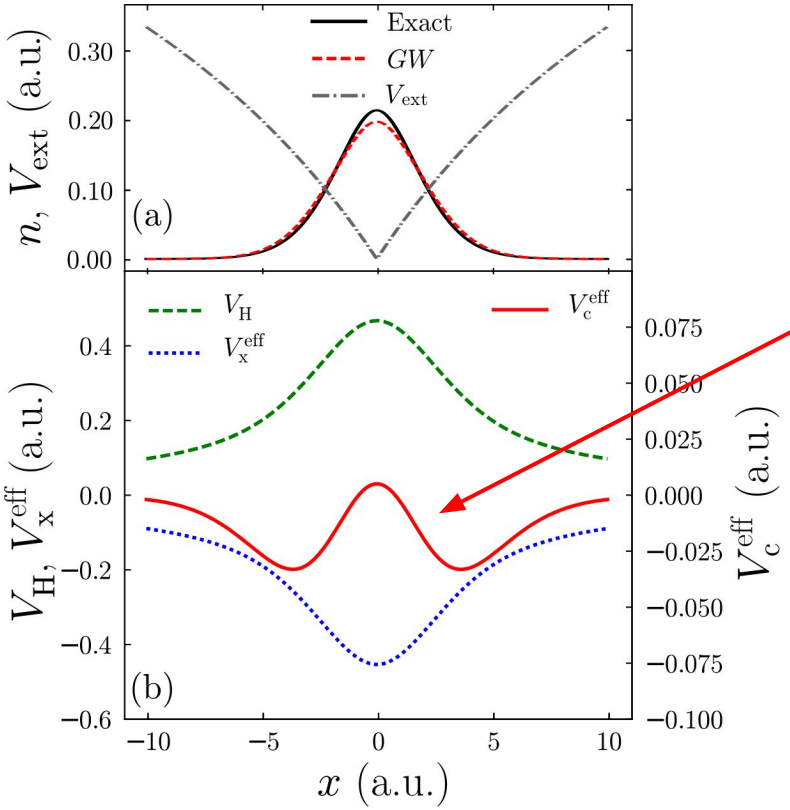
This remaining error is termed the **self-screening error** as it can be thought of each electron screening it's own presence.

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?

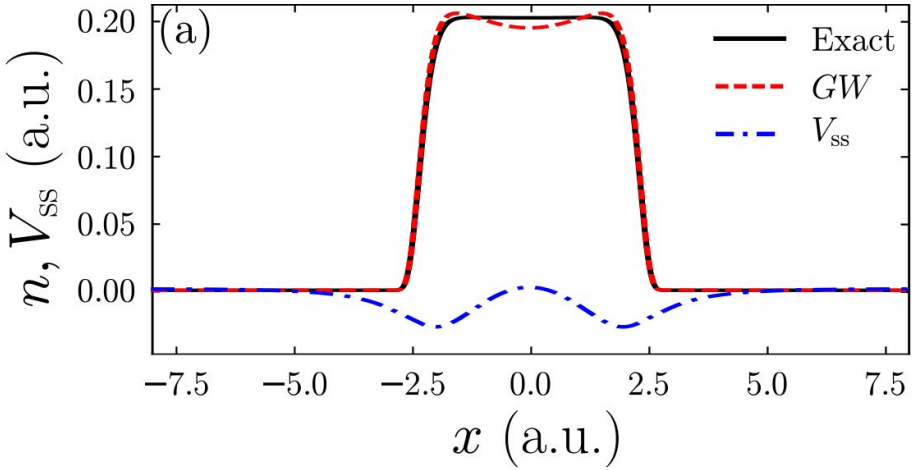


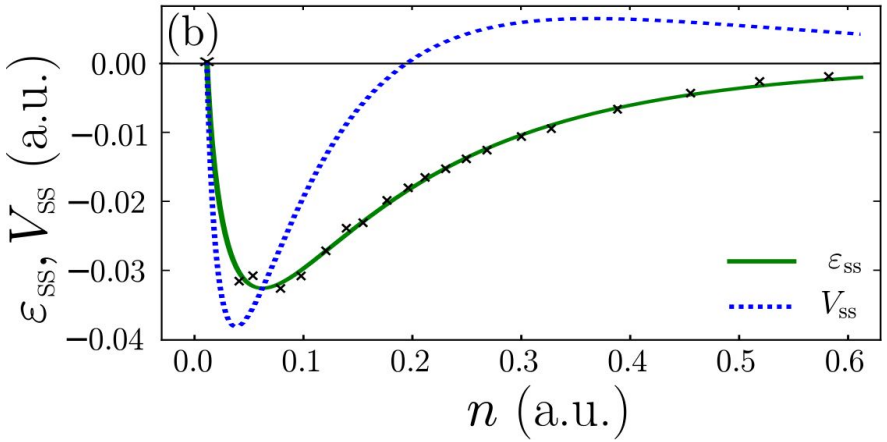
$$V^{\text{eff}}(x) = \frac{1}{\phi(x)} \int \Sigma(x, x', \varepsilon)\phi(x')dx'$$

Self-screening potential!

- Finite systems of electrons in 1D where the SE can be solved exactly.
- Electrons treated as spinless to approach the level of exchange and correlation in a real system for a given computational effort.
- Can be performed with any given external potential.

Our local density self-screening correction

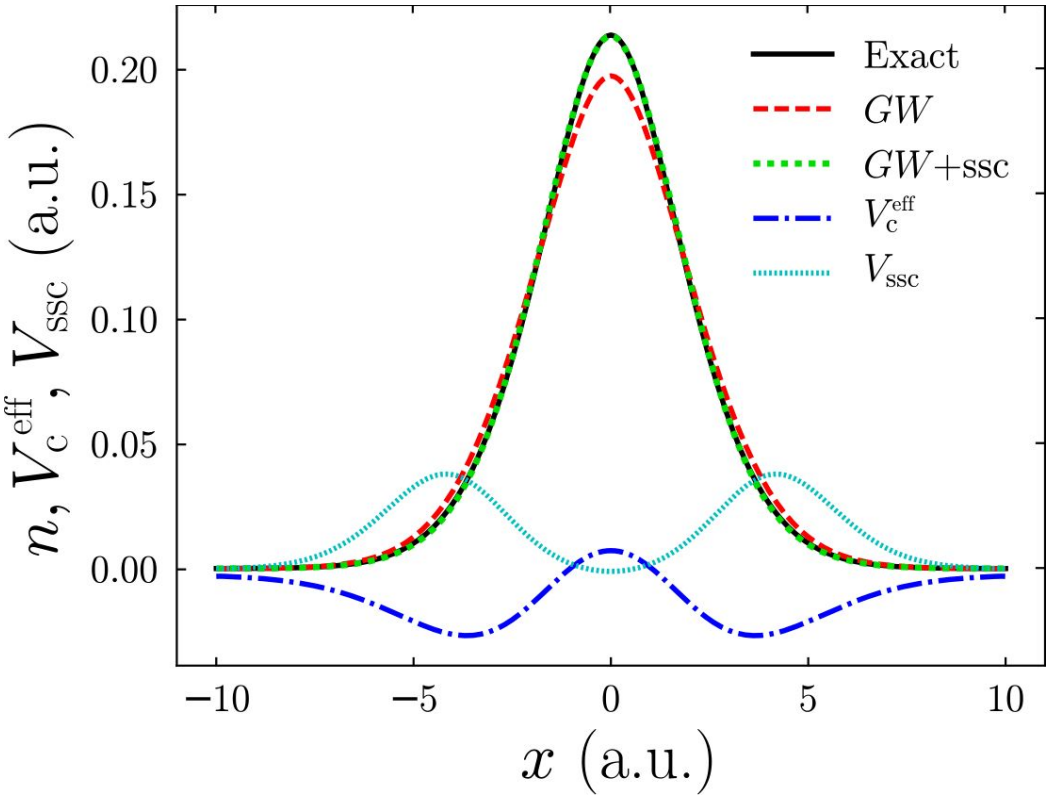




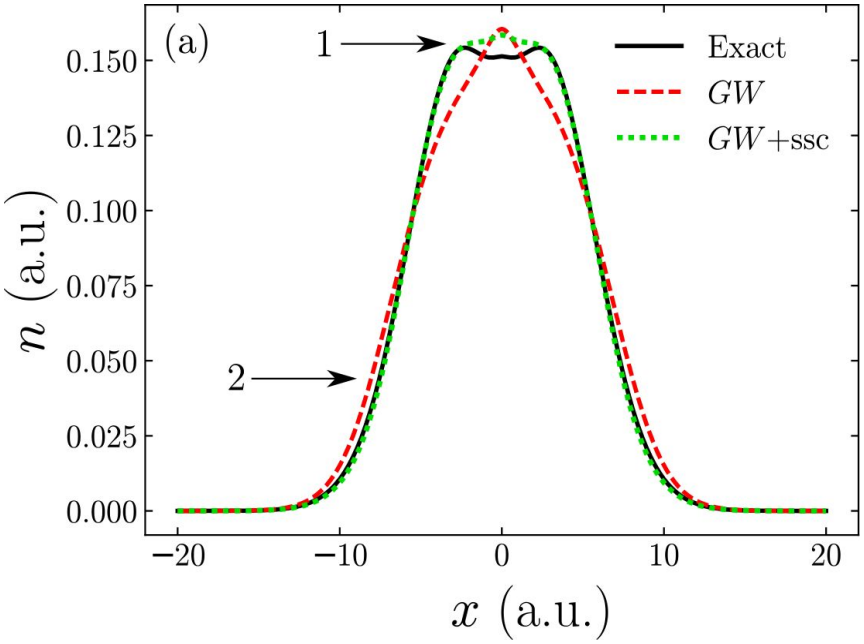
$$V_{\mathrm{ssc}}[n(x)] = ane^{-bn^c}(2 - bcn^c)$$

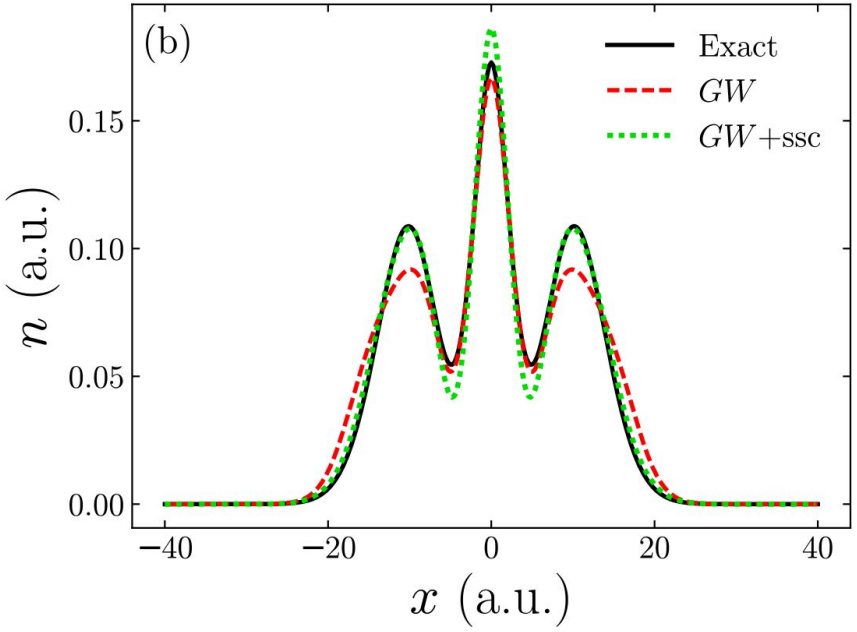
$$a = 4.09268, b = 9.20609, c = 0.53652$$

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 is subject to 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 over *GW*

Thanks for Listening!

Paper: J. Wetherell, M. J. P. Hodgson and R. W. Godby, Physical Review B (Rapid Communications) **97**, 121102 (2018).

ArXiv: 1802.06826

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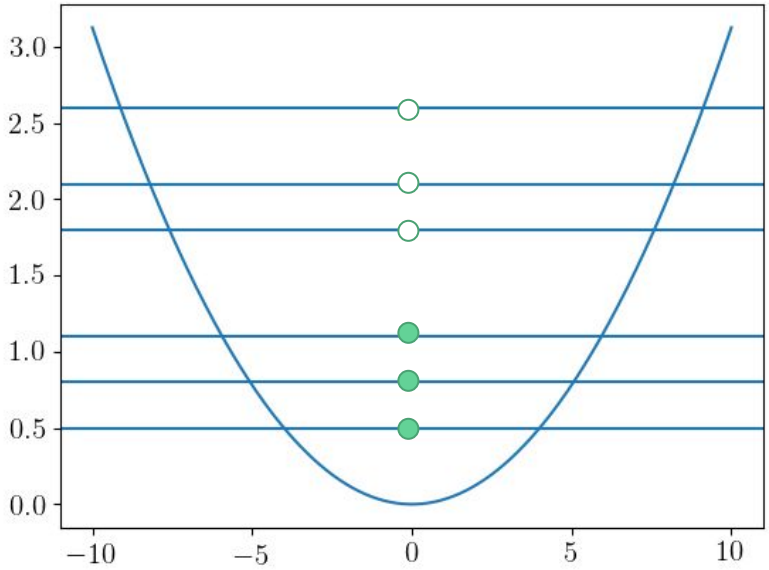
1. The *GW* approximation is subject to the self-screening error
2. We construct a local density functional to correct this error
3. The density and ionisation energies from our *GW*+ssc is a significant improvement over *GW*

Extra slides

The many-body Green's function



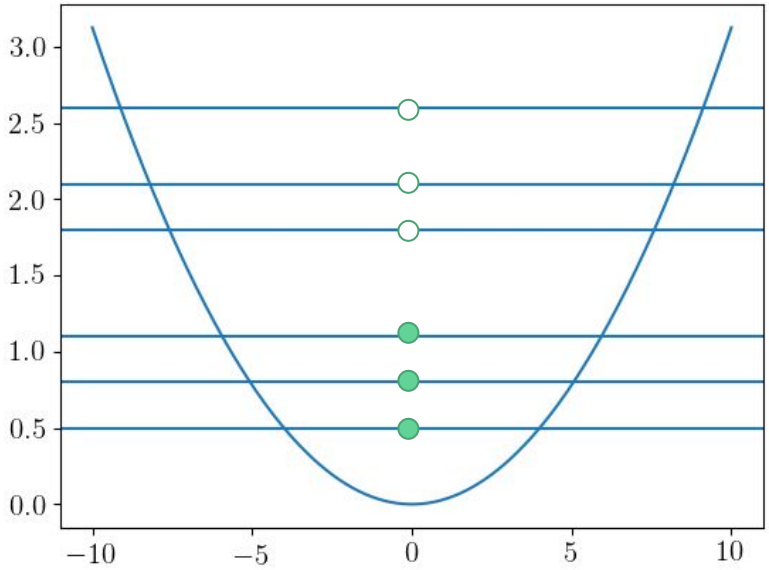
If we add an electron at t=0 and remove it at t, what is the probability amplitude it was added at position x_1 and removed at x_2?

$$\phi_4(x_1)$$

$$\phi_4^*(x_2)e^{-i\varepsilon_4 t}$$

$$\phi_4(x_1)\phi_4^*(x_2)e^{-i\varepsilon_4 t}$$

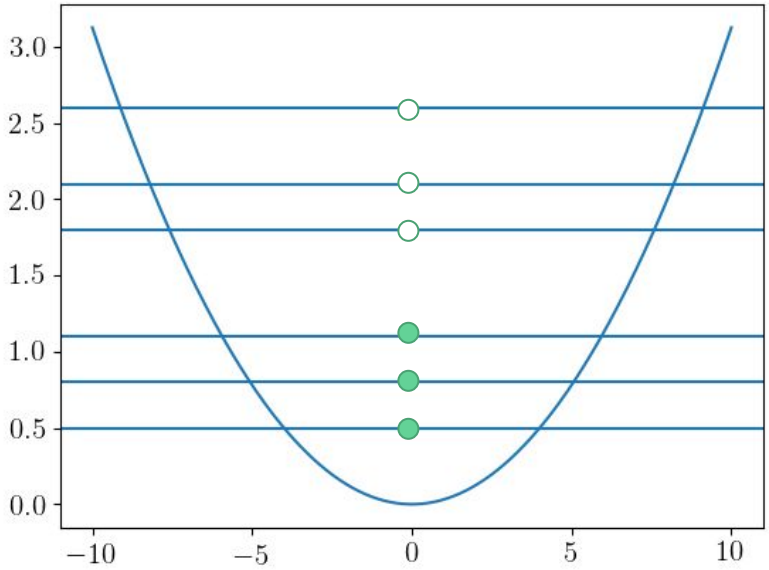
The many-body Green's function



If we add an electron at t=0 and remove it at t, what is the probability amplitude it was added at position x_1 and removed at x_2?

$$\sum_{n}^{\text{unocc}} \phi_n(x_1)\phi_n^*(x_2)e^{-i\varepsilon_n t}$$

The many-body Green's function

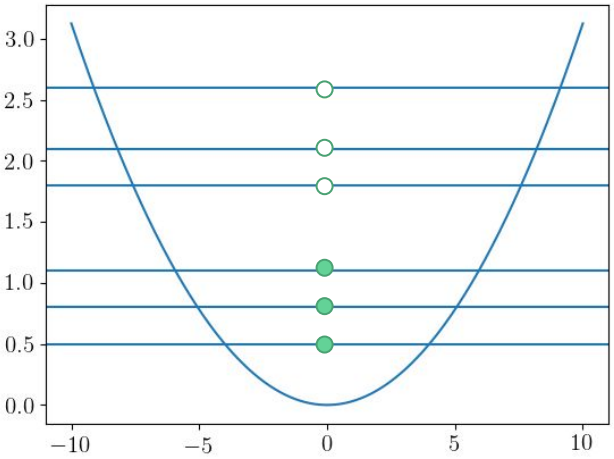


If we add a hole at t=0 and remove it at t, what is the probability amplitude it was added at position x_1 and removed at x_2?

$$\sum_{n}^{\text{occ}} \phi_n(x_1)\phi_n^*(x_2)e^{-i\varepsilon_n t}$$

The many-body Green's function

$$iG_0(x_1, x_2, t) = \begin{cases} \sum_n^{\text{unocc}} \phi_n(x_1)\phi_n^*(x_2)e^{-i\varepsilon_n t} : t > 0 \\ \sum_n^{\text{occ}} \phi_n(x_1)\phi_n^*(x_2)e^{-i\varepsilon_n t} : t \leq 0 \end{cases}$$



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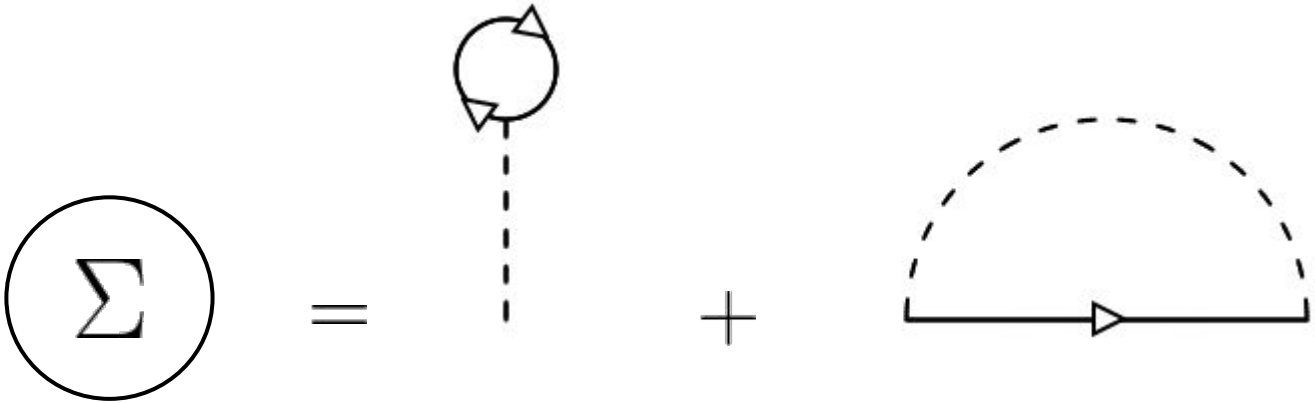
$$iG_0(x_1, x_2, t) = \langle \Phi_0 | T[\psi(x_2, t_2)\psi^\dagger(x_1, t_1)] | \Phi_0 \rangle$$

The many-body Green's function

$$iG_0(x_1, x_2, t) = \langle \Phi_0 | T[\psi(x_2, t_2)\psi^\dagger(x_1, t_1)] | \Phi_0 \rangle$$

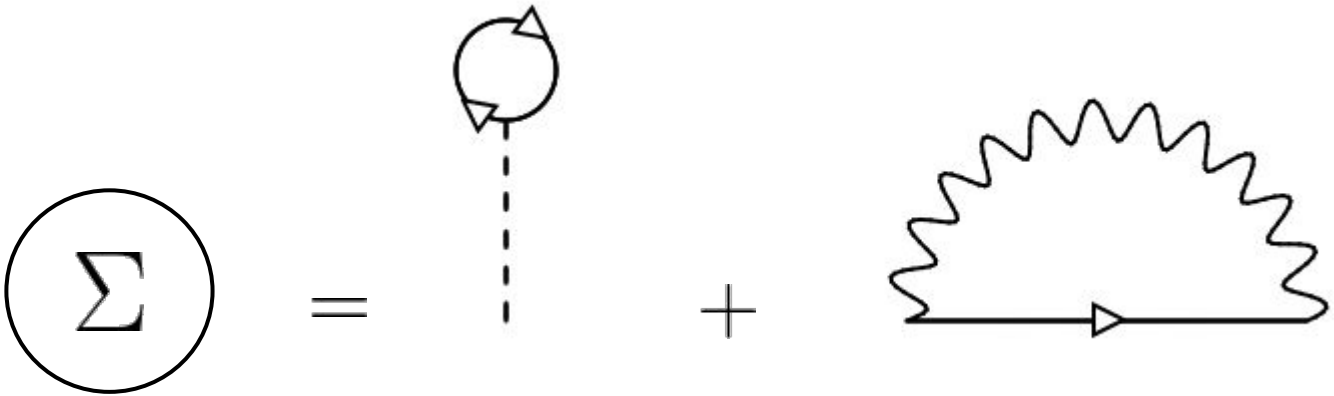
$$iG(x_1, x_2, t) = \langle \Psi_0 | T[\psi(x_2, t_2)\psi^\dagger(x_1, t_1)] | \Psi_0 \rangle$$

The Hartree-Fock self-energy



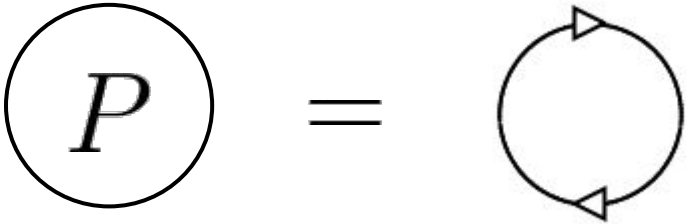
$$\Sigma_{\mathrm{HF}} = V_{\mathrm{H}} + Gv$$

The *GW* Approximation



$$\Sigma_{\mathrm{GW}} = V_{\mathrm{H}} + GW$$

The Random Phase Approximation (RPA)



$$P(x_1, x_2, t) = iG(x_1, x_2, t)G(x_2, x_1, -t)$$