Unphysical and physical solutions in many-body theories: from weak to strong correlation

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Nonlinear Dyson equations

We often solve Dyson-like equations which are non-linear:

$$X = X_0 + X_0 K[X] X$$

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Example : Hartree Fock

$$G = G_0 + G_0 \Sigma^{HF}[G] G \qquad \Sigma^{HF}[G] = v_H[G] + v_x[G]$$

$$v_H[G](\mathbf{r}, t) = -i \int d\mathbf{r}' \, G(\mathbf{r}', t, \mathbf{r}', t^+) v_c(\mathbf{r}, \mathbf{r}')$$

$$v_x[G](\mathbf{r}, t) = \imath \int d\mathbf{r}' \, G(\mathbf{r}, t, \mathbf{r}', t^+) v_c(\mathbf{r}, \mathbf{r}')$$

Dyson equation in one point

One-point model (OPM): one point in space, time and spin ($G \to y; v_c \to u; \Sigma \to s$).

Exact self-energy: $\tilde{s}[y_0, u] = -\frac{1}{2} u y_0 \Longrightarrow y = y_0 + y_0 \tilde{s}[y_0, u] y$

Real life: self-energy is a function of $y \Longrightarrow y = y_0 + y_0 s[y, u] y$

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Example: the HF self-energy in one point:
$s[y, u] = -\frac{1}{2} u y \Longrightarrow Y^{\pm}_{HF} = \frac{1}{V}\left[-1 \pm \sqrt{1 + 2V}\right] \quad (Y = y/y_0, V = u y_0^2)$

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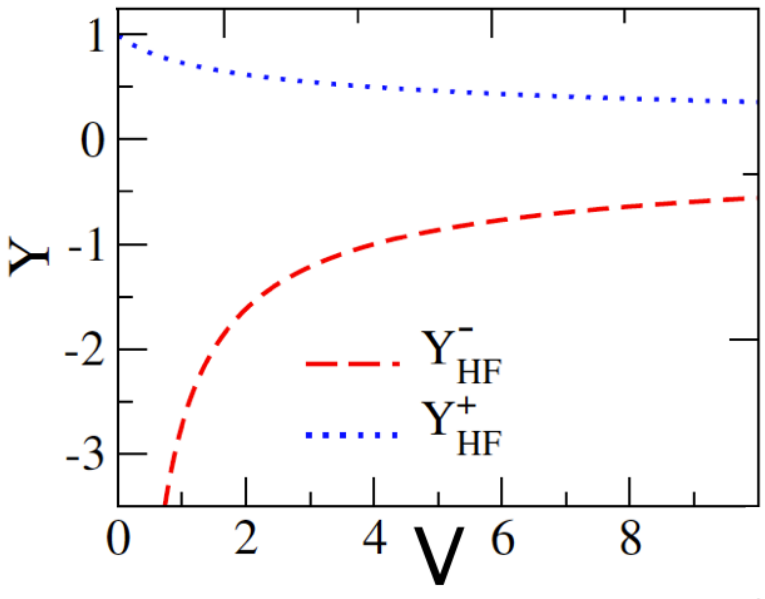
Two solutions:

physical: Y^{+}_{HF}

unphysical: Y^{-}_{HF}



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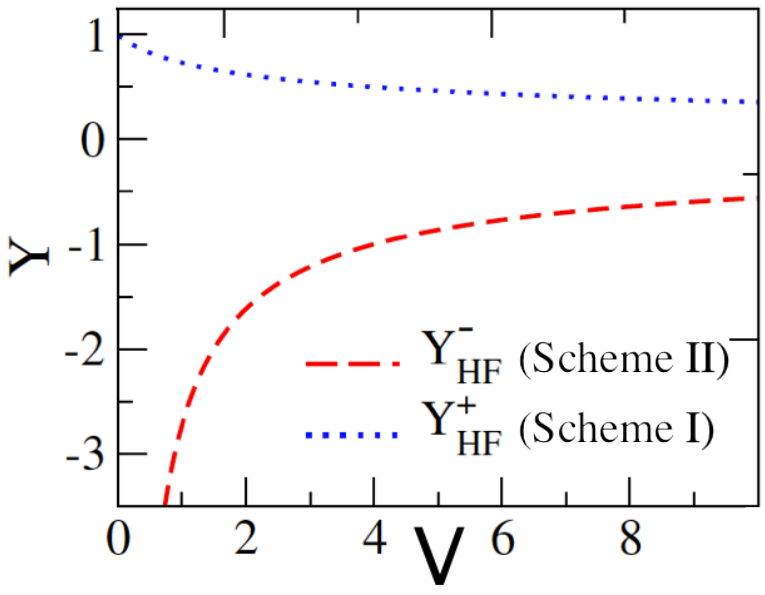
HF equations are solved by iterating

Scheme I : $Y^{(n+1)} = \frac{2}{2+VY^{(n)}}$

Scheme II : $Y^{(n+1)} = \frac{2}{VY^{(n)}} - \frac{2}{V}$

continued fractions of Y^{+}_{HF} and Y^{-}_{HF}



Real materials: absorption spectrum of LiF from TDDFT

Optical absorption ($\mathrm{Im}[\epsilon_M]$)

$$\epsilon^{-1} = 1 + v_c\chi \qquad \chi(1,2) = L(1,2,1^+,2^+)$$

$$\text{BSE:} \qquad L = L_0 + L_0(\omega)\Xi[L]L \qquad \Xi[L] = v_c - W[L]$$

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$$f_H = v_c \quad f_{xc}[\chi] = \frac{1 + v_c\chi(\omega = 0)}{\chi_0(\omega = 0)} \quad \text{bootstrap kernel (PRL 107, 186401)}$$

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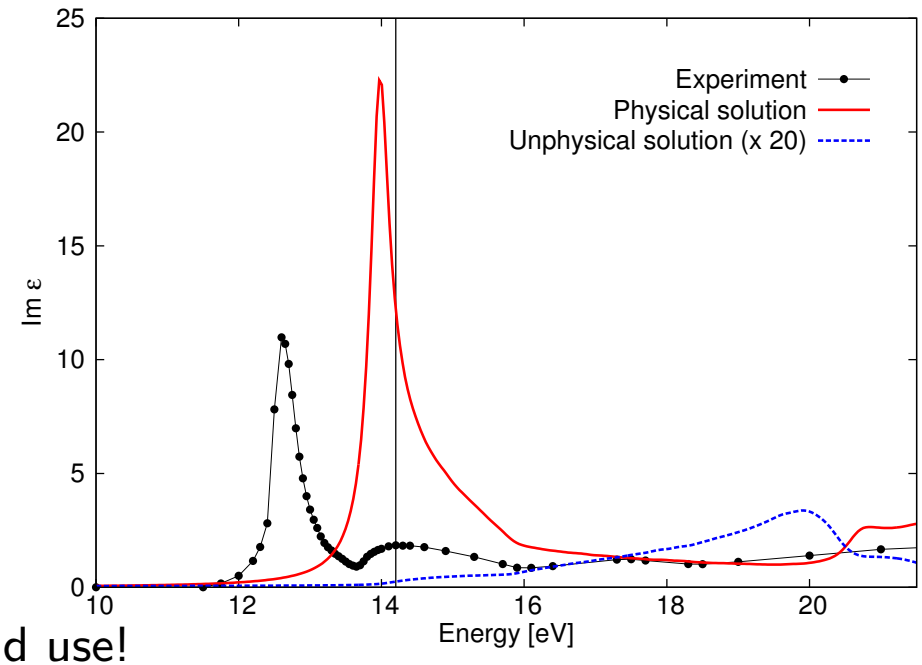
Scheme I : physical solution

Scheme II : unphysical solution



The OPM tells us which scheme we should use!

The map $G_0 \leftarrow G$

Instead of $\Sigma[G_0]$ we prefer to use $\Sigma[G]$ (less diagrams, conserving)

Possible thanks to the Luttinger-Ward (LW) functional

$$\Sigma[G_0] \rightarrow \Sigma[G_0[G]] \rightarrow \Sigma[G]$$

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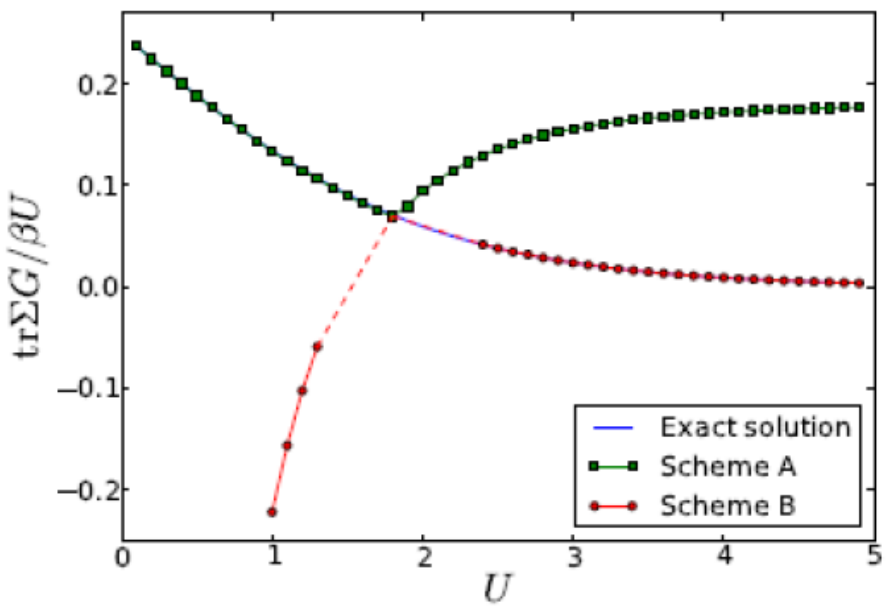
Kozik *et al.* [PRL 114, 156402 (2015)] performed numerical calculations on Hubbard atom with two iterative schemes

- $\Sigma[G]$ has at least two branches
- Nonexistence of Luttinger-Ward



Can we use the OPM to reproduce and analyze these results?

The map $G_0 \leftarrow G$ in the OPM

Exact self-energy: $\tilde{s}[z_0] = -\frac{1}{2} u z_0$

Dyson equation: $z_0 = y + \frac{1}{2} u y z_0^2$ (y is known and z_0 is to be determined)

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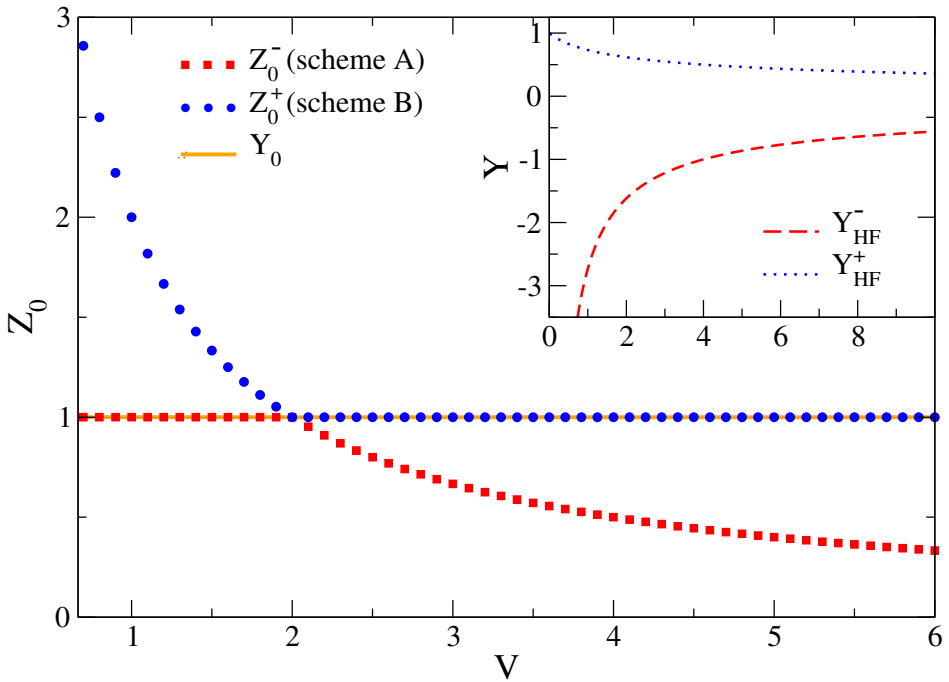
Two solutions:

$$z_0^{\pm} = \frac{1}{uy}\left(1 \pm \sqrt{1-2uy^2}\right) \underbrace{\Longrightarrow}_{Z_0 = z_0/y_0} Z_0^{\pm} = \frac{2+V \pm \sqrt{(2-V)^2}}{2V},$$



The sign of the square root has to be changed to stay on physical solution!

Iteration schemes

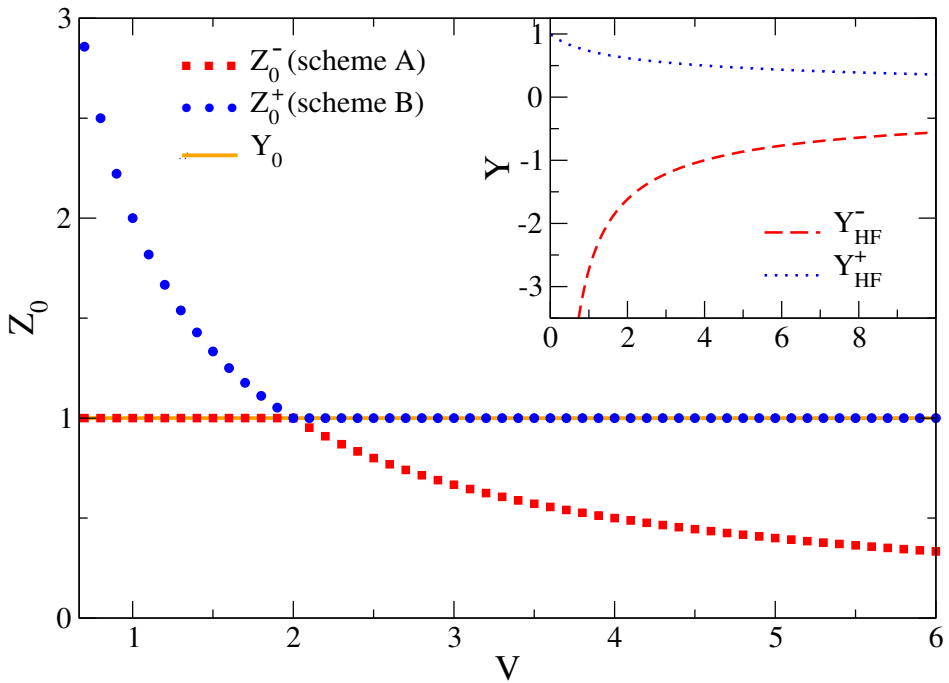
Two possible iterative schemes (same as Kozik *et al.*) are

$$\frac{1}{Z_0^{(n+1)}} = 1 + \frac{1}{2}V(1 - Z_0^{(n)}) \qquad \textbf{(A)},$$

$$\frac{1}{Z_0^{(n+1)}} = -1 - \frac{1}{2}V(1 - Z_0^{(n)}) + \frac{2}{Z_0^{(n)}} \qquad \textbf{(B)}.$$

Scheme A: continued fraction of Z_0^-

Scheme B: continued fraction of Z_0^+



We should change iteration scheme at $V = 2$!

How can we detect if anything is wrong if the exact solution is not available?

Two-particle correlation function

The OPM highlights the (reducible) polarizability χ as critical quantity; it changes sign at $V = 2$:

$$\frac{\chi}{\chi_0} = 2\frac{2-V}{(2+V)^2},$$

$V > 2$: perturbation expansion of exact solution ($Y = \frac{1}{1+V/2}$) diverges.

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Compare to Schaefer et al., PRL 110, 246405 (2013):

Hubbard model: Breakdown of perturbation theory is linked to an eigenvalue of 2-particle correlation function becoming negative.

Defining the domain: OPM

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No definition of domain $\rightarrow$ multiple solutions

By imposing exact constraints one can eliminate unphysical solutions.

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Example:

A physical G_0 is a sum of simple poles, each with a strength normalized to one:

$$G_0(\mathbf{r}, \mathbf{r}', \omega) = \sum_s \frac{\phi_s(\mathbf{r})\phi_s^*(\mathbf{r}')}{\omega - \epsilon_s}$$

Corresponding constraint in the OPM: $Z_0 = 1$ (physical solution)

In practice, it is often not obvious how to impose this constraint.

Exact self-energy functional of G in the OPM

In the OPM we can construct the exact self-energy as a functional of y:

$$s^{\pm}[y,u] = -\frac{1}{2}uy_0[y] = -\frac{1}{2y}\left(1 \pm \sqrt{1-2uy^2}\right)$$

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Expanding the square root (infinite convergence radius $\forall u$):

$$s^{\pm}[y,u] = -\frac{1}{2y} \mp \frac{1}{2y} \pm \frac{1}{2}u\left[y + \frac{uy^3}{2} + \ldots\right].$$

leads to LW perturbation expansion for $V < 2$ (s^-), first order is HF, etc.

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What about $s^+(V > 2)$?

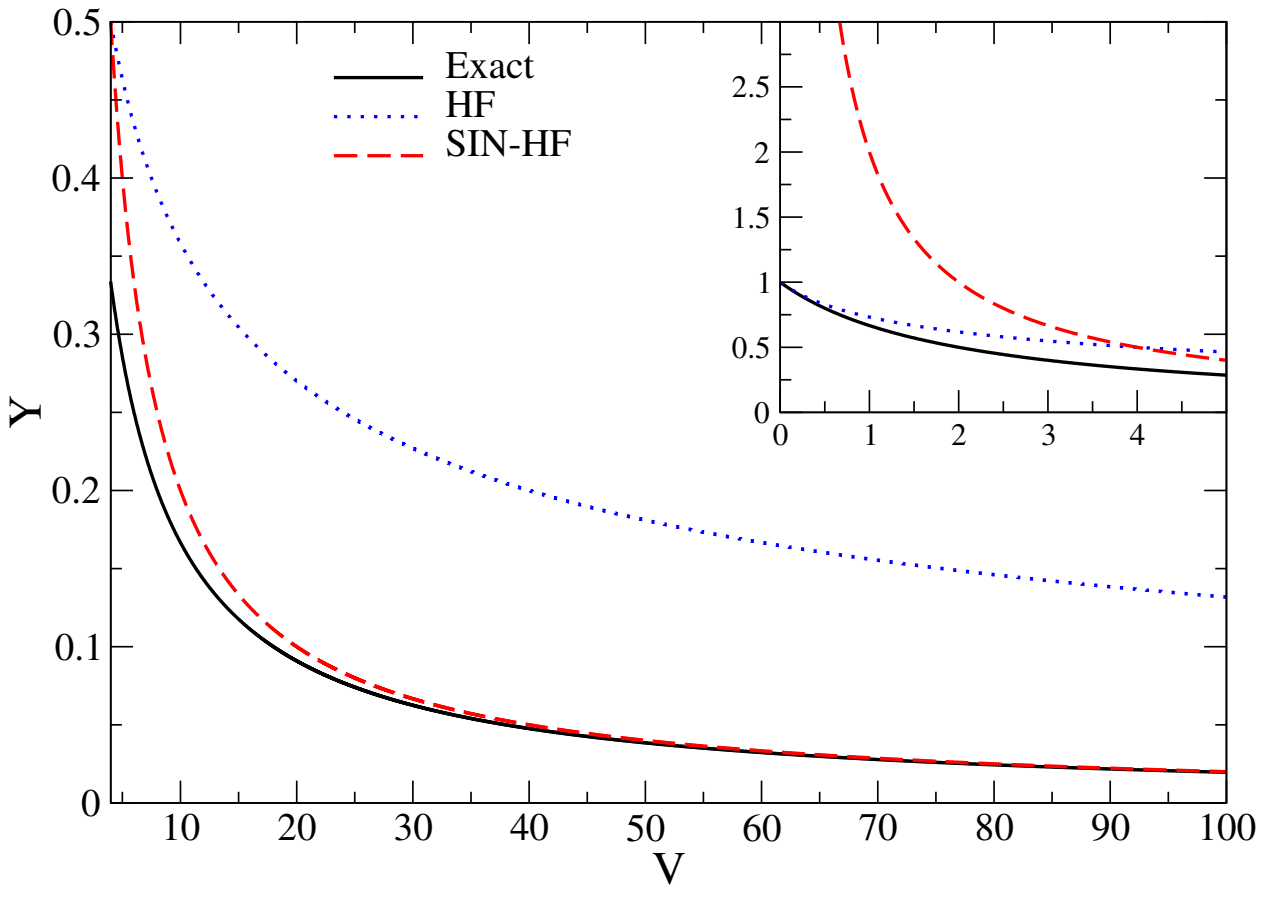
$-\frac{1}{y}$: first term in a self-energy expansion for strong interaction (SIN).
Expansion for strong interaction: $s^{\mathrm{SIN-PT}} = -\frac{1}{y} - s^{\mathrm{PT}}$

Expansions for both weak ($V < 2$) and strong ($V > 2$) interaction!

SIN-HF

First order for weak interaction: HF, $s^{\mathrm{HF}} = -\frac{1}{2}uy$

First order for strong interaction: SIN-HF, $s^{\mathrm{SIN-HF}} = -\frac{1}{y} - s^{\mathrm{HF}}$



Conclusions and Outlook

- Unphysical solutions in *ab initio* calculations for real materials.

OPM:

- With a proper constraint $G_0 \leftarrow G$ is unique (LW well-defined)
- 2-particle correlation function indicates when to switch iteration scheme
- Perturbation expansions can be found for both weak and strong interaction

Beyond the OPM:

- Can we find similar analytical results in the Hubbard atom? (Hamiltonian)
- What about the map $v_c \leftrightarrow$ W? ($W < v_c$)

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see also:
Lani *et al.*, New J. Phys. 14, 013056 (2012)
Berger *et al.*, New J. Phys. 16, 113025 (2014)

Defining the domain: static self-energy

Is the following a sufficient constraint for a static self-energy?

$$G_0(\mathbf{r}, \mathbf{r}', \omega) = \sum_s \frac{\phi_s(\mathbf{r})\phi_s^*(\mathbf{r}')}{\omega - \epsilon_s}$$

Suppose the Dyson equation has two solutions G_0 and G_0' (fixed G).
The difference of the two Dyson equations is

$$[G_0']^{-1} = G_0^{-1} - \Sigma[G_0] + \Sigma[G_0']$$

In the diagonal basis of G_0 this becomes

$$[G_0']^{-1} = \delta_{ll'}(\omega - \epsilon_l) - \Sigma_{ll'}[G_0] + \Sigma_{ll'}[G_0']$$

For a static Σ the off-diagonal elements of $[G_0']^{-1}$ must be static too and equal to the $\omega \to \infty$ limit in which they vanish (bounded spectrum).

Therefore G_0 and G_0' are diagonal in the same basis $\to G_0' = G_0$

See also R. Eder, arXiv:1407.6599 (2014)