The one-point model: solving equations in pointland

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- Adrian Stan
- Bernardo Mendoza

Motivation

One-point model (OPM): One point in space, time and spin.

- functions become variables and functionals become functions.

$$f(\mathbf{r}, \sigma, t) \rightarrow f$$
$$F[g(\mathbf{r}, \sigma, t)] \rightarrow F(g)$$

- Integrals and sums can be dropped.

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Features

- retains the structure of the full equations
- insight into the solutions of complicated equations (Kadanaff-Baym; Hedin)
- physics much reduced

Hedin's equations

A closed set of equations for the one-body Green's function.

$$G(1,2) = G_H(1,2) + G_H(1,3)\Sigma_{xc}(3,4)G(4,2)$$

$$\Sigma_{xc}(1,2) = iG(3,2)W(4,2)\Gamma(4,1,3)$$

$$W(1,2) = v_c(1,2) + v_c(1,3)P(3,4)W(4,2)$$

$$P(1,2) = -iG(2,3)G(4,2)\Gamma(1,3,4)$$

$$\Gamma(1,2,3) = \delta(1,2)\delta(1,3) + G(4,5)G(6,7)\frac{\delta\Sigma_{xc}(2,3)}{\delta G(4,7)}\Gamma(1,5,6)$$

Hedin's equations in one point

$G \to y$, $\Sigma_{xc} \to s_{xc}$, $W \to u$, $v_c \to v$, $P \to p$, $\Gamma \to g$.

$$
\begin{aligned}
y &= y_H + y_H s_{xc} y \\
s_{xc} &= yug \\
u &= v + vpu \\
p &= \pm y^2 g \\
g &= 1 + \frac{ds_{xc}(y)}{dy} y^2 g
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$$

Molinari found a perturbative solution using the $+$ sign ($y_H = 1$):

$$s = v_H + s_{xc} = 2v + 10v^2 + 74v^3 + 706v^4 + \cdots$$

The prefactors equal the number of diagrams at each order in v.

Pavlyukh and Hübner found an implicit solution of Hedin's equations ($+$ sign).

Molinari, PRB 71, 113102 (2005); Molinari and Manini, EPJB 51, 331 (2006)
Pavlyukh and Hübner, J. Math. Phys. 48, 052109 (2007)

Kadanoff-Baym equation

A closed equation for the 1-GF is given by the Kadanoff-Baym equation:

$$G(1,2;[\varphi]) = G_0(1,2) + \int d3\, G_0(1,3) v_H(3;[\varphi]) G(3,2;[\varphi])$$
$$+ \int d3\, G_0(1,3)\varphi(3) G(3,2;[\varphi]) + i \int d34\, G_0(1,3) v_c(3^+,4) \frac{\delta G(3,2;[\varphi])}{\delta \varphi(4)}$$

The equilibrium Green's function: $G(1,2) = G(1,2;[\varphi = 0])$

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Functional differential equation is nonlinear due to $v_H = -ivG$.

Linearize v_H around $\phi = 0$.

$$G(1,2;[\tilde{\varphi}]) = G_H(1,2) + \int d3 G_H(1,3)\tilde{\varphi}(3) G(3,2;[\tilde{\varphi}]) + i \int d34 G_H(1,3) W(3^+,4) \frac{\delta G(3,2;[\tilde{\varphi}])}{\delta\tilde{\varphi}(4)}$$

with $W = \epsilon^{-1} v$ and $\tilde{\varphi} = \epsilon^{-1}\varphi$

Lani, Romaniello, Reining, New J. Phys. 14, 013056 (2012)

linearized Kadanoff-Baym equation

Linearized KBE in one point

$$y(x) = y_H + y_H x y(x) + u y_H y'(x).$$

General solution $(x = 0)$:

$$y_u = -\sqrt{\frac{\pi}{2u}} \exp\left[\frac{1}{2uy_H^2}\right]\left\{\mathrm{erf}\left(\sqrt{\frac{1}{2uy_0^2}}\right) + C(y_H, u)\right\}$$

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Initial condition:

$$\lim_{u \to 0} y_u = y_H \quad \longrightarrow \quad C = -1$$

Physical solution

$$y_{phys} = -\sqrt{\frac{\pi}{2u}} \exp\left[\frac{1}{2uy_H^2}\right] \left\{ \operatorname{erf}\left(\sqrt{\frac{1}{2uy_0^2}}\right) - 1 \right\}$$

Lani, Romaniello, Reining, New J. Phys. 14, 013056 (2012)

GW and self-consistency

In one point

$$y = y_H + y_H s_{xc} y$$
$$s_{xc} = -uy$$

Quadratic equation:

$$y = y_H - y_H u y^2 \quad \rightarrow \quad y_u = \frac{\pm\sqrt{1 + 4uy_H^2} - 1}{2uy_H}$$

Physical solution: $+$ ($\lim_{u\to 0} y_u = y_H$)
Unphysical solution: - ($\lim_{u\to 0} y_u \neq y_H$)

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Physical solution: $+$ ($\lim_{u\to 0} y_u = y_H$)
Unphysical solution: - ($\lim_{u\to 0} y_u \neq y_H$)

In practice one iterates to obtain the self-consistent solution.

$$G^{(n+1)} = (1 - \Sigma_{xc}[G^{(n)}]G_H)^{-1} G_H \quad \rightarrow \quad y^{(n+1)} = \frac{y_H}{1 + uy_H y^{(n)}} \quad \rightarrow \quad \textit{physical}$$

$$\Sigma_{xc}[G^{(n+1)}] = G_H^{-1} - [G^{(n)}]^{-1} \quad \rightarrow \quad y^{(n+1)} = -\frac{1}{uy_H} + \frac{1}{uy^{(n)}} \quad \rightarrow \quad \textit{unphysical}$$

Lani, Romaniello, Reining, New J. Phys. 14, 013056 (2012)

GW: exact solutions

So far u (W) and y_H (G_H) were fixed.
What happens if we remove these constraints?

$$u = \frac{v}{1 + vy^2} \qquad y_H = \frac{y_0}{1 + y_0 vy}$$

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The GW Dyson equation in one point is a quartic equation

$$y = \frac{y_0(1 + vy^2)}{1 + vy^2 + y_0 v^2 y^3} \qquad \left(G = [G_0^{-1} - \Sigma_{GW}]^{-1}\right)$$

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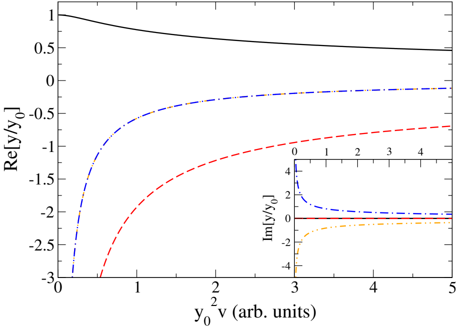
Four solutions: 1 physical + 3 unphysical :



AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

GW: iterative solution

Usually the GW Dyson equation is solved iteratively:

$$y_{n+1} = \frac{y_0(1 + vy_n^2)}{1 + vy_n^2 + y_0 v^2 y_n^3} \qquad \left(G = [G_0^{-1} - \Sigma_{GW}]^{-1}\right)$$

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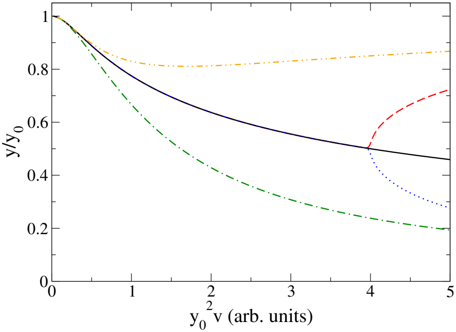
Results :



Beyond a certain interaction strength the iterative result is not equal to physical result

AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

Attracting and repelling fixed points

Attracting fixed point: iteration converges to y_{GW}

Repelling fixed point: iteration does not converge to y_{GW}

Attracting and repelling fixed points

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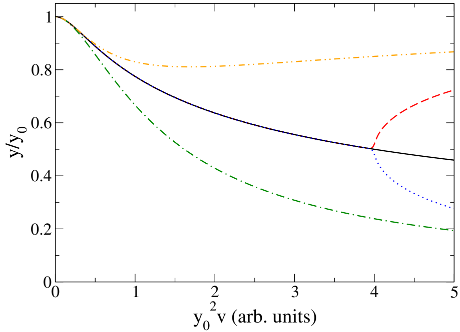
y_{GW} is attracting when $y_0^2 v < 4$ y_{GW} is repelling when $y_0^2 v > 4$



AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

Alternative iteration schemes

Iteration schemes that do converge to y_{GW} for all v are:

$$y_{n+1} = \frac{y_0(1 + 2vy_n^2)}{1 + y_0 v y_n + v y_n^2 + y_0 v^2 y_n^3} \qquad (G = G_0 + G_0 \Sigma_{GW} G)$$

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Or iterate y for fixed u, update u, iterate y, etc.:

$$u_n = \frac{v}{1 + vy_n^2} \qquad \left(W = (1 - v_c GG)^{-1} v_c\right)$$

$$y_{n+1} = \frac{y_0}{1 + y_0(v - u_n)y_n} \qquad \left(G = [G_0^{-1} - \Sigma_{GW_{fixed}}]^{-1}\right)$$

AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

The full KBE

Full (non-linearized) KBE in one point ($\varphi \to z$):

$$y(z) = y_0 - vy_0 y^2(z) + y_0 z y(z) + vy_0 y'(z).$$

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General solution ($z = 0$):

$$y_v = y_0 - C\left[\frac{C}{y_0} + \frac{1}{y_0^2} e^{\frac{1}{2v y_0^2}} \left(C\sqrt{\frac{\pi}{2v}}\mathrm{erf}\left[\frac{1}{\sqrt{2v y_0^2}}\right] - 1\right)\right]^{-1}$$

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The physical solution should tend to y_0 when $v \to 0$:

$$y_{phys} = y_0 \qquad (C = 0)$$

One point KBE: perfect cancellation between the two terms containing v.

Full functional problem: partial cancellation.

AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

Generalized KBE in the one-point model

To mimic the partial cancellation in one point we introduce a parameter λ:

$$y(z) = y_0 - v y_0 y^2(z) + y_0 z y(z) + \lambda v y_0 y'(z).$$

Generalized KBE in the one-point model

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$$y(z) = y_0 - vy_0 y^2(z) + y_0 z y(z) + \lambda v y_0 y'(z).$$

The physical solution for $\lambda = \frac{1}{2}$:

$$y_{phys} = \frac{2y_0}{2 + vy_0^2}$$

Dyson equation:

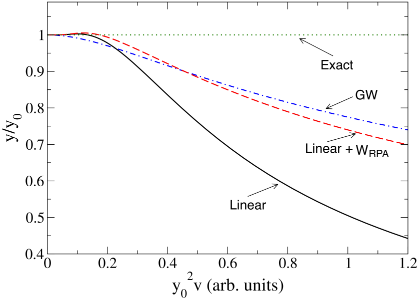
$$y = y_0 + y_0 s y \quad \rightarrow \quad s = -\frac{1}{2} v y_0$$

The exact self-energy is a functional of y_0.

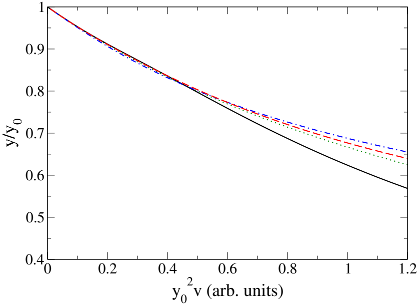
AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

Comparison to approximate methods

$\lambda = 1$



$\lambda = \frac{1}{2}$



$$W_{RPA} = (1 - v_c GG)^{-1} v_c$$

In one point G obtained from the linearized KBE can best be combined with W_{RPA}

AB, Romaniello, Tandetzky, Mendoza, Brouder, Reining, New J. Phys. 16, 113025 (2014)

Tarantino, Mendoza, Romaniello, AB, Reining, J. Phys Condens. Matter 20, 135602 (2018)

Real life: absorption spectrum of LiF from TDDFT

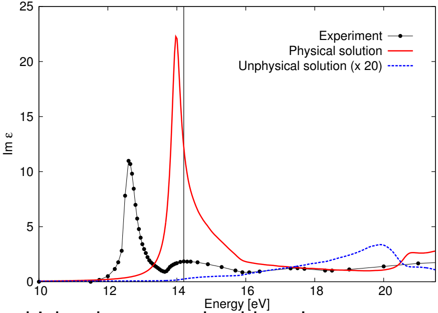
Does this problem occur in real life?

$$\epsilon(\omega) = (1 + v_c\chi(\omega))^{-1}$$

where

$$\chi(\omega) = \chi_0(\omega) + \chi_0(\omega) f_{Hxc}[\chi]\chi(\omega)$$

$$f_{Hxc}[\chi] = v_c + \frac{1 + v_c\chi(\omega = 0)}{\chi_0(\omega = 0)} \qquad \text{bootstrap kernel}$$



The OPM tells us which scheme we should use!

Stan, Romaniello, Rigamonti, Reining, AB, New J. Phys. 17, 093045 (2015)

Uniqueness of the map $G_0 \leftarrow G$

Σ is a well-defined functional of G_0: $\Sigma[G_0]$.
In practice $\Sigma[G] = \Sigma[G_0[G]]$: sum rules and conservation laws.

$\Sigma[G]$: the map $G_0 \leftarrow G$ should be unique

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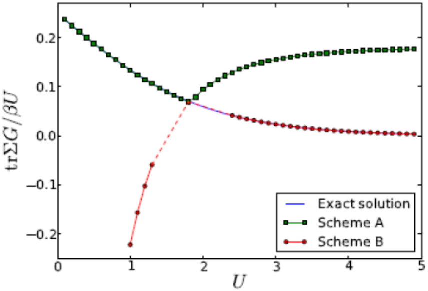
Numerical calculations on Hubbard atom with two iterative schemes.
y axis corresponds to double occupancy



Kozik, Ferrero, Georges, PRL 114, 156402 (2015)

A careful definition of the domain of G_0 and G is missing $\longrightarrow$ unphysical solutions

The map $G_0 \leftarrow G$ in the OPM

Exact self-energy: $\tilde{s}[z_0] = -\frac{1}{2} u z_0$
Dyson equation: $z_0 = y + \frac{1}{2} v y z_0^2$

y is known and z_0 is to be determined.

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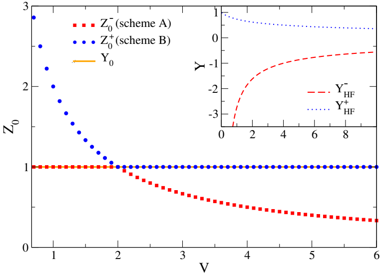
y is known and z_0 is to be determined.

Two solutions:

$$z_0^{\pm} = \frac{1}{vy}\left(1 \pm \sqrt{1 - 2vy^2}\right) \underbrace{\Longrightarrow}_{Z_0 = z_0/y_0;\, V = vy_0^2} Z_0^{\pm} = \frac{2 + V \pm \sqrt{(2-V)^2}}{2V},$$



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

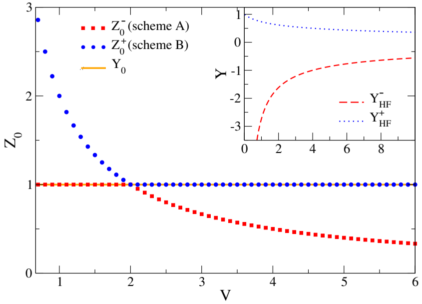
Stan, Romaniello, Rigamonti, Reining, AB, New J. Phys. 17, 093045 (2015)
Rossi and Werner, J. Phys. A 48, 485202 (2015)

Iteration schemes

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

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

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



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

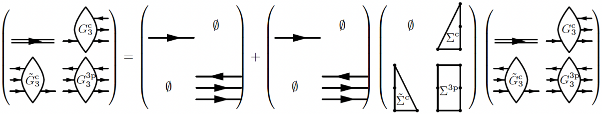
OPM: polarizability χ is critical quantity: changes sign at $V = 2$.

Stan, Romaniello, Rigamonti, Reining, AB, New J. Phys. 17, 093045 (2015)

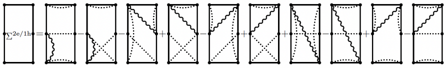
Rossi and Werner, J. Phys. A 48, 485202 (2015)

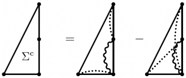
The multi-channel Dyson equation

Coupling G_1 with G_3:



The multi-channel self-energy $\Sigma_3(v_c)$:





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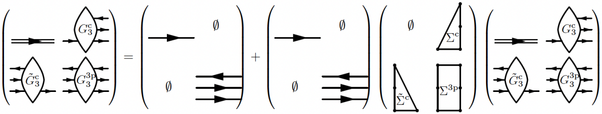

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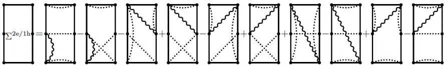

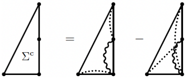

Riva, Romaniello, AB, Phys. Rev. Lett. 131, 216401 (2023)

In one point:

$$\begin{pmatrix} y_1 & y_c \\ \tilde{y}_c & y_3 \end{pmatrix} = \begin{pmatrix} y_0 & 0 \\ 0 & y_0^3/2 \end{pmatrix} + \begin{pmatrix} y_0 & 0 \\ 0 & y_0^3/2 \end{pmatrix} \begin{pmatrix} 0 & 2v \\ 2v & 10v \end{pmatrix} \begin{pmatrix} y_1 & y_c \\ \tilde{y}_c & y_3 \end{pmatrix}$$

Iteration yields the number of skeleton diagrams at each order in v

$$s \propto 2v^2 + 10v^2 + 50v^3 + 250v^4 + \cdots$$

Conclusions

- The OPM simplifiies complicated equations such that they can be solved exactly.
- The OPM can be used to analyse the solutions of these equations
- The OPM can be used to detect and analyse potential problems in finding the physical solution.