Functionals of Green's functions: why and how?

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Palaiseau Theoretical Spectroscopy Group

Functionals of Green's functions: why and how?

1. Life is a functional……..2. of what? …….3. or of what else?
4. To be fair with DFT
5. What we want and what we choose
6. The total energy with Green's functions
7. Other observables
8. The tasks, and…….9. what is really our task?
10. Approximation strategies, ingredients
11. Use of exact constraints
12. Use of generating functional equations
13. A halt on perturbation theory
14. Where to start from?
15. Use of nearsightedness
16. Summary
17. Some suggestions, to be discussed

T=0, N fixed

$$O = \langle \hat{O} \rangle$$

$$O = \int ... \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N) \sum_{i,j,...} O(x_i, x_j, ...) \Psi(x_1, ...x_N)$$

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$$O = \int \ldots \int dx_1 \ldots dx_N \Psi^*(x_1, \ldots . x_N) \sum_{i,j,\ldots} O(x_i, x_j, \ldots) \Psi(x_1, \ldots x_N)$$

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$$O = O[\Psi]$$

$$\Psi \longrightarrow O$$

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$$O = \langle \hat{O} \rangle$$

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_{\alpha} e^{-\beta(E_\alpha - \mu N_\alpha)} \langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle$$

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$$Z = \sum_{\alpha} e^{-\beta(E_\alpha - \mu N_\alpha)}$$

$$O = \langle \hat{O} \rangle$$

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_{\alpha} e^{-\beta(E_\alpha - \mu N_\alpha)} \langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle$$

$$\frac{1}{Z} \mathrm{Tr} \left\{ e^{-\beta(\hat{H} - \mu \hat{N})} \hat{O} \right\}$$

$$\hat{O}$$

$$\hat{H} = -\frac{\hbar^2}{2m_e}\sum_i \nabla_i^2 \quad + \sum_i v_{\text{ext}}(\mathbf{r}_i) \quad + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

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$$O = O[\Psi] \longrightarrow \tilde{O}[v_{\text{ext}}]$$

(and N or chemical potential)

$$O = \frac{1}{Z}\mathrm{Tr}\left\{e^{-\beta(\hat{H}-\mu\hat{N})}\hat{O}\right\}$$

Trace: → huge integrals

→ huge sum

→ operators do not commute in general

→ we didn’t simplify

Strategy!

$O = O[\Psi]$ Simple functional of complicated function

$\tilde{O}[v_{\mathrm{ext}}]$ **Complex functional of simple function**

$$O = O[\Psi]$$

$$\downarrow$$

$$\tilde{O}[v_{\mathrm{ext}}]$$

$$\downarrow$$

$$\mathcal{O}[Q]???$$

$$O = \int ... \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N) \sum_{i,j,...} O(x_i, x_j, ...) \Psi(x_1, ...x_N)$$

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Expectation value of a local one-body operator:

$$O = \int ... \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N) \sum_{i,j,...} O(x_i, x_j, ...) \Psi(x_1, ...x_N)$$

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$$O_1 = \int ... \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N) \sum_{i} O_1(x_i) \Psi(x_1, ...x_N)$$

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$$O_1 = N \int ... \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N) O_1(x_1) \Psi(x_1, ...x_N)$$

$$O_1 = \int dx_1 \, O_1(x_1) \, N \int dx_2 ... dx_N \, \Psi^*(x_1, ...x_N) \Psi(x_1, ...x_N)$$

$$O_1 = \int dx_1 \, O_1(x_1) n(x_1)$$

Only the density is needed!!!

DFT: not only

$$O_1 = \int dx_1 \, O_1(x_1) n(x_1)$$

$$O = O[\Psi]$$

$$\tilde{O}[v_{\text{ext}}]$$

$$\mathcal{O}[n]$$

…….but for all O:

Comparison:

$$O = O[\Psi]$$

* explicit functional known
* input complicated
* input difficult to calculate
* functional difficult to evaluate

$$\tilde{O}[v_{\mathrm{ext}}]$$

* explicit functional known
* input simple
* input known
* functional difficult to evaluate

$$\mathcal{O}[n]$$

* explicit functional (often) unknown
* input simple
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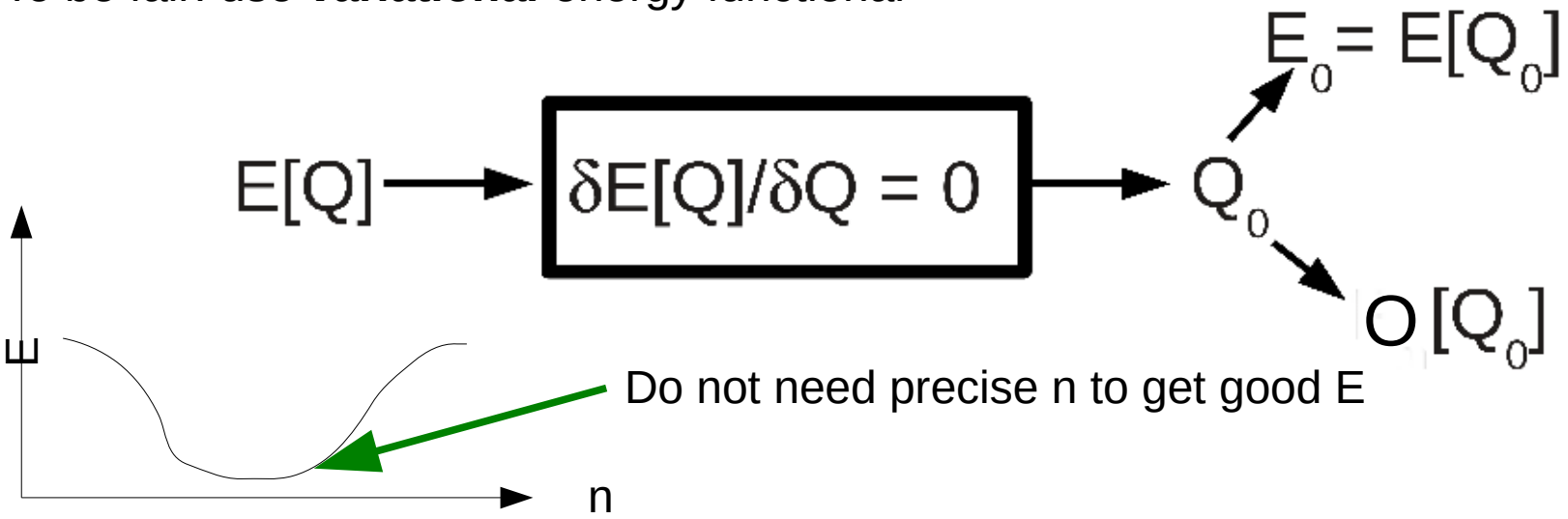
$$\mathcal{O}[n]$$

* explicit functional (often) unknown
* input simple
* input difficult to calculate
* functional difficult to evaluate?

To be fair: use **variational** energy functional



BUT: other O not variational → need good n → need good fctl E[n], so:

$$\mathcal{O}[n]$$

* explicit functional for O (often) unknown
* input simple, known how to calculate
* for this, energy functional also needed
* functional difficult to evaluate?

“DFT leads to efficient calculations…..”

Proposed reformulation:

“We hope that DFT helps us to find approximations
that lead to efficient calculations…..”

“……for n and/or E[n] ……and maybe other O[n]…..”

Note: Hartree helps

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Expectation value of the kinetic energy operator:

$$O = \int \ldots \int dx_1 \ldots dx_N \, \Psi^*(x_1, \ldots . x_N) \sum_{i,j,\ldots} O(x_i, x_j, \ldots) \Psi(x_1, \ldots x_N)$$

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$$E_{\text{kin}} = -\int \ldots \int dx_1 \ldots dx_N \, \Psi^*(x_1, \ldots . x_N) \sum_{\cdot} \frac{\nabla_i^2}{2} \Psi(x_1, \ldots x_N)$$

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$$= -\int dx_1 \left[\frac{\nabla_1'^2}{2} N \int \ldots \int dx_2 \ldots dx_N \, \Psi^*(x_1, \ldots . x_N) \Psi(x_1', x_2, \ldots x_N) \right]_{|x_1' \to x_1}$$

$$= -\int dx_1 \left[\frac{\nabla_1'^2}{2} \rho(x_1, x_1') \right]_{|x_1' \to x_1}$$

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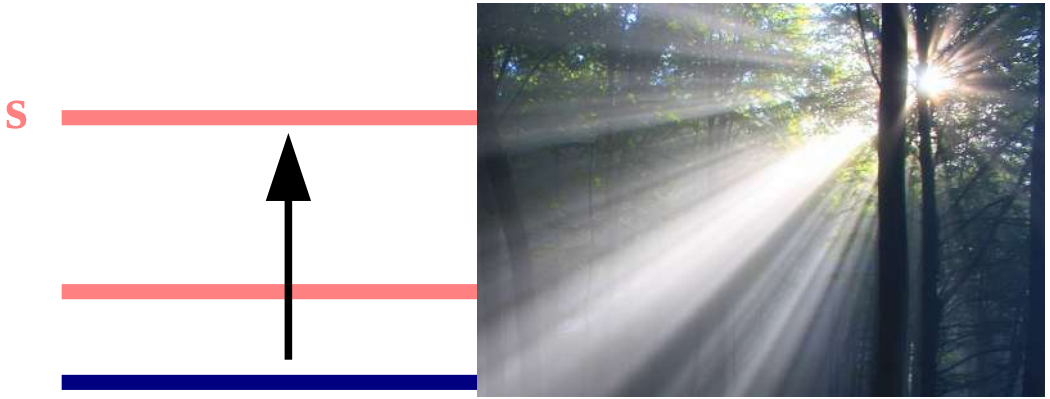
Suggests RDMFT

$$= -\int dx_1 \left[\frac{\nabla_1'^2}{2} \rho(x_1, x_1') \right]_{|x_1' \to x_1}$$

Spectroscopy: have to describe transitions

$$f_{ds}(t) = N \int dx_1 ... dx_N \, \Psi^*(x_1, ...x_N; t) d(x_1) e^{i\omega t} \Psi_s(x_1, ...x_N; t)$$



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Phase factor: excitation energy

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For the transition amplitude

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Phase factor: excitation energy

For the transition amplitude

$$G^{>}(x_1, x_2, \omega) = -2\pi i \sum_{\alpha\lambda} \omega_\alpha \mathrm{f}_{\alpha\lambda}(x_1) \mathrm{f}^*_{\alpha\lambda}(x_2) \delta(\omega + E_\alpha - E_\lambda)$$

$$\mathrm{f}_{\alpha\lambda}(x_1) = \langle \alpha | \hat{\psi}(x_1) | \lambda \rangle$$

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Spectroscopic observables are more easily expressed as functionals of Green's functions

Phase factor: $e^{i\omega t}$ energy

→ GFFT

For the transition amplitude

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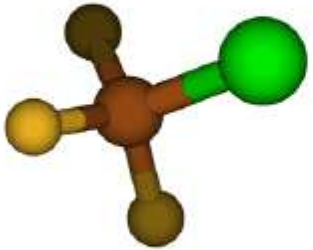
$$G(x_1, x_1', t, t') = -i\langle N|T[\hat{\Psi}(x_1, t)\hat{\Psi}^\dagger(x_1', t')]|N\rangle$$

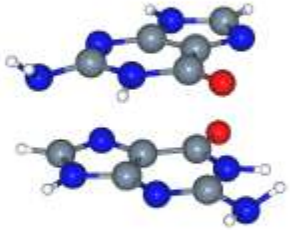
$\Psi(x_1, x_2, ..., x_N; t)$

CI, QMC



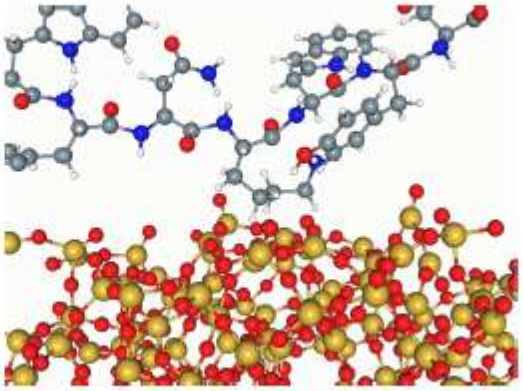
$G(x_1, x_1', t, t')$

Green's Functions



$n(\mathbf{r}; t)$

Density Functionals



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Simple expression for expectation values of 1-body operators...

$$\langle \hat{O} \rangle = -i \int dx_1 \, O(x_1) \lim_{t' \to t^+} G^T(x_1, t; x_1, t')$$

$$\rho(x_1, x_2) = -iG^T(x_1, t, ; x_2, t^+)$$

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...and for the total energy (Galitskii-Migdal):

$$E = \frac{1}{2} \int dx \lim_{t' \to t^+} \left[\frac{\partial}{\partial t} - ih(x) \right] G(x, t, x', t')_{x' \to x}$$

V. M. Galitskii and A. B. Migdal, “Application of quantum field theory methods to the many body problem [translation: Soviet Phys. JETP 7, 96–104 (1958)],” Zh. Eksp. Teor. Fiz. 34:139–150, 1958.

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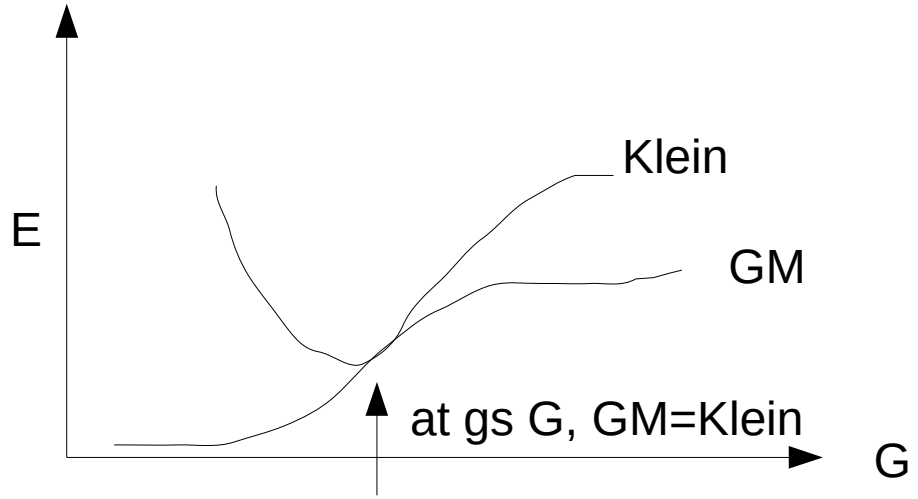
Explicit, simple, but…...NOT variational!

Variational functional:

$$\Omega_{Klein}[G] = \Phi[G] - \mathfrak{Tr}(G_0^{-1}G - 1) - \mathfrak{Tr}\ln(G_0 G^{-1}) + \Omega^0$$

A. Klein, “Perturbation theory for an infinite medium of fermions. II,” Phys. Rev. 121:950, 1961



Others possible, of course (e.g. LW)

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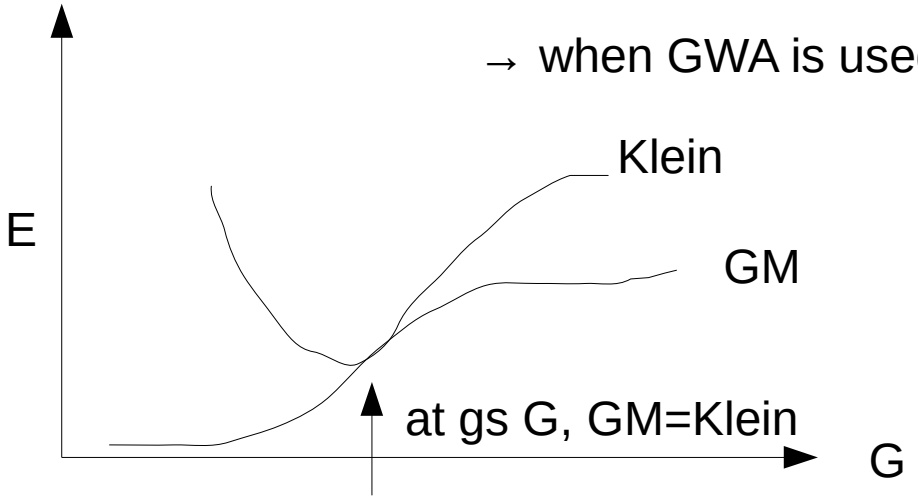
Remarks:

→ at solution flat, but not shown to be a minimum

→ since variational, can evaluate e.g. with i.p. GF

→ still have to find xc functional

→ when GWA is used, KS GF yields DFT-RPA



Others possible, of course (e.g. LW)

$$\Sigma = \frac{\delta \Phi}{\delta G}$$

Plays the role of xc potential.

$$G = (G_0^{-1} - \Sigma)^{-1}$$

Plays the role of KS equations
(that can be formulated as Dyson eqs)

Theory	Kohn–Sham DFT	$G-\Sigma$ functionals
Quantity calculated	Static density $n(\mathbf{r})$	Dynamic Green's function $G(\mathbf{r},\mathbf{r}',\omega)$
Approach	Auxiliary system of independent particles with static local potential $v_{\mathrm{xc}}(\mathbf{r})$	System described by dynamic non-local self-energy $\Sigma(\mathbf{r},\mathbf{r}',\omega)$
Exact formulation	Universal $\Omega_{\mathrm{xc}}[n]$ $v_{\mathrm{xc}}(\mathbf{r})=\frac{\delta\Omega_{\mathrm{xc}}}{\delta n(\mathbf{r})}$	Luttinger–Ward $\Phi[G]$ $\Sigma(\mathbf{r},\mathbf{r}',\omega)=\frac{\delta\Phi}{\delta G(\mathbf{r},\mathbf{r}',\omega)}$

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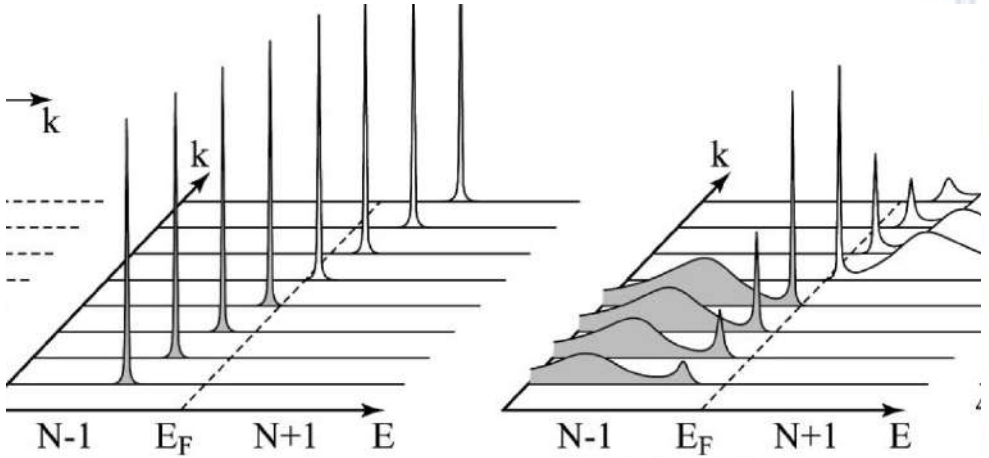
Spectral function

$$A_{\mathbf{k}}(\omega) = \frac{1}{\pi} |\mathrm{Im}\, G_{\mathbf{k}}(\omega)|$$



From Damascelli et al., RMP 75, 473 (2003)

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$$\tilde{\mathcal{O}}[G]$$

* more explicit functionals known, including E and A
* input reasonably simple, known how to calculate
* for this, **variational** energy functional also needed
* functional difficult to evaluate

for other observables?

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$\tilde{\mathcal{O}}[G]$

* more explicit functionals known, including E and A
* input reasonably simple, known how to calculate
* for this, **variational** energy functional also needed
* functional difficult to evaluate for oter observables?

→ approximate E[G] or directly the self-energy

→ from this, calculate G (or find G from elsewhere)

→ if needed, approximate the functional expression $\tilde{\mathcal{O}}[G]$

→ evalulate $\tilde{\mathcal{O}}[G]$ at the correct *G*

$\tilde{\mathcal{O}}[G]$

* more explicit functionals known, including E and A
* input reasonably simple, known how to calculate
* for this, **variational** energy functional also needed
* functional difficult to evaluate?

→ approximate E[G] or directly the self-energy

→ from this, calculate G (or find G from elsewhere)

→ if needed, approximate the functional expression $\tilde{\mathcal{O}}[G]$

→ evalulate $\tilde{\mathcal{O}}[G]$ at the correct *G*

Note: the $\tilde{\mathcal{O}}[G]$ that we know explicitly are all linear in *G*

→ what is really our task?

→ approximate E[G] or directly the self-energy

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→ *Only simple approximations are useful.*
We know the exact results already.

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→ *Only simple approximations are useful. We know the exact results already.*

Holds for all MB theories.

→ what is really our task?

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→ if needed, approximate the functional expression $\tilde{\mathcal{O}}[G]$

→ evalulate $\tilde{\mathcal{O}}[G]$ the correct *G*

→ *Only simple approximations are useful.*
We know the exact results already.

Note: "DFT is computationally simple"
……only because of the simple approximations

Functionals of Green's functions: why and how?

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My favorite approximation strategies:

→ Use of exact constraints

→ Use of generating functional equations

→ Perturbation Theory, starting from a…….

→ ……..model

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Use of exact constraints daily bread in DFT, see e.g.

"strongly constrained and appropriately normed" (SCAN) meta-GGA
(17 exact constraints!)
Sun, J., Ruzsinszky, A., and Perdew, J.P.,PRL 115, 036402 (2015).

Less so, I would say, in GFFT
(with exceptions, of course, e.g. Y. Takada PRL 87, 226402 (2001).

But one often used constraint: symmetries → conservation laws
(particle number, total momentum, total angular momentum, total energy)

$$\Sigma = \frac{\delta \Phi}{\delta G}$$, with xc functional built following diagrammatic rules, leads to fulfillment of conservation laws.

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Problem: beyond the first order approximations, these approx violate other exact constraints
→ they may give negative spectral functions

G. Stefanucci, Y. Pavlyukh, A.-M. Uimonen, and R. van Leeuwen, “Diagrammatic expansion for positive spectral functions beyond GW: Application to vertex corrections in the electron gas,” Phys. Rev. B 90:115134, 2014, and later work.

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A. D. Jackson and R. A. Smith, “High cost of consistency in Green’s-function expansions,” Phys. Rev. A 36:2517–2518, 1987.

→ You must choose what is the most important physics for your application

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From EoM and generating functional

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3})\left\{[u(\bar{3}) + v_{Hu}(\bar{3})]G_u(\bar{3},2) + iv_c(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)}\right\}$$

$$1 \equiv (\mathrm{r}_1, \sigma_1, t_1) \qquad f(\bar{1})g(\bar{1}) \equiv \int d1\, f(1)g(1) \qquad G_u \equiv G[u]$$

$$v_H(3) = -iv_c(3-\bar{5})G(\bar{5},\bar{5}^+)$$

J. Schwinger, PNAS. 37: 452 (1951)

L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, W. A. Benjamin, New York, 1964

R.M. Martin, L. Reining, D.M. Ceperley, “Interacting Electrons:Theory and Computational Approaches”, Cambridge (2016)

Giovanna Lani, Pina Romaniello, Arjan Berger, Matteo Guzzo, Adrian Stan, Lorenzo Sponza, Christine Giorgetti, Matteo Gatti, Walter Tarantino, Bernardo Mendoza, J. Sky Zhou, Marilena Tzavala, Stefano Di Sabatino, Pierluigi Cudazzo, John Rehr, Joshua Kas

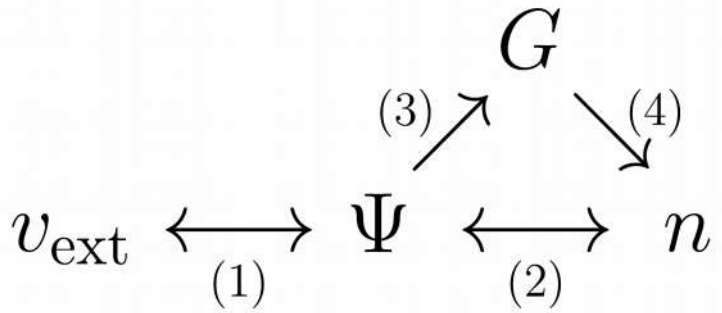
Note: for DFT and RDMFT, see R. Fukuda et al., Progress of Theoetical Physics 92, 833 (1994)

Why not solve it with an ansatz?

But: additional difficulty with interacting Green's functions: what is a Green's function?

→ problem to define the domain

$$G(1,2) \equiv -i \langle \Psi_0 | \mathbf{T}[\hat{\psi}(1)\hat{\psi}^\dagger(2)] | \Psi_0 \rangle$$



$$n(x_1,t) = \langle N|\hat{\Psi}^\dagger(x_1,t)\hat{\Psi}(x_1,t)|N\rangle = -iG(x_1,x_1,t,t^+)$$

→ Change off-diagonals: cannot be "GF"

→ Even for a non-interacting GF,
which energies and wavefunctions belong to a local potential?

$$G_0^T(x_1,x_2,\omega) = \lim_{\eta\to 0^+} \sum_\ell \frac{\psi_\ell(x_1)\psi_\ell^*(x_2)}{\omega - \varepsilon_\ell + i\eta\,\mathrm{sgn}(\varepsilon_\ell - \mu)}$$

Common approximations

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3})\left\{[u(\bar{3}) + v_{Hu}(\bar{3})]G_u(\bar{3},2) + iv_c(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)}\right\}$$

$$\frac{\delta G(3,2)}{\delta u(4)} = -G(3,\bar{5})\frac{\delta G^{-1}(\bar{5},\bar{6})}{\delta u(4)}G(\bar{6},2) \approx G(3,4)G(4,2)$$

$$G_u(1,2) \approx G^0(1,2) + G^0(1,\bar{3})\{[u(\bar{3}) + v_{Hu}(\bar{3})]G_u(\bar{3},2) + iv_c(\bar{3},\bar{4})G(\bar{3},\bar{4})G(\bar{4},2)\}$$

Fock self-energy ($u \rightarrow 0$)

Common approximations

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3})\left\{[u(\bar{3}) + v_{Hu}(\bar{3})]G_u(\bar{3},2) + iv_c(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)}\right\}$$

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$$u_{\rm cl}(1) = u(1) + v_{Hu}(1)$$

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3})u_{\rm cl}(\bar{3})G_u(\bar{3},2) + iG^0(1,\bar{3})v_c(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)}$$

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$$G(1,2) = G^0(1,2) + G^0(1,\bar{3})u_{\rm cl}(\bar{3})G_u(\bar{3},2) + iG^0(1,\bar{3})W_u(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u_{\rm cl}(\bar{4}^+)}; \quad G_u(\bar{3},\bar{4}^+)G_u(\bar{4}^+,2)$$

GW approx. ($u \to 0$)

Common approximations

$$G(1,2) = G^0(1,2) + G^0(1,\bar{3})u_{\rm cl}(\bar{3})G_u(\bar{3},2) + iG^0(1,\bar{3})W_u(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u_{\rm cl}(\bar{4}^+)}$$

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G^0 Σ G

Dyson equation: approximate Σ

Hedin's equations

L. Hedin, “New method for calculating the one-particle Green’s function with application to the electron-gas problem,” Phys. Rev. 139:A796–823, 1965

$$G_u(1,1') = G_{\rm cl}(1,1') + iG_{\rm cl}(1,\bar{2})W_u(\bar{2},\bar{3})\frac{\delta G_u(\bar{2},1')}{\delta u_{\rm cl}(\bar{3}^+)}$$

Can be solved exactly in linear response and for the case of isolated orbital

$$G(\tau) = G_{\rm cl}(\tau)\mathcal{F}(\tau) \qquad \mathcal{F}(t_1 - t_2) = \exp\left[-i\int_{t_1}^{t_2} dt' \int_{t'}^{t_2} dt'' \, \mathcal{W}(t't'')\right]$$

$$A(\omega) = \frac{\Gamma}{\pi} e^{-\frac{\lambda}{\omega_p^2}} \left[\frac{1}{(\omega - \varepsilon^{QP})^2 + \Gamma^2} + \right.$$
$$+ \frac{\lambda}{\omega_p^2} \frac{1}{(\omega - \varepsilon^{QP} + \omega_p)^2 + \Gamma^2} +$$
$$+ \frac{1}{2}\left(\frac{\lambda}{\omega_p^2}\right)^2 \frac{1}{(\omega - \varepsilon^{QP} + 2\omega_p)^2 + \Gamma^2} +$$
$$\left. + \frac{1}{6}\left(\frac{\lambda}{\omega_p^2}\right)^3 \frac{1}{(\omega - \varepsilon^{QP} + 3\omega_p)^2 + \Gamma^2} + \ldots \right]$$

indep. of $u_{\rm cl}$

$$G_u(1,1') = G_{\rm cl}(1,1') + iG_{\rm cl}(1,\bar{2})W_u(\bar{2},\bar{3})\frac{\delta G_u(\bar{2},1')}{\delta u_{\rm cl}(\bar{3}^+)}$$

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Functional of $\Sigma_{\rm GW}$

$$A(\omega) = \frac{\Gamma}{\pi} e^{-\frac{\lambda}{\omega_p^2}}\left[\frac{1}{(\omega-\varepsilon^{QP})^2+\Gamma^2} + \right.$$
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$$\left. + \frac{1}{6}\left(\frac{\lambda}{\omega_p^2}\right)^3 \frac{1}{(\omega-\varepsilon^{QP}+3\omega_p)^2+\Gamma^2} + \ldots\right]$$

indep. of $u_{\rm cl}$

→ Cumulant expansion in bosons

L. Hedin, Physica Scripta **21**, 477 (1980), ISSN 0031-8949.
L. Hedin, J. Phys.: Condens. Matter **11**, R489 (1999).
P. Nozieres and C. De Dominicis, Physical Review **178**, 1097 (1969), ISSN 0031-899X.
D. Langreth, Physical Review B **1**, 471+ (1970).

Sodium: Aryasetiawan et al., PRL 77, 19

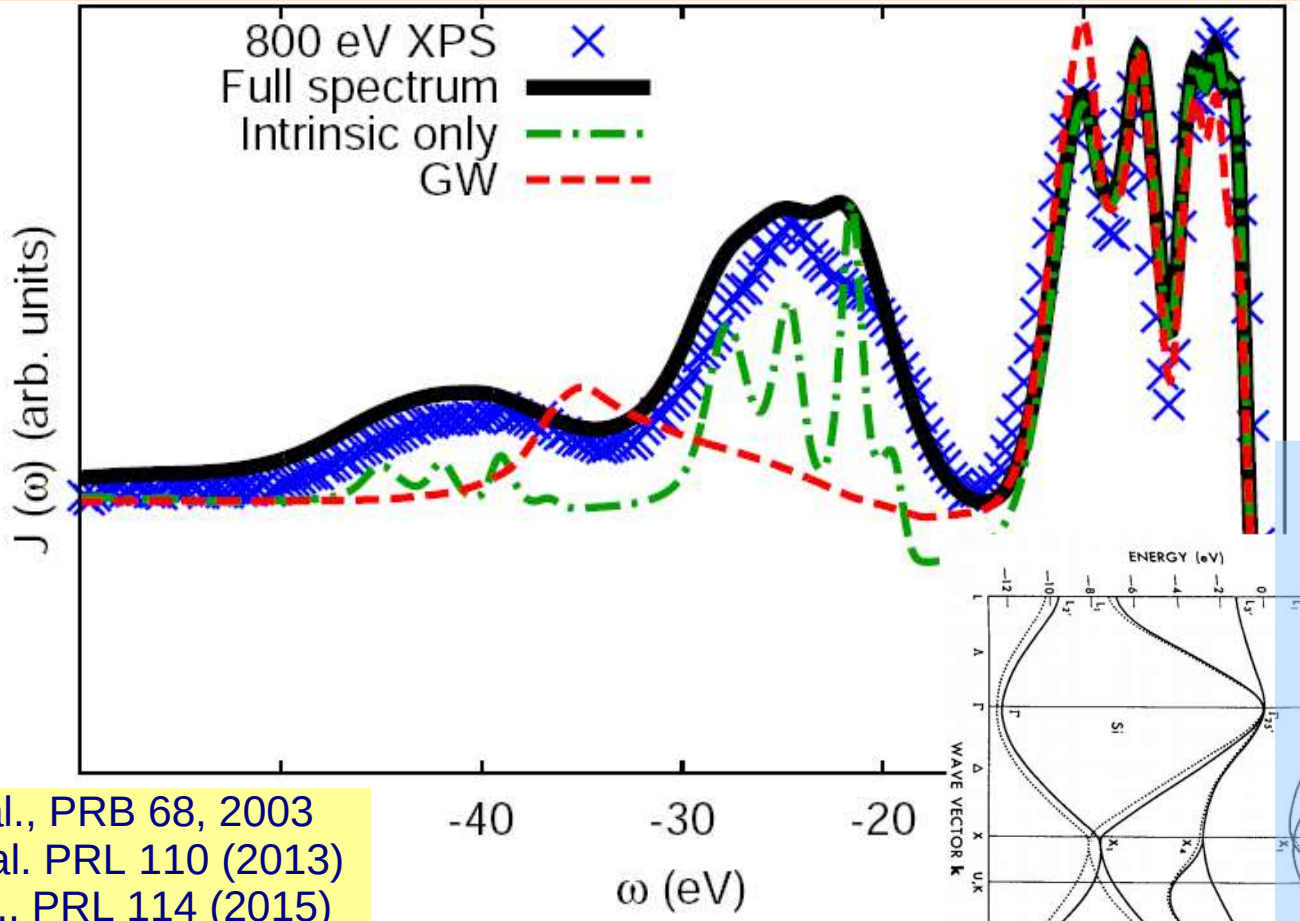
Silicon: Kheifets et al., PRB 68, 2003

In DMFT context: Casula, Rubtsov, Biermann, PRB 85, 035115 (2012)

Here: → the first in a series of approximations
→ link to GW
→ prescription for ingredients

→ The one-body spectral function of silicon

M. Guzzo et al., PRL 107, 166401 (2011) in collab. with J. Kas and J. Rehr, M. Silly and F. Sirotti



Kheifets et al., PRB 68, 2003
Lischner et al. PRL 110 (2013)
Caruso et al., PRL 114 (2015)

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Isolated orbital:

Marilena Tzavala et al., “Nonlinear response in the cumulant expansion for core-level photoemission”,
Phys. Rev. Research 2, 033147 (2020)

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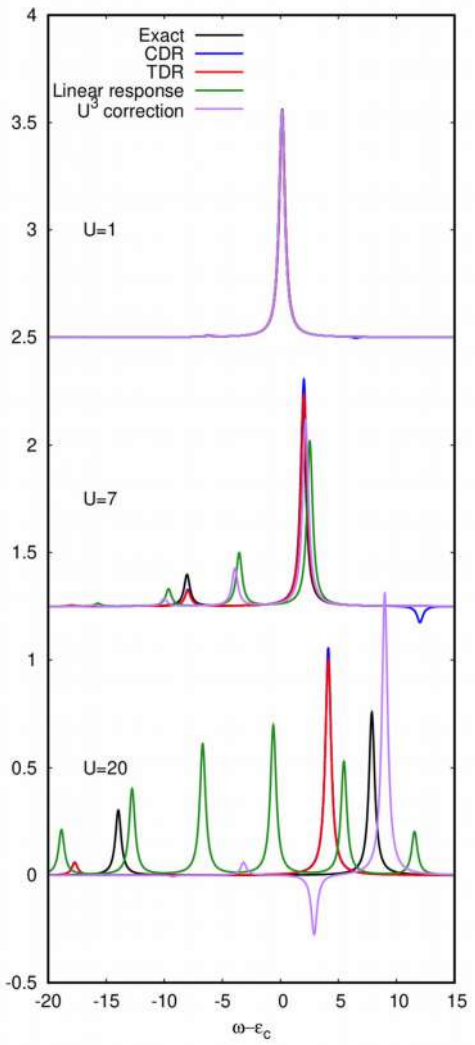
Phys. Rev. Research 2, 033147 (2020)

$$\hat{H} = \epsilon_0 \hat{c}^\dagger \hat{c} + \epsilon_a^0 \hat{n}_a + \epsilon_b^0 \hat{n}_b - U\hat{n}_h\hat{n}_a - t(\hat{c}_a^\dagger \hat{c}_b + \hat{c}_b^\dagger \hat{c}_a)$$



Functionals of Green's functions: why and how?

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Iteration → perturbation series

* in v or W or whatsoever you want (there is not THE perturbation expansion)

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Iteration → perturbation series

* in v or W or whatsoever you want (there is not THE perturbation expansion)

* how good is PT? Problems?

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3}) \left\{ [u(\bar{3}) + v_{Hu}(\bar{3})] G_u(\bar{3},2) + i v_c(\bar{3},\bar{4}) \frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)} \right\}$$

$$y(z) = y_0^0 + y_0^0 z y(z) - y_0^0 \nu y(z) y(z) + \frac{1}{2} y_0^0 \nu \frac{dy}{dz}$$

Giovanna Lani, Pina Romaniello, Lucia Reining, New Journal of Physics 14 (2012) 013056
Arjan Berger et al., New Journal of Physics 16 (2014) 113025
Adrian Stan et al., New Journal of Physics 17 (2015) 093045
Walter Tarantino et al 2018 J. Phys.: Condens. Matter 30 135602

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→ Multiple solutions. Good one? What are the others?

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$$y(z) = \left[\frac{1}{y_0(z)} + \frac{v y_0(z)}{2}\left(1 + \frac{y_0(z)\sqrt{\frac{v}{\pi}}\exp\left[-\frac{1}{v y_0^2(z)}\right]}{\operatorname{erf}\left[\frac{1}{\sqrt{v y_0^2(z)}}\right] - \frac{1}{C\left(v, y_0^0\right)}}\right)^{-1}\right] .$$

$$y_0(z) = y_0^0 + y_0^0 z y_0(z)$$

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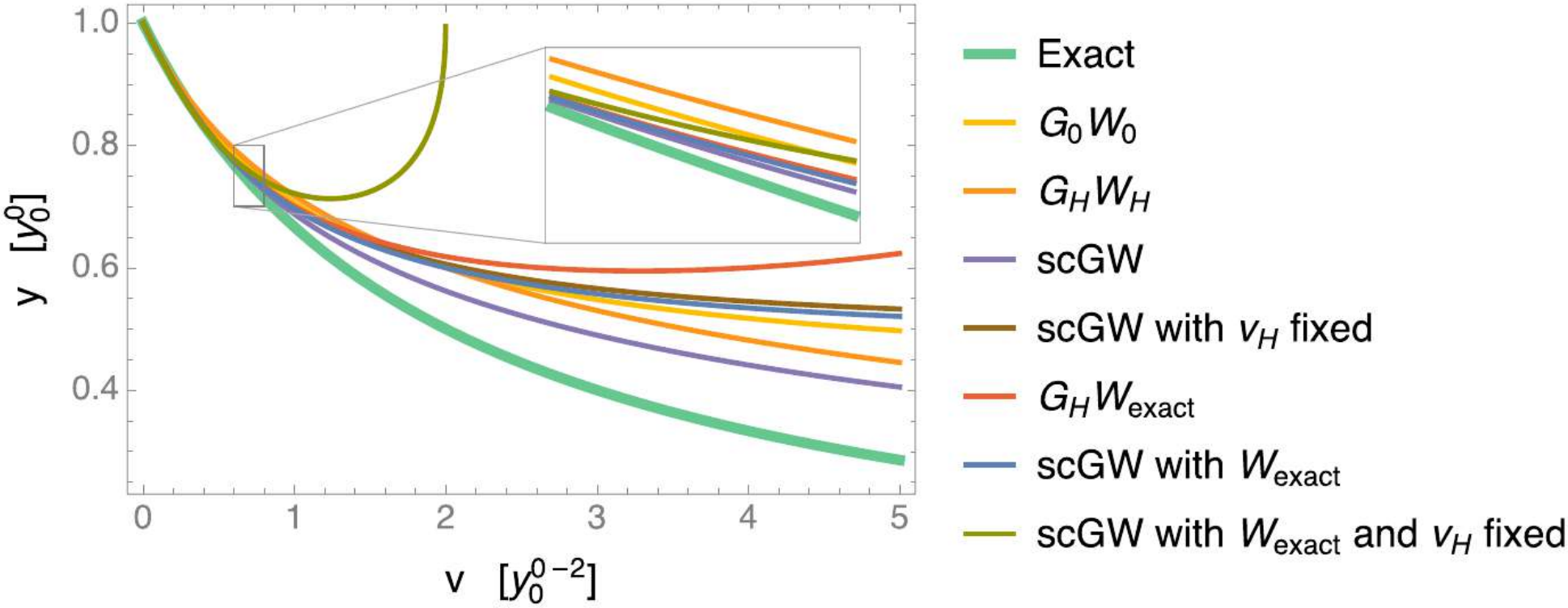
* Asymptotic expansion of error function
* Assume *C* Taylor expandable

} $C = 0$

"Physical solution": $y(z) = \dfrac{2y_0(z)}{2 + \nu y_0^2(z)}$ $\qquad y_\nu(z) = y_0(z) \sum_{n=0}^{\infty} \left(-\dfrac{y_0^2(z)}{2} \nu \right)^n$

Yields perturbation expansion

Model to understand behavior



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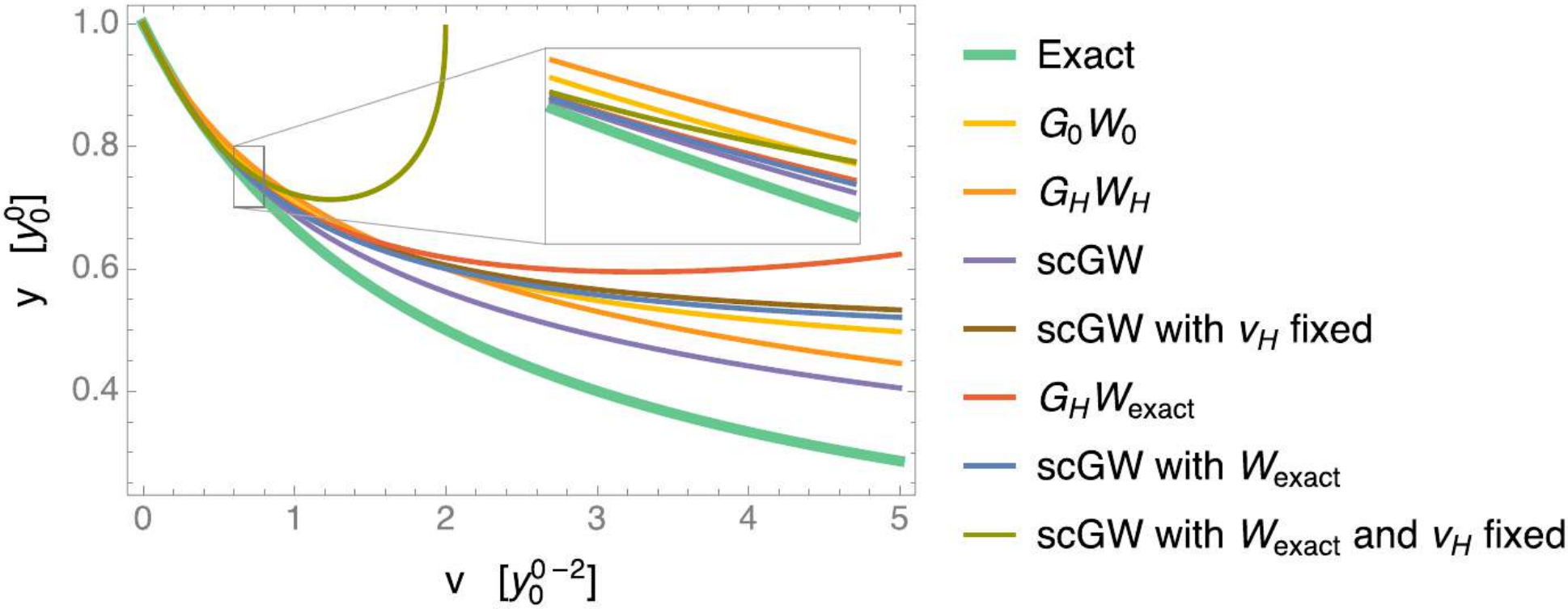
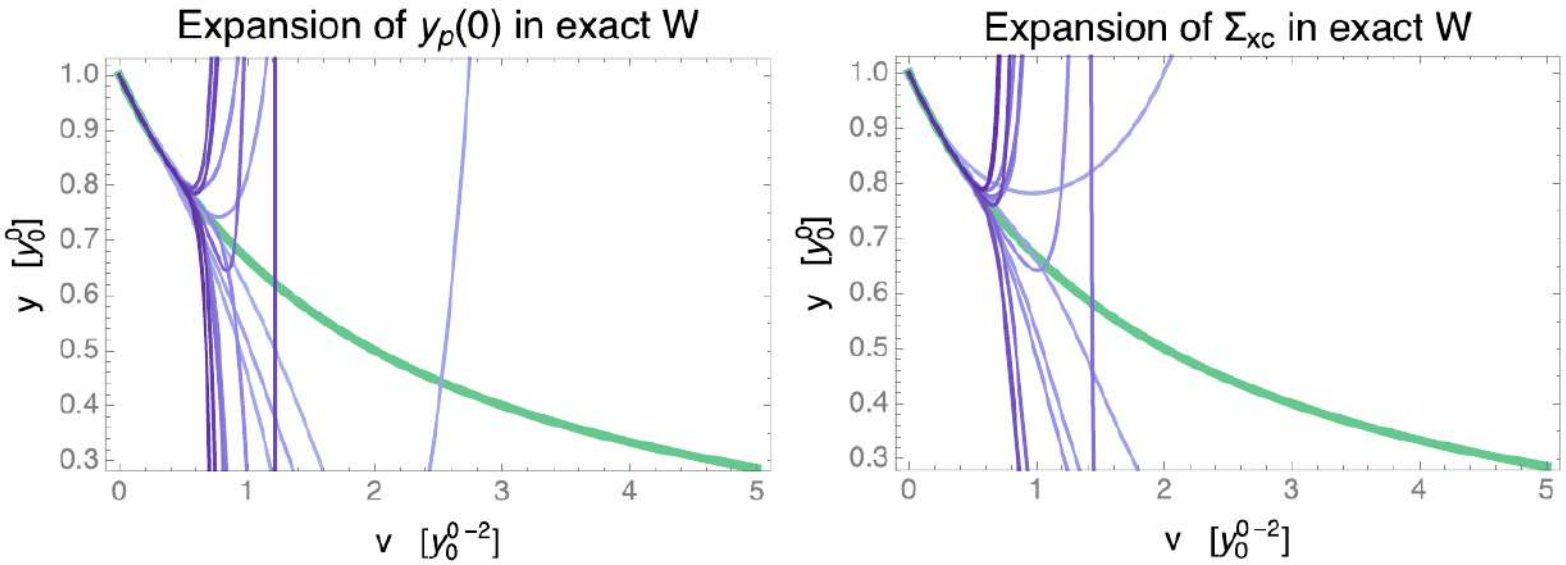


Asymptotic convergence

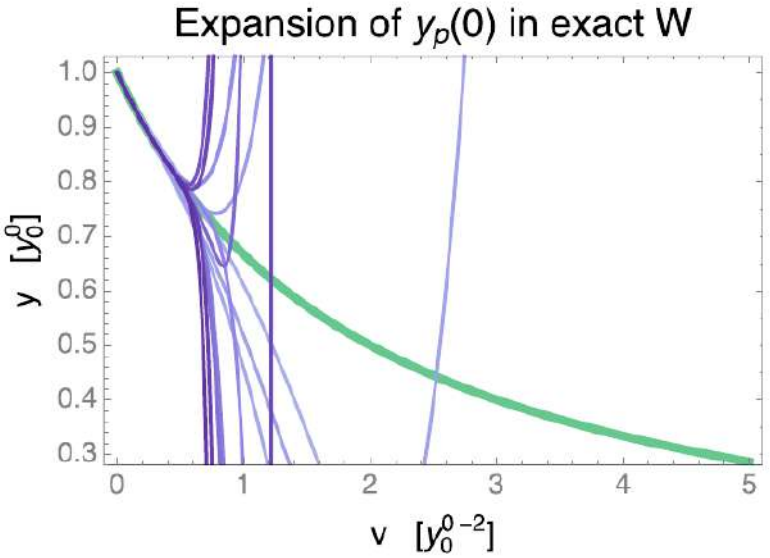
Model to understand behavior

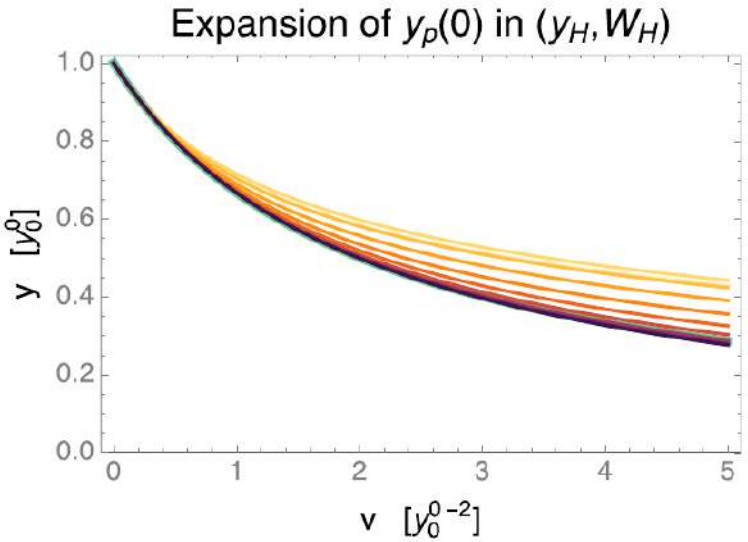


W. Tarantino et al., J. Phys.: Condens. Matter 30 (2018) 135602

Model to understand behavior

Expansion in screened interaction





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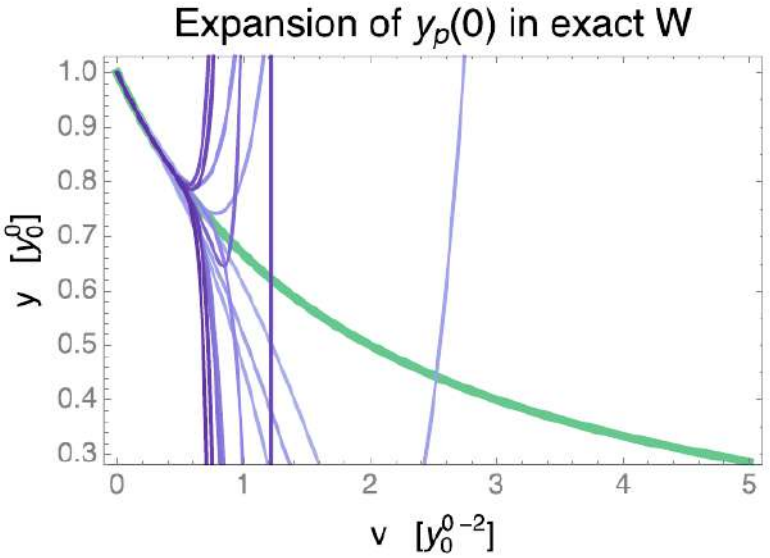
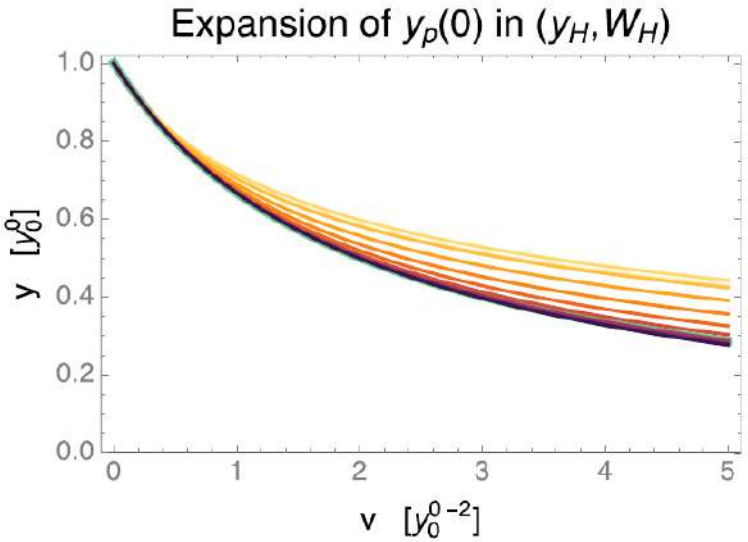




W. Tarantino et al., J. Phys.: Condens. Matter 30 (2018) 135602

RPA-like (to be interpreted in full problem) interaction seems good choice

Iteration → perturbation series

* in v or W or whatsoever you want

* this is a perturbation series for G. Could also decide to iterate for self-energy:

From the EoM.....

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3})\left\{[u(\bar{3}) + v_{Hu}(\bar{3})]G_u(\bar{3},2) + iv_c(\bar{3},\bar{4})\frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)}\right\}$$

.....and the definition of Σ

$$G(1,2) = G_0(1,2) + iG_0(1,\bar{3})\Sigma(\bar{3},\bar{5})G(\bar{5},2)$$

Derive the differential equation for the self-energy:

$$\Sigma(1,2) = iv_c(1,\bar{4})M^{-1}_{1\bar{3};\bar{4}\bar{4}}G^{-1}(\bar{3},2)$$

with $$M_{\alpha\beta;\gamma\delta} \equiv \left(G^{-1}(\alpha,\gamma)G^{-1}(\delta,\beta) - \frac{\delta\Sigma(\alpha,\beta)}{\delta G(\gamma,\delta}\right)$$

→ This creates the functional(s) Σ(G)! How many?

→ Multiple solutions. Good one? What are the others?

$$y(z) = y_0^0 + y_0^0 z y(z) - y_0^0 \nu y(z) y(z) + \frac{1}{2} y_0^0 \nu \frac{dy}{dz}$$

$$G_u(1,2) = G^0(1,2) + G^0(1,\bar{3}) u_{\rm cl}(\bar{3}) G_u(\bar{3},2) + i G^0(1,\bar{3}) v_c(\bar{3},\bar{4}) \frac{\delta G_u(\bar{3},2)}{\delta u(\bar{4}^+)}$$

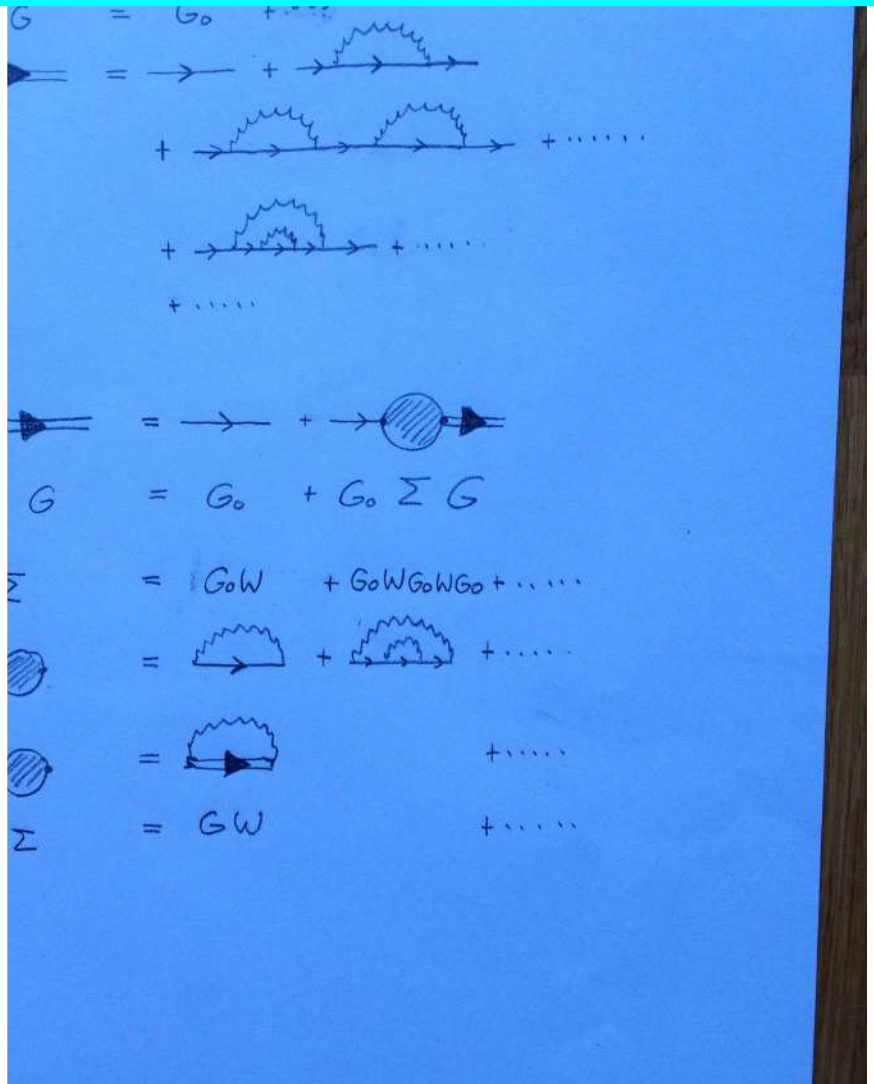
→ Full problem: even more solutions since

$$i v_c(3,\bar{4}) \frac{\delta G_u(3,2)}{\delta u(\bar{4}^+)} = G_0^{-1}(3,\bar{1}) G(\bar{1},2) - \delta(3,2) - u_{\rm cl}(3) G_u(3,2)$$

→ How to specify the conditions “continuity” and “fctl derivative”?

→ Parametrize “good G's”.....**domain?**

→ From $\Sigma[G^0]$ to $\Sigma_b[G]$: is bold perturbation theory valid?



$G[G_0,W]$

$\Sigma = S[G_0,W]$

$\Sigma = S'[G,W]$

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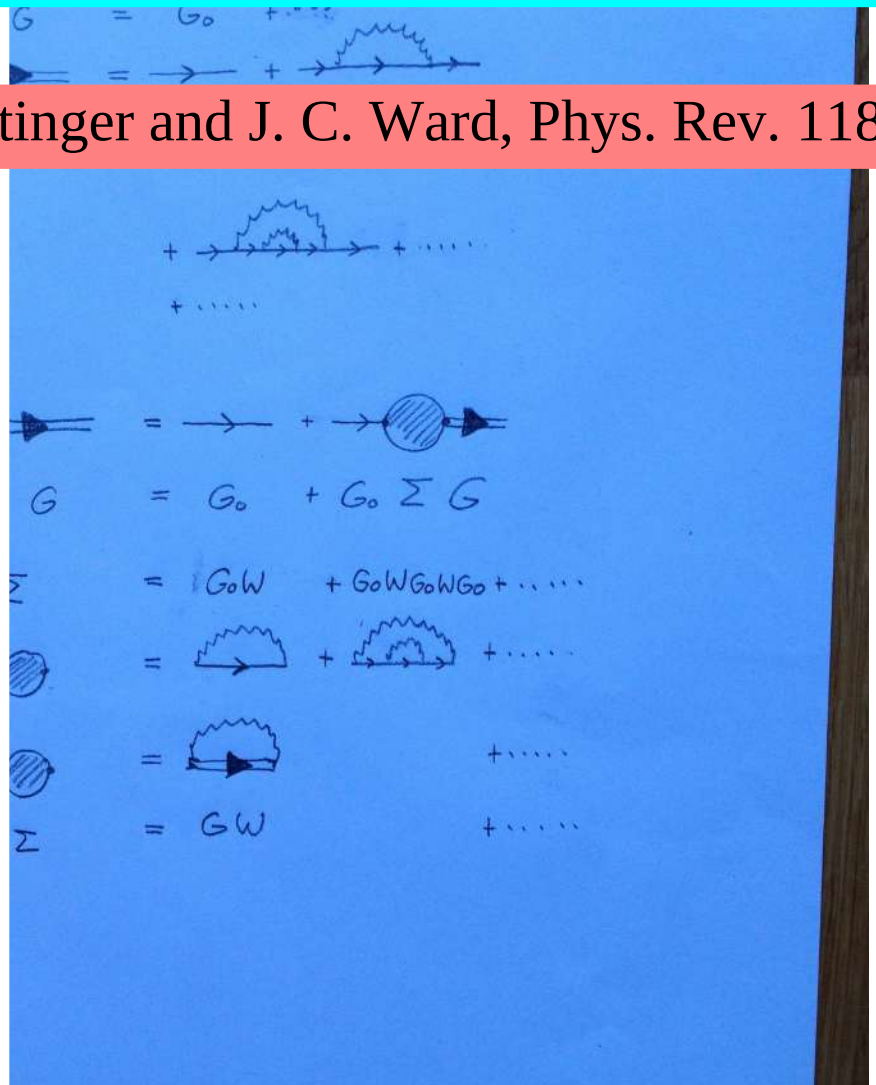
J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960)



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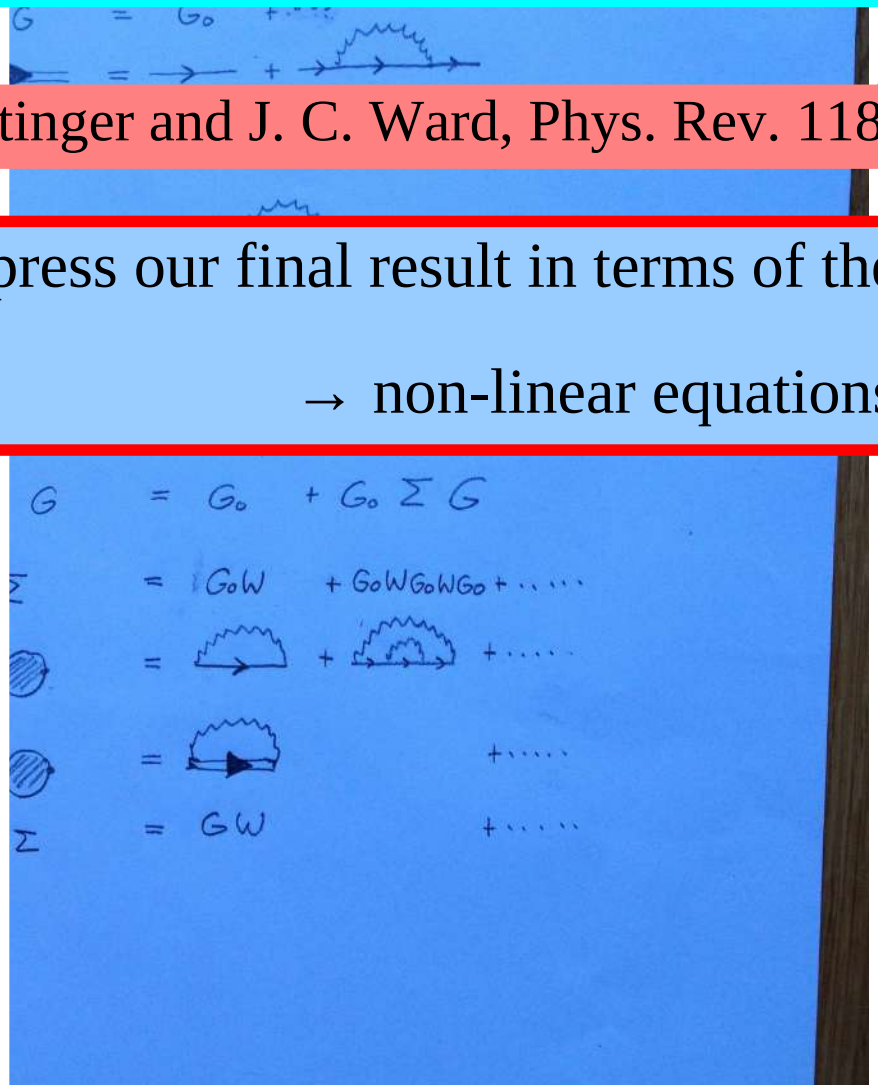

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We express our final result in terms of the final result

→ non-linear equations

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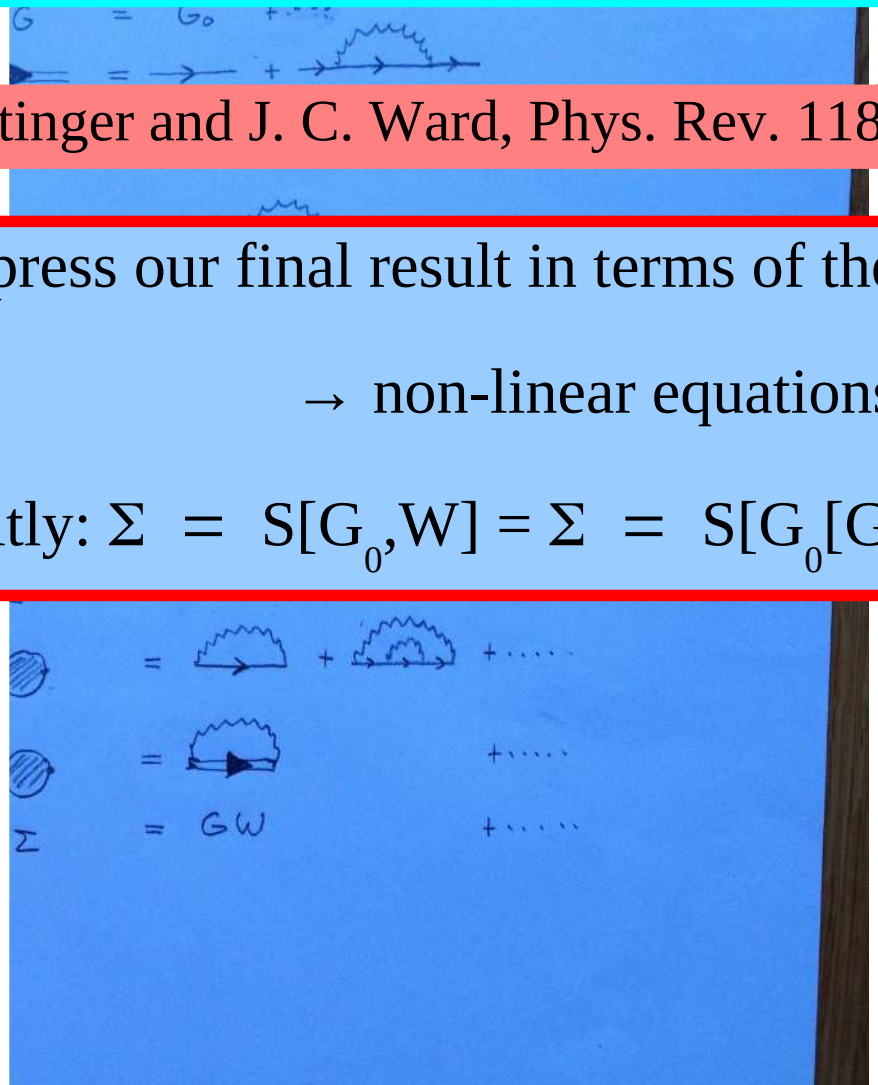

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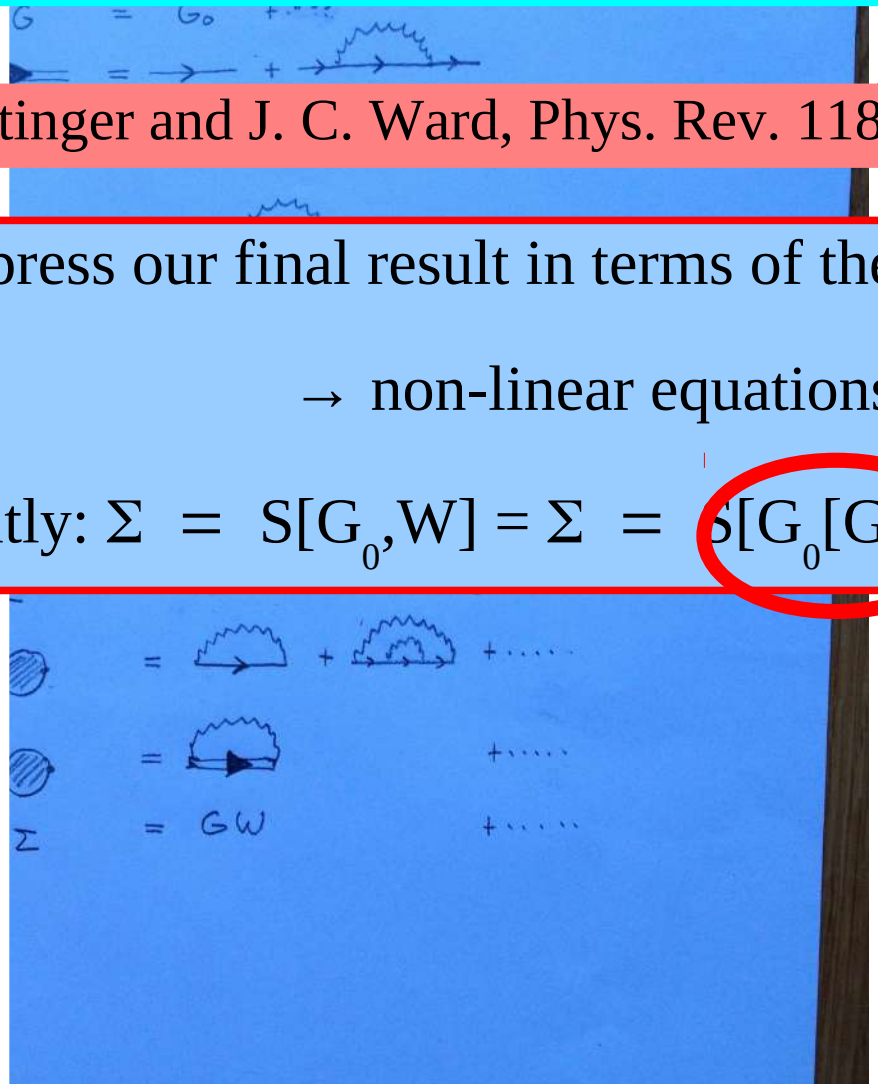

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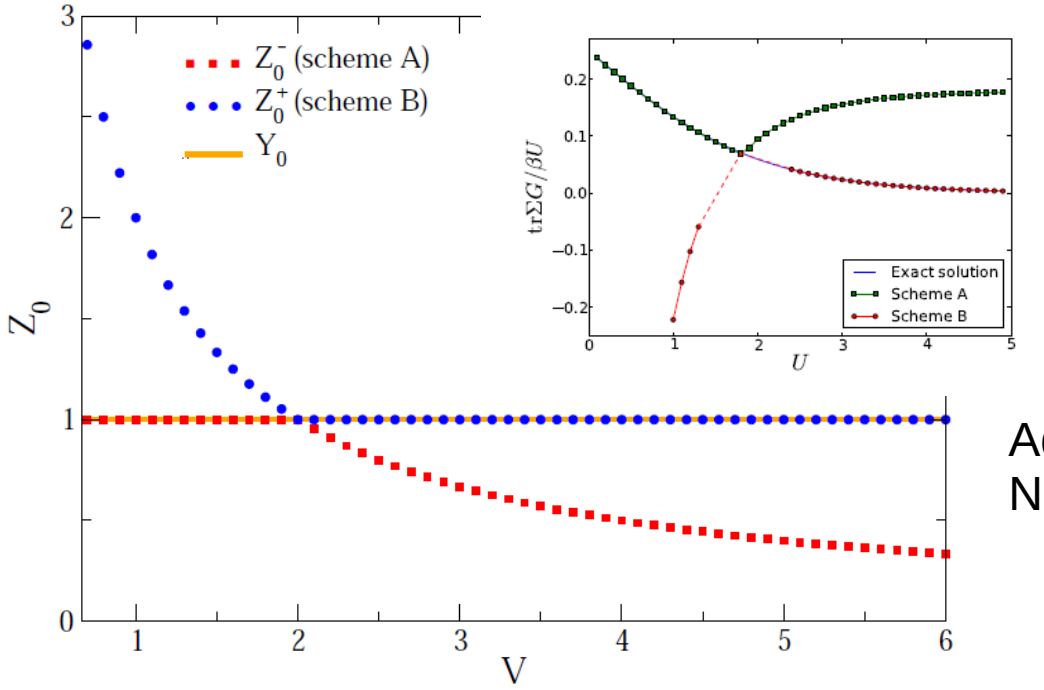

Kozik E, Ferrero M and Georges A
2015 Phys. Rev. Lett. 114 156402,
Nonexistence of the Luttinger-Ward Functional and Misleading Convergence of Skeleton Diagrammatic Series for Hubbard-Like Models

Adrian Stan et al.,
New Journal of Physics 17 (2015) 093045

Skeleton series OK in weak interaction regime
Complementary series from second solution in large interaction regime

See also Tarantino et al.,Self-consistent Dyson equation and self-energy functionals: An analysis and illustration on the example of the Hubbard atom, PRB 96, 045124 (2017)

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→ Could one tune the starting model so much that PT is no longer necessary?

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which means, O(0) is perfect: the model replaces the real system.

You don’t like this. But let us again learn from DFT.

$$O = \int \ldots \int dx_1 \ldots dx_N \, \Psi^*(x_1, \ldots . x_N) \sum_{i,j,\ldots} O(x_i, x_j, \ldots) \Psi(x_1, \ldots x_N)$$

$O = O[\Psi]$ Simple functional of very complex function

$O = \tilde{O}[n]$ Very complex functional of simple function

Moreover, *n(r)* not known a priori…..

Kohn-Sham DFT strategy:

1. auxiliary system with xc potential → *n(r)*

2. “take xc energy, potential from somewhere else”

LDA: $v_{\mathrm{xc}}([n], r) \approx v_{\mathrm{xc}}^{HEG}(n_r^h) \qquad n_r^h = n(r)$

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Why is this good?

1. Kohn-Sham system: have to approximate only one compact object

2. LDA: Do an advanced (QMC) calculation in the HEGs

   - but do it only **once and forever, and for everyone**!

D. M. Ceperley and B. J. Alder
Phys. Rev. Lett. 45, 566 (1980)

Starting from the LDA:

* expand, see e.g. Kohn, W.; Sham, L. J. Phys. Rev. 1965, 140, A1133–A1138,
Palummo, M., et al. Phys. Rev. B 1999, 60, 11329–11335

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* do better, see e.g…….

W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965);
E. Fermi, Rend. Accad. Naz. Lincei 6, 602 (1927); L. Thomas, Proc. Cambridge Phil. Soc. 33, 542 (1927); S.-K. Ma and K. A. Brueckner, Phys. Rev. 165, 18 (1968); S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. 58, 1200 (1980); O. Gunnarsson, M. Jonson, and B. Lundqvist, Solid State Commun. 24, 765 (1977); J. A. Alonso and L. Girifalco, Solid State Commun. 24, 135 (1977); J. A. Alonso and L. A. Girifalco, Phys. Rev. B 17, 3735 (1978); O. Gunnarsson, M. Jonson, and B. I. Lundqvist, Phys. Rev. B 20, 3136 (1979); O. Gunnarsson and R. Jones, Phys. Scr. 21, 394 (1980); R. Cuevas-Saavedra, D. Chakraborty, S. Rabi, C. Crdenas, and P. W. Ayers, J. Chem. Theory Comput. 8, 4081 (2012); D. C. Langreth and J. P. Perdew, Phys. Rev. B 21, 5469 (1980); J. P. Perdew and W. Yue, Phys. Rev. B 33, 8800 (1986); J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996); J. P. Perdew, S. Kurth, A. Zupan, and P. Blaha, Phys. Rev. Lett. 82, 2544 (1999); J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Phys. Rev. Lett. 100, 136406 (2008); J. Sun, A. Ruzsinszky, and J. P. Perdew, Phys. Rev. Lett. 115, 036402 (2015); J. F. Dobson, in Electronic Density Functional Theory, Recent Progress and New Directions, edited by J. F. Dobson, G. Vignale, and M. P. Das (Springer, Boston, MA,New York, 1998) pp. 261–284.J. Jung, P. Garcıa-Gonzalez, J. F. Dobson, and R. W. Godby, Phys. Rev. B 70, 205107 (2004); P. Garcıa-Gonzalez, J. E. Alvarellos, and E. Chacon, Phys. Rev. A 54, 1897 (1996); T. Olsen and K. S. Thygesen, Phys. Rev. B 86, 081103 (2012); T. Olsen and K. S. Thygesen, Phys. Rev. Lett. 112, 203001 (2014); C. E. Patrick and K. S. Thygesen, J. Chem. Phys. 143, 102802 (2015); P. S. Schmidt, C. E. Patrick, and K. S. Thygesen, Phys. Rev. B 96, 205206 (2017); D. Lu, J. Chem. Phys. 140, 18A520 (2014); G. Vignale and M. Rasolt, Phys. Rev. Lett. 59, 2360 (1987); A. Zangwill and P. Soven, Phys. Rev. A 21, 1561 (1980); E. K. U. Gross and W. Kohn, Phys. Rev. Lett. 55, 2850 (1985); J. F. Dobson, M. J. Buenner, and E. K. U. Gross, Phys. Rev. Lett. 79, 1905 (1997); T. K. Ng, Phys. Rev. Lett. 62, 2417 (1989); G. Vignale and W. Kohn, Phys. Rev. Lett. 77, 2037 (1996); G. Vignale, C. A. Ullrich, and S. Conti, Phys. Rev. Lett. 79, 4878 (1997); I. V. Tokatly, Phys. Rev. B 75, 125105 (2007); X. Gao, J. Tao, G. Vignale, and I. V. Tokatly, Phys.
Rev. B 81, 195106 (2010); V. U. Nazarov, I. V. Tokatly, S. Pittalis, and G. Vignale, Phys. Rev. B 81, 245101 (2010); P. E. Trevisanutto, A. Terentjevs, L. A. Constantin, V. Olevano, and F. D. Sala, Phys. Rev. B 87, 205143 (2013); M. Panholzer, M. Gatti, and L. Reining, Phys. Rev. Lett. 120, 166402 (2018); G. Giuliani and G. Vignale, Quantum Theory of the Electron Liquid (Cambridge University Press, 2005);
R. M. Martin, Electronic Structure: Basic Theory and Practical Methods (Cambridge University Press, 2004)

Starting from the LDA:

* expand, see e.g. Kohn, W.; Sham, L. J. Phys. Rev. 1965, 140, A1133–A1138,
Palummo, M., et al. Phys. Rev. B 1999, 60, 11329–11335

* do better, see e.g…….

* exactify & approximation strategy: Connector Theory
Marco Vanzini et al., arXiv:1903.07930v3,
Ayoub Aouina, Matteo Gatti, Lucia Reining, Faraday Discussions 224, 27 (2020)

Kohn-Sham DFT approximation strategy:

1. auxiliary system with xc potential → *n(r)*

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LDA:

$$v_{\mathrm{xc}}([n], r) \approx v_{\mathrm{xc}}^{HEG}(n_r^h)$$

$$n_r^h = n(r)$$

→ we use a model to simulate the real system

→ we use a different model to simulate the real system in each point

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W. Kohn, Phys. Rev. Lett., 1996, 76, 3168–3171.
21 E. Prodan and W. Kohn, Proc. Natl. Acad. Sci. U. S. A., 2005, 102, 11635–11638.

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→ **Can we use nearsightedness in GFFT?**

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What is nearsightedness in GFFT?

$$\Sigma(\mathbf{r}_1, \mathbf{r}_2, \omega) \qquad\qquad \Sigma(\mathbf{r}_1, \mathbf{r}_2; t_1 - t_2)$$

Around some average point? At which frequency? Or for each time difference?

Note: we are in a static system, this is not a question of making an adiabatic approx.

The answer of DMFT (or Spectral Density Functional Theory)

A. Georges et al., Rev. Mod. Phys. 68, 13 (1996)

S. Y. Savrasov and G. Kotliar, Phys. Rev. B 69, 245101 (2004), and references therein

The answer of DMFT (or Spectral Density Functional Theory)

Site/orbital basis

Target: $n(\mathbf{r})$

$$A_{\ell\ell}(\omega) = \frac{1}{\pi}|\mathrm{Im}\, G_{\ell\ell}(\omega)|$$

Aux. pot. $v_{\mathrm{xc}}([n], r)$

$$\Sigma^{\mathrm{loc}}_{\ell}(\omega) \neq \Sigma_{\ell\ell}(\omega)$$ (in full Dyson eq.)

Note: general auxiliary system,

Matteo Gatti, et al.,
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$$G = G_{\mathrm{aux}} + G_{\mathrm{aux}}[\Sigma - V_{\mathrm{aux}}]G$$

$$T\{G_{\mathrm{aux}}[\Sigma - V_{\mathrm{aux}}]G\} = 0$$

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Nearsightedness approx. $n^h_r = n(r)$

LDA

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Nearsightedness approx. $n^h_r = n(r)$

LDA Single-site DMFT

The answer of DMFT (or Spectral Density Functional Theory)

		Site/orbital basis
Target:	$n(\mathbf{r})$	$A_{\ell\ell}(\omega) = \frac{1}{\pi}\lvert\mathrm{Im}\, G_{\ell\ell}(\omega)\rvert$
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Nearsightedness approx.	$n^h_r = n(r)$	$G^{AIM}_{\ell}(\omega) = G_{\ell\ell}(\omega)$
	LDA	Single-site DMFT

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Nearsightedness approx.	$n^h_r = n(r)$	$G^{AIM}_{\ell}(\omega) = G_{\ell\ell}(\omega)$
	LDA	Single-site DMFT

Note: in HEG, interacting and non-interacting density are the same.
In the AIM, interacting and non-interacting spectral functions are not the same!!!

Beyond the fox and the grapes…….

For 1 electron: $$\Sigma_{\mathrm{x}}(\mathbf{r}_1, \mathbf{r}_2) = \frac{\sqrt{n(\mathbf{r}_1) n(\mathbf{r}_2)}}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

More in general, we may expect that $\Sigma(\mathbf{r}_1, \mathbf{r}_2, \omega)$

depends essentially on $n(\mathbf{r}_1),\ \ n(\mathbf{r}_2)$

Generalized nearsightedness…….needs model that is not local and not homogeneous.

To be explored

See A. Aouina et al., Faraday Discussions 224, 27 (2020).
More generally, inhomogeneous model systems, e.g.
P-F Loos et al., J. Chem Phys. 140, 18A524 (2014) and 146, 114108 (2017)

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