

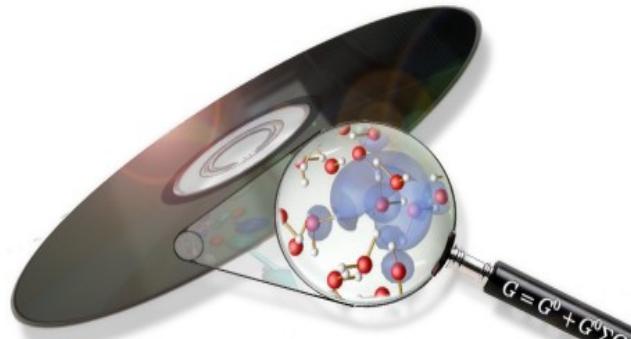
Methods, models and materials: Joining forces to deal with the many-body problem

Lucia Reining
Palaiseau Theoretical Spectroscopy Group & Friends



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Methods, models and materials: Joining forces to deal with the many-body problem

- Functionals,
and strategies to find them
- The connector project,
or how to play Lego together
- The homogeneous electron gas,
trouble with our methods, and promising combinations
- Insert concerning MBPT+TDDFT,
the total energy
- A Christmas advocacy

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$$O = O[\Psi] = \langle \Psi | \hat{O} | \Psi \rangle$$

- * well-known expression

- * difficult to use

$$O = O[\Psi] = \langle \Psi | \hat{O} | \Psi \rangle$$

- * well-known expression

- * difficult to use

$$O = \tilde{O}[Q]$$

- * Q might also fully describe the observable, but be simpler

- * Q might itself be an observable

- * The problem is then to know Q , and to know $\tilde{O}[Q]$

Descriptor

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

The problem is then to know Q

Descriptor

Auxiliary “potential”

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

$$v_{\text{xc}}(\mathbf{r}; [n])$$

The problem is then to know Q

P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)

W. Kohn and L. J. Sham, Phys. Rev. 140, A113 (1965)

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→ Mostly try to approximate $E[n]$

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* *Not many observables are easy to express in terms of the density*

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

$v_{xc}(\mathbf{r}; [n])$

The problem is then to know Q , and to know $\tilde{O}[Q]$

→ Mostly try to approximate $E[n]$

- * *Not many observables are easy to express in terms of the density*
- * *Therefore, we often replace the observable of the real material by that of the KS system*

Descriptor

Auxiliary “potential”

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

$$v_{\text{xc}}(\mathbf{r}; [n])$$

$$G(\mathbf{r}, \mathbf{r}', \omega)$$

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega; [G])$$

→ Known functionals $A_{\mathbf{k}}(\omega; [G])$

$$E = \tilde{E}[G]$$

→ Often try to approximate $\epsilon(\mathbf{q}, \omega; [G])$

Descriptor

Auxiliary “potential”

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

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$$G(\mathbf{r}, \mathbf{r}', \omega)$$

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega; [G])$$

$$G_{\ell\ell}(\omega)$$

$$\Sigma_{\ell}^{loc}(\omega; [G^{loc}]) \quad \text{DMFT}$$

→ Known functional $A_{\ell\ell}(\omega; [G_{\ell\ell}])$

→ Often approximate $A_{\mathbf{k}}(\omega; [G^{loc}])$

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

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

Descriptor

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$$G(\mathbf{r}, \mathbf{r}', \omega)$$

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Auxiliary “potential”

$$v_{\text{xc}}(\mathbf{r}; [n])$$

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More:

RDMFT: T. L. Gilbert, Phys. Rev. B 12, 2111 (1975);
R. Requist and O. Pankratov, Phys. Rev. B 77, 235121 (2008)

General: M. Gatti, et al., PRL 99, 057401 (2007);
M. Vanzini, et al., Faraday Discussions 224, 424-447 (2020)

Descriptor

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

$$G(\mathbf{r}, \mathbf{r}', \omega)$$

Auxiliary “potential”

$$v_{\text{xc}}(\mathbf{r}; [n])$$

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega; [G])$$

None of the auxiliary potentials, interactions etc. is known

Perturbation expansions in MBPT often used

And besides this?

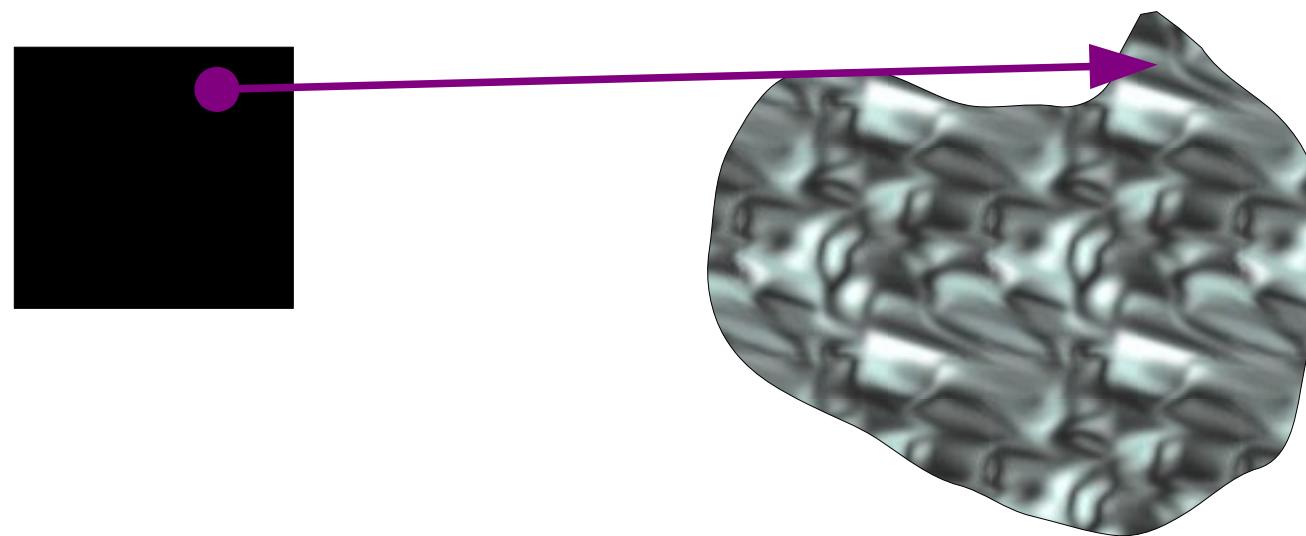
→ Often approximate $A_{\mathbf{k}}(\omega; [G_{\ell\ell}])$

Further: see M. Gatti, et al., PRL 99, 057401 (2007);
M. Vanzini, et al., Faraday Discussions 224, 424-447 (2020)

Typical DFT approximation strategy

$$v_{\text{xc}}(\mathbf{r}; [n]) \rightarrow v_{\text{xc}}(n_{\mathbf{r}}^h)$$

Material



W. Kohn and L. J. Sham, Phys. Rev. 140:A1133–1138, 1965

Typical DFT approximation strategy

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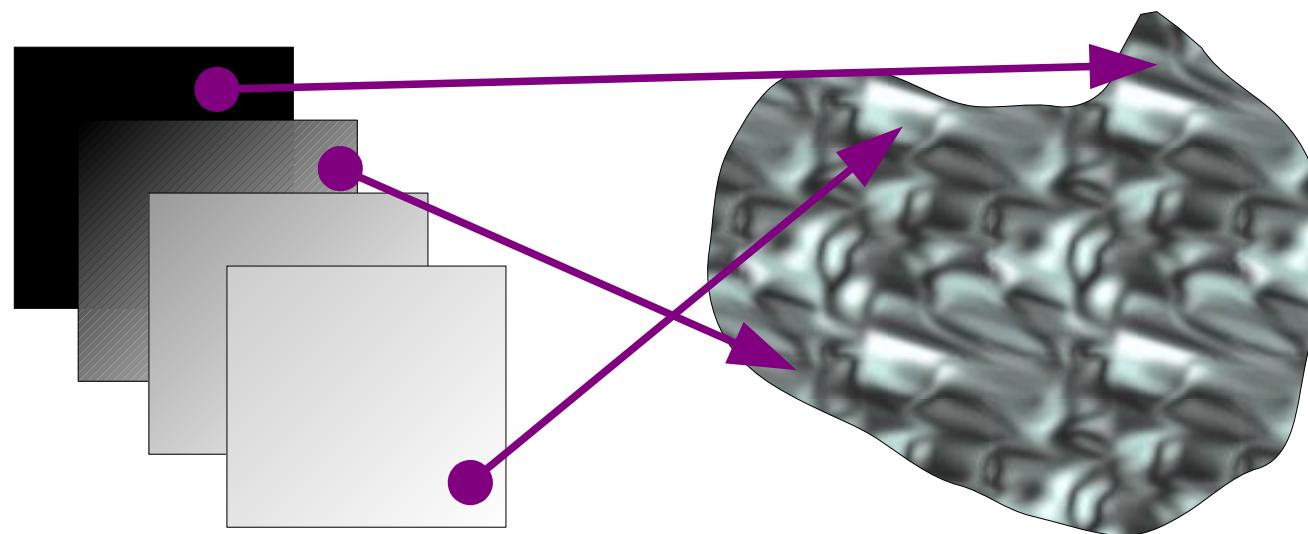
$$n_r^h = n(r)$$

Local Density Approximation (LDA)

Homogeneous
electron gas



Material



W. Kohn and L. J. Sham, Phys. Rev. 140:A1133–1138, 1965

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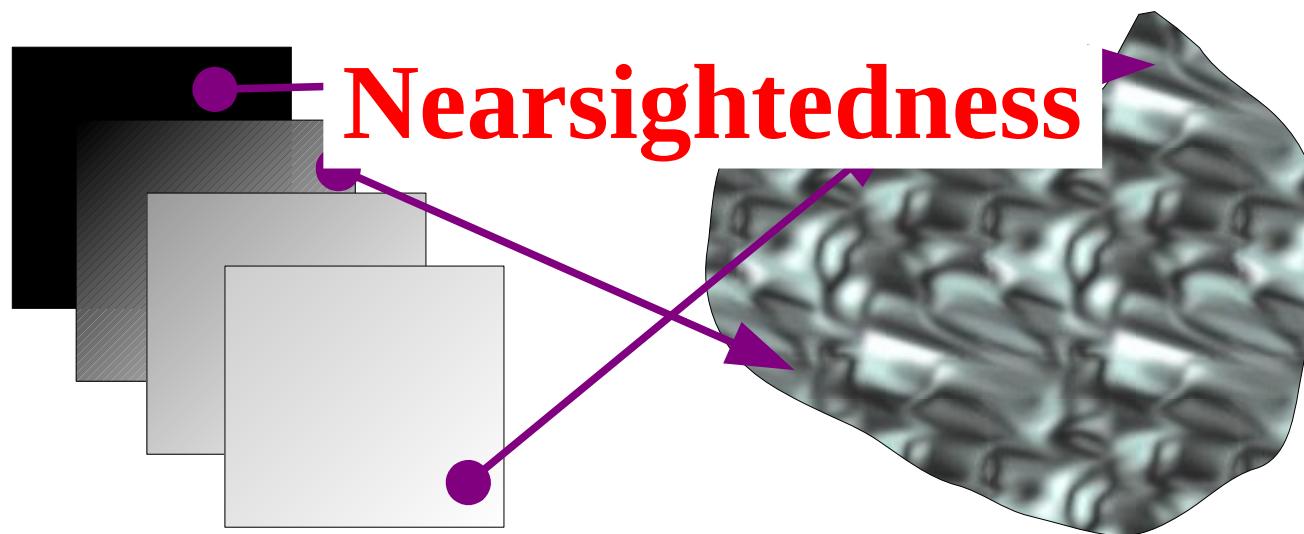
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“Same local density”
Local Density Approximation (LDA)



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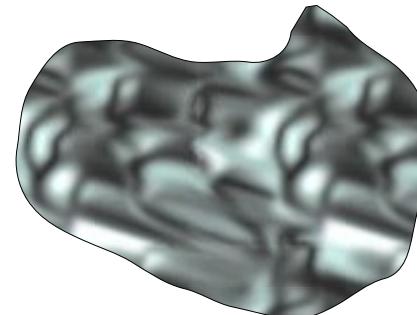
GFFT approximation strategy **of DMFT**

$$\Sigma_{\ell}^{loc}(\omega)$$

$$G_{jj}(\omega)$$

$v_{xc}(\mathbf{r}, [n])$ $n_r^h = n(r)$ Local Density Approximation (LDA)

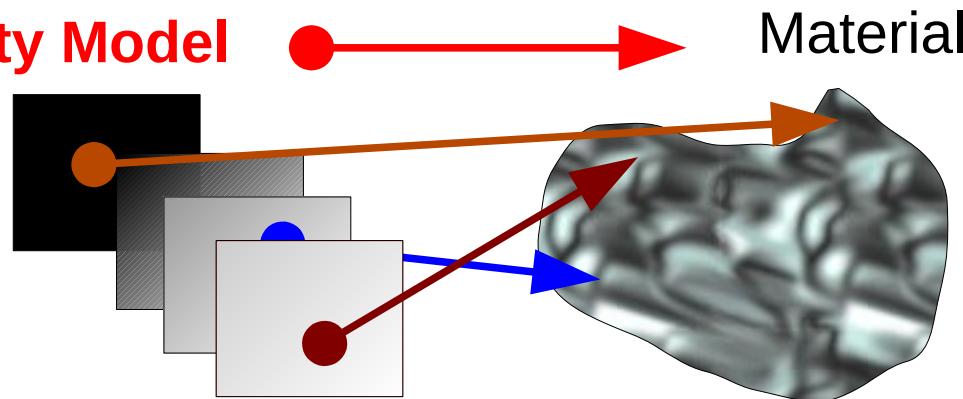
Material



GFFT approximation strategy **of** DMFT

$$\Sigma_{\ell}^{loc}(\omega)$$

Anderson Impurity Model



GFFT approximation strategy **of** DMFT

$$\Sigma_{\ell}^{loc}(\omega)$$

$$G_{\ell\ell}(\omega)$$

Single site DMFA

$$\Sigma_{\ell}^{loc}(\omega, [G_{\ell\ell}])$$

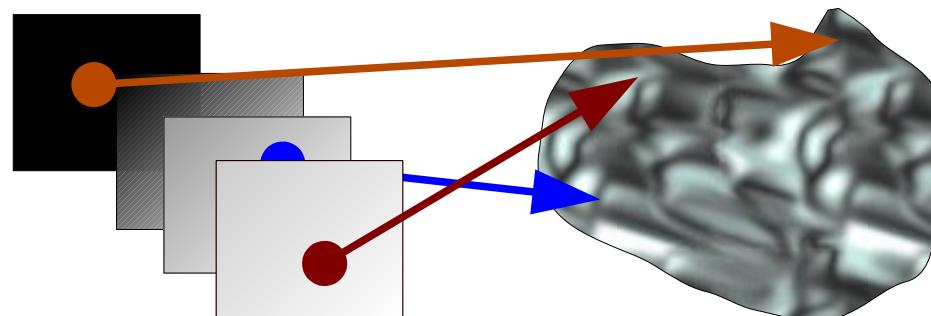
“Same local spectral function”

Nearsightedness

Anderson Impurity Model



Material



General strategy

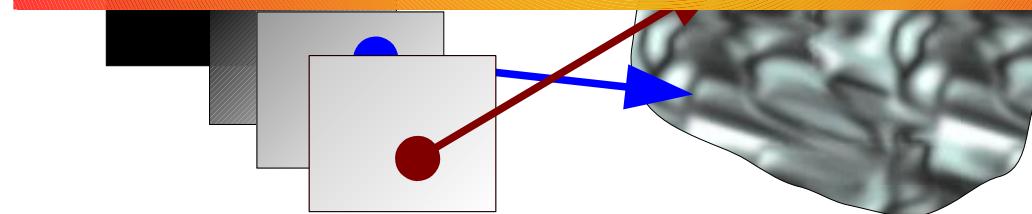
$$\Sigma_{\ell}^{loc}(\omega)$$

$$G_{\ell\ell}(\omega)$$

→ Take from a model

$$\Sigma_{\ell}^{loc}(\omega)$$

Anderson Impurity → Suppose nearsightedness



“Same local spectral function” →

Typical DFT approximation strategy

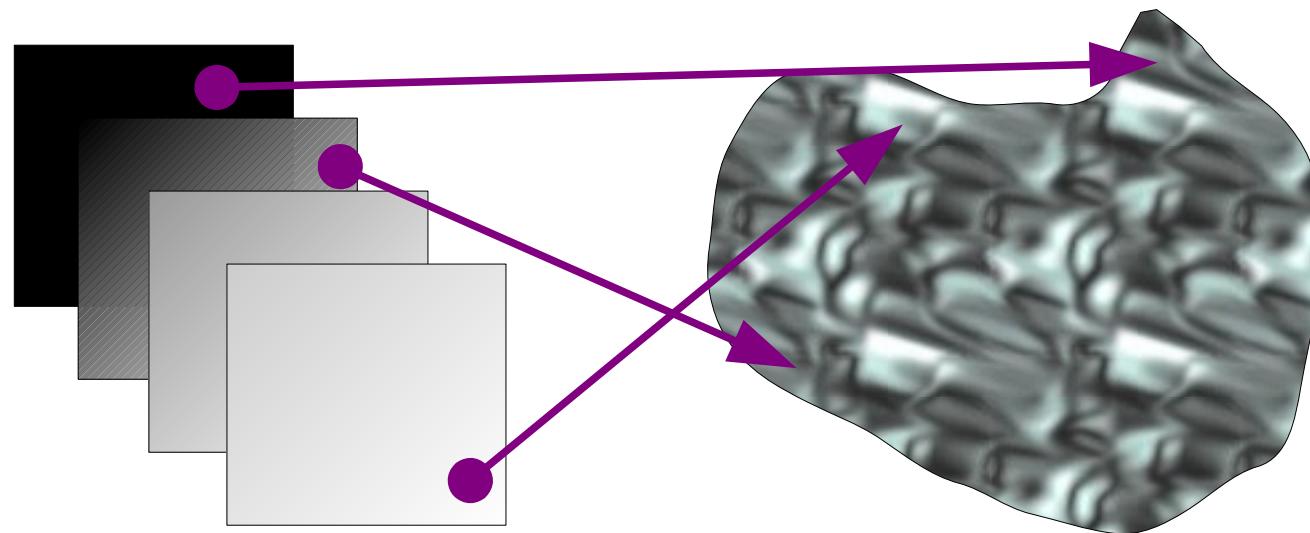
$$v_{\text{xc}}(\mathbf{r}; [n]) \rightarrow v_{\text{xc}}(n_{\mathbf{r}}^h) \quad n_r^h = n(r)$$

Local Density Approximation (LDA)

**Homogeneous
electron gas**



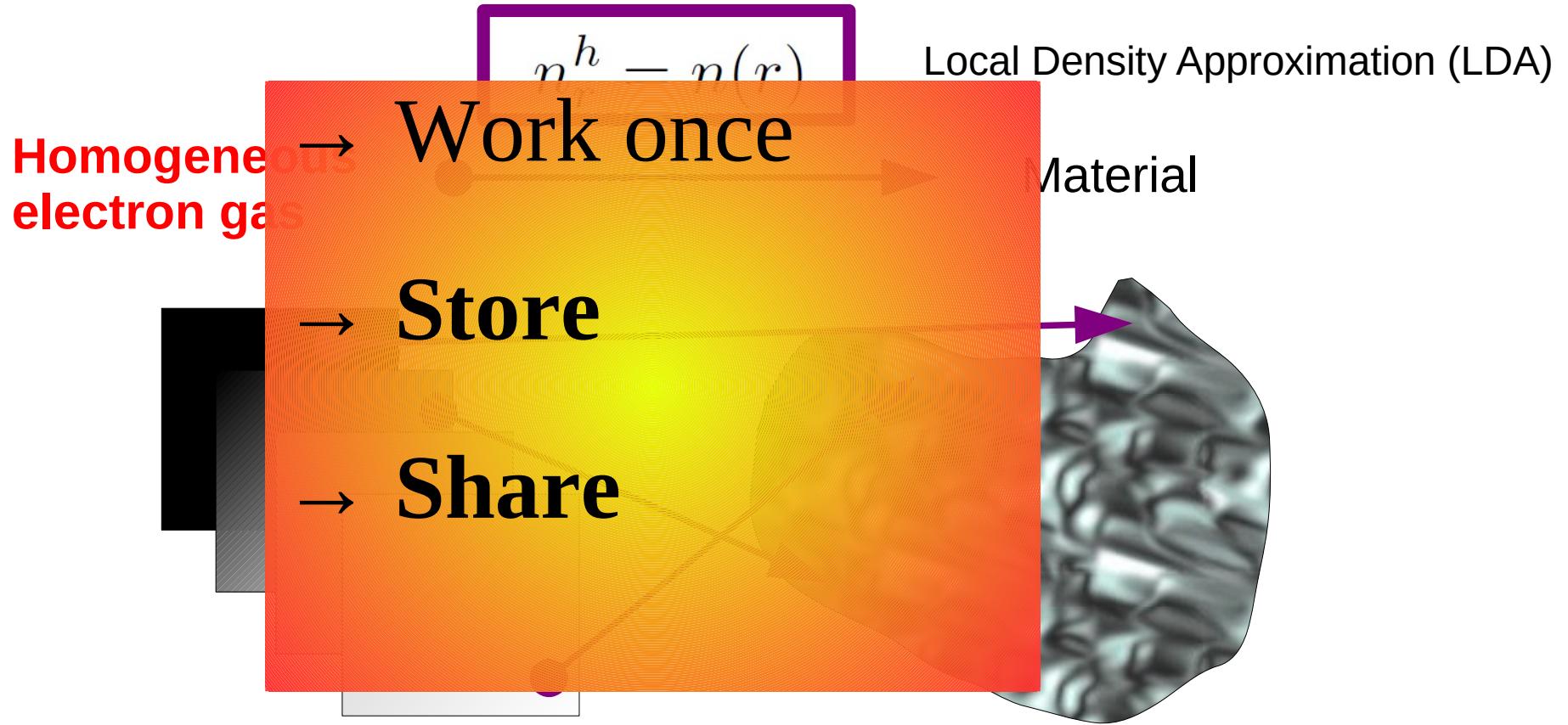
Material



W. Kohn and L. J. Sham, Phys. Rev. 140:A1133–1138, 1965

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

Typical DFT approximation strategy



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$$\Sigma_{\ell}^{loc}(\omega; [G^{loc}]) \quad \text{DMFT}$$

Store & interpolate ?

Descriptor

Auxiliary “potential”

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

$$v_{\text{xc}}(\mathbf{r}; [n])$$

$$\underline{G(\mathbf{r}, \mathbf{r}', \omega)}$$

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega; [G])$$

$$G_{\ell\ell}(\omega)$$

$$\Sigma_{\ell}^{loc}(\omega; [G^{loc}]) \quad \text{DMFT}$$

Nearsightedness ?

We definitely want to learn

from DFT-LDA and related approximations!!!

LDA

Homog
electron gas



W. Kohn and L. J. Sham, Phys. Rev. 140:A1133–1138, 1965

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

Homogeneous
electron gas

Extend DFT-LDA approximation strategy

- beyond nearsightedness
- beyond DFT

proximation (LDA)

→ Work once

→ Store

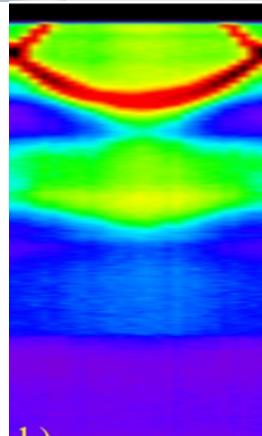
→ Share

W. Kohn and L. J. Sham, Phys. Rev. 140:A1133–1138, 1965

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



$$\hat{H}\Psi_\lambda(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N) = E_\lambda\Psi_\lambda(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N)$$





Faster





Better understanding

Faster



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Methods, models and materials: Joining forces to deal with the many-body problem



Ayoub Aouina



Marco Vanzini



Martin Panholzer

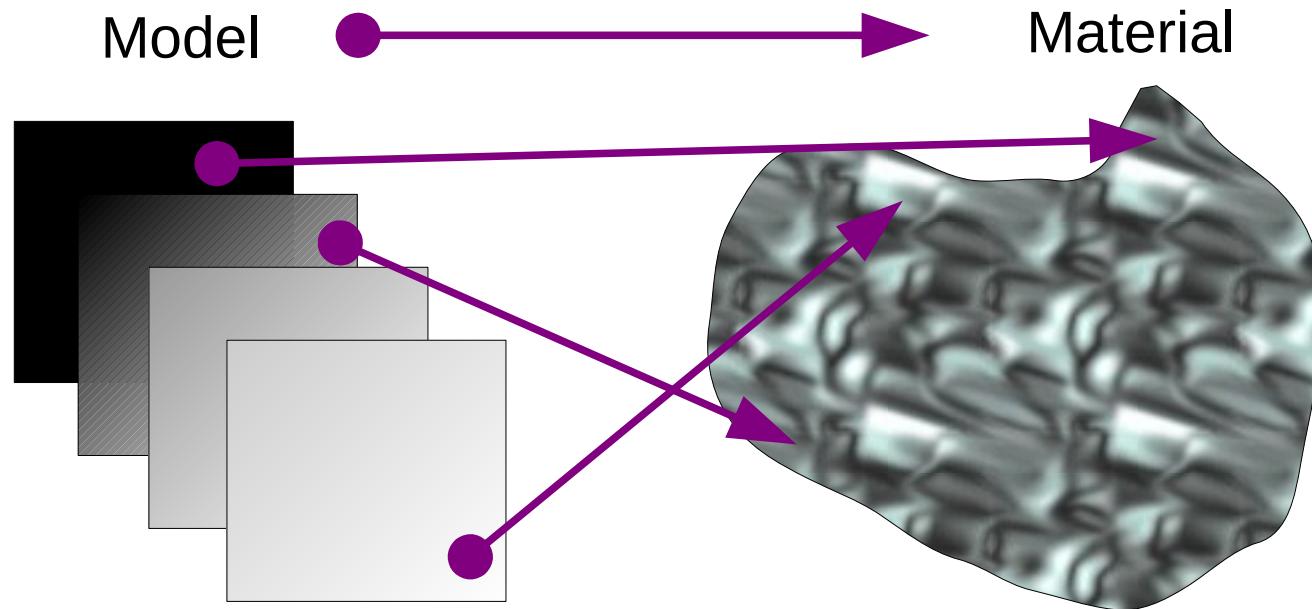


Matteo Gatti



Beyond nearsightedness

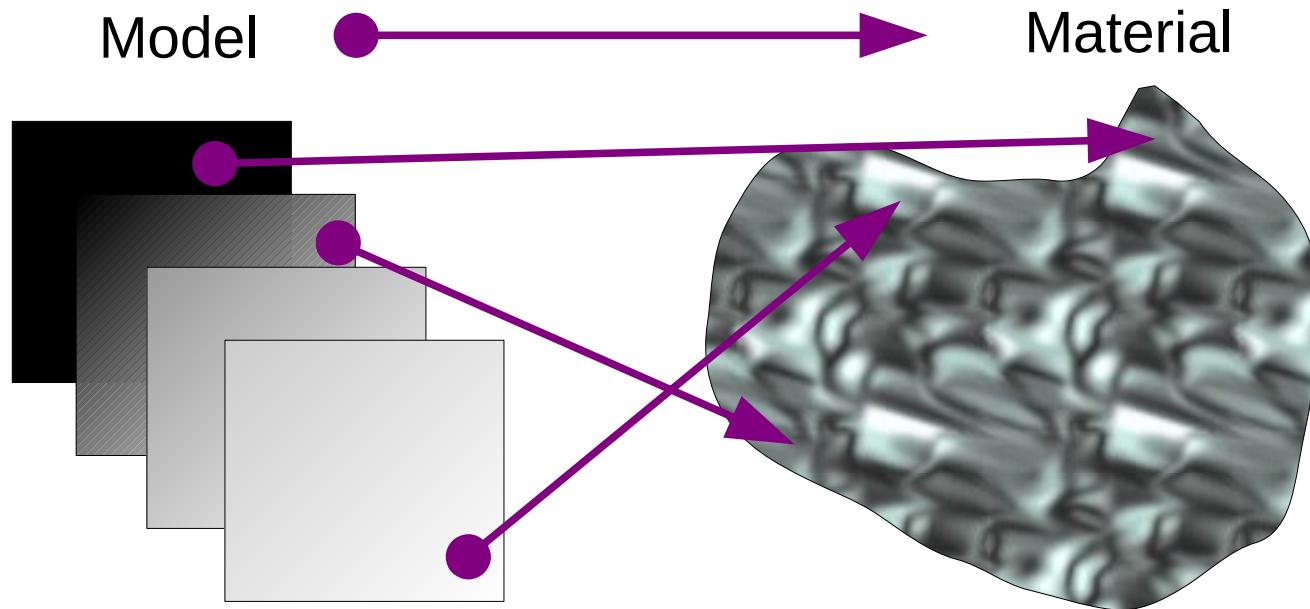
In every point, we can replace the result in the material
by that in one of the model realizations



Aouina, Gatti, Reining, Faraday Discussions 224, 27 (2020)
Vanzini, Aouina, Panholzer, Gatti, Reining, NPJ Comp Mat (2022)

Beyond nearsightedness

$$v_{\text{xc}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

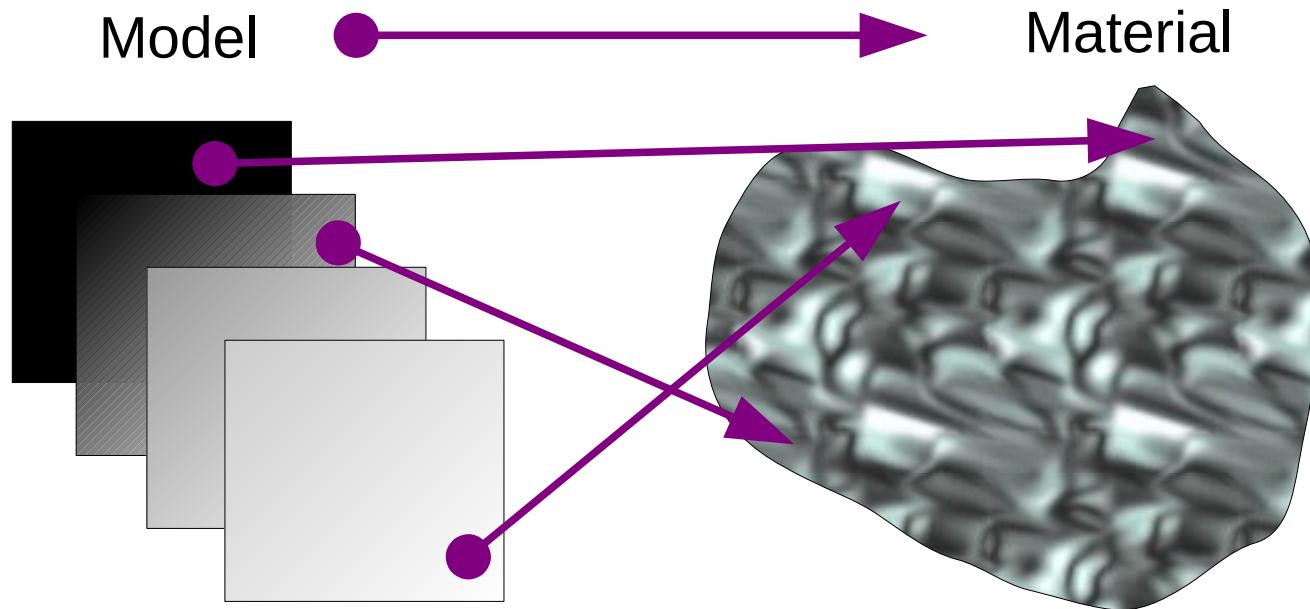


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Beyond nearsightedness

Exact:

$$v_{\text{xc}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

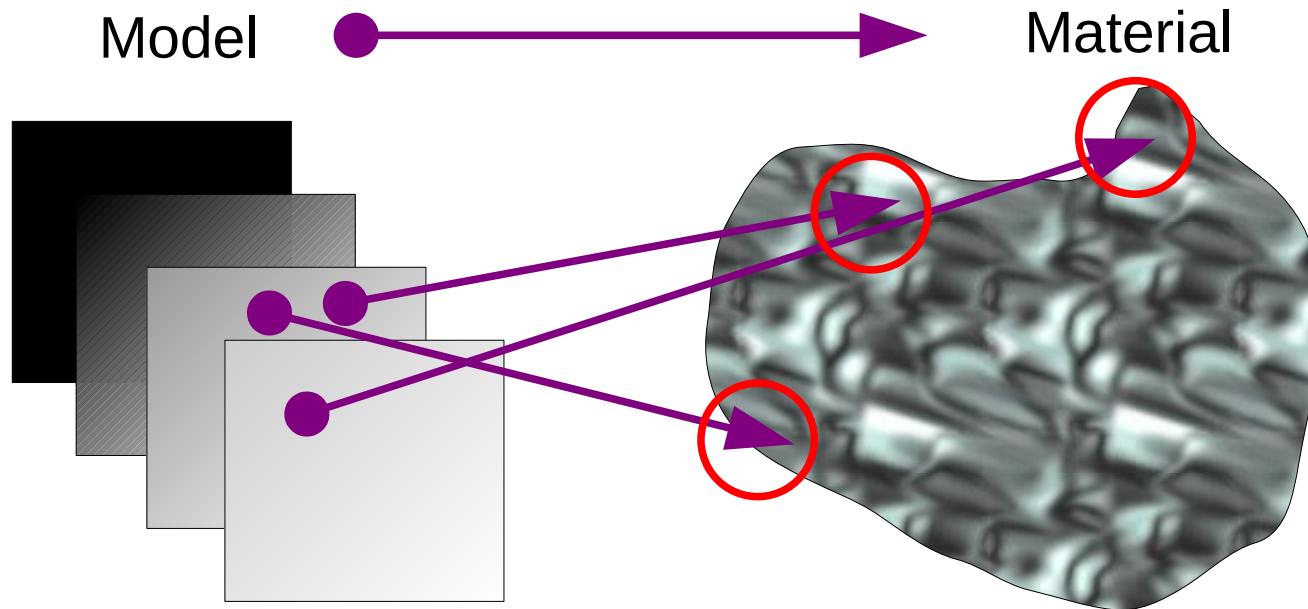


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Beyond nearsightedness

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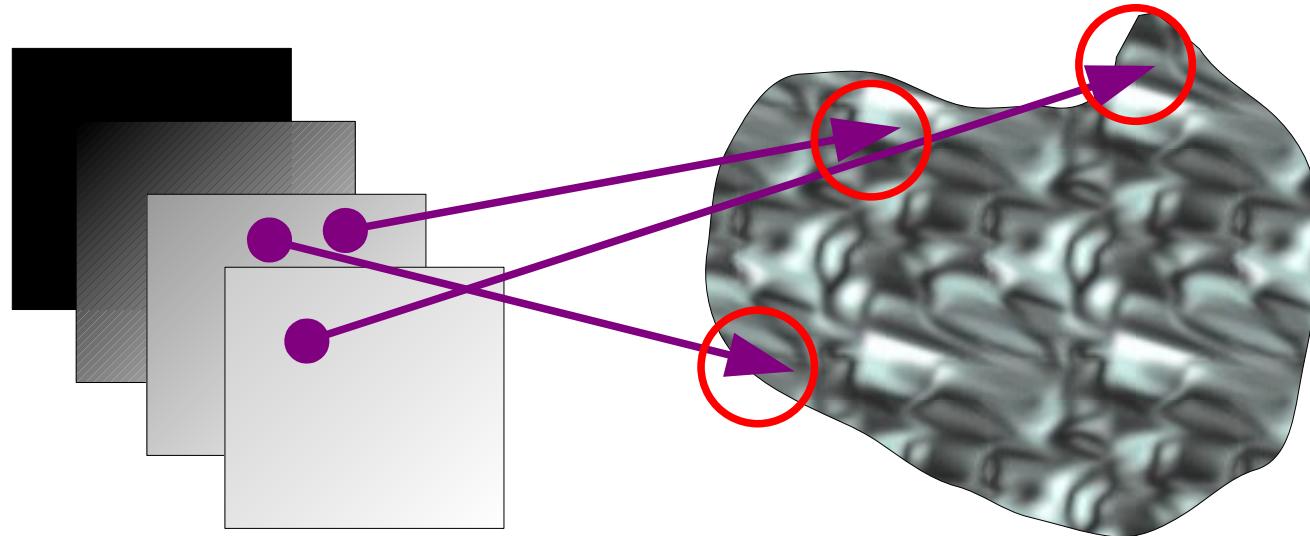
$$v_{\text{xc}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

“Connector”

???

Model

Material



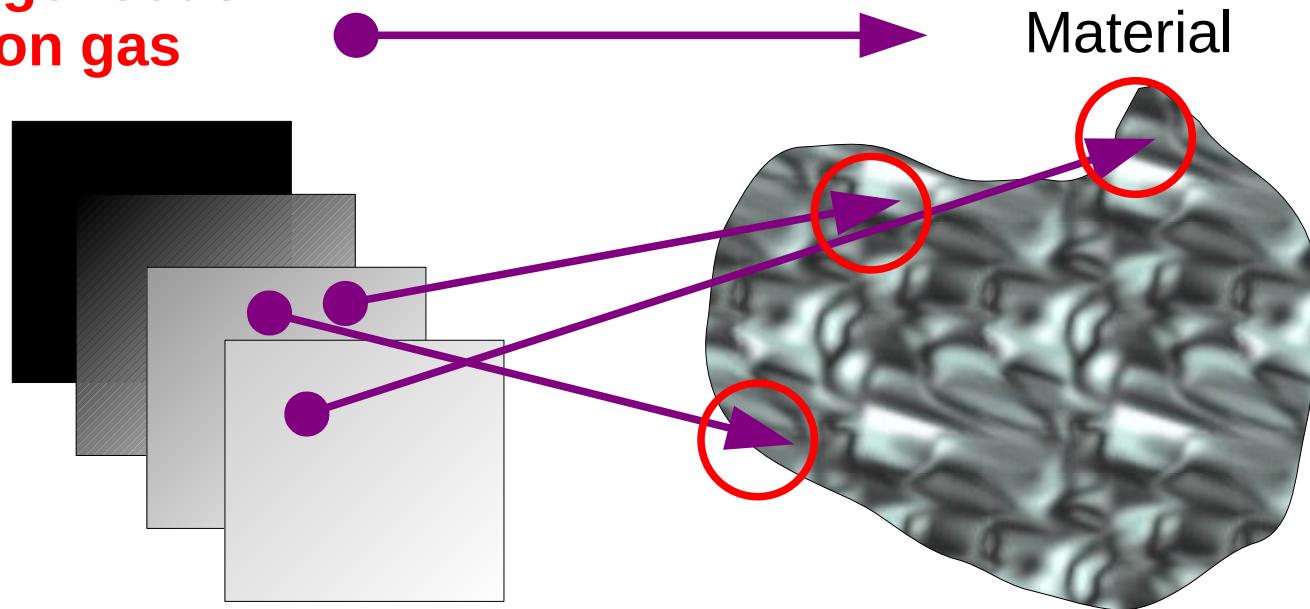
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Homogeneous
electron gas

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???

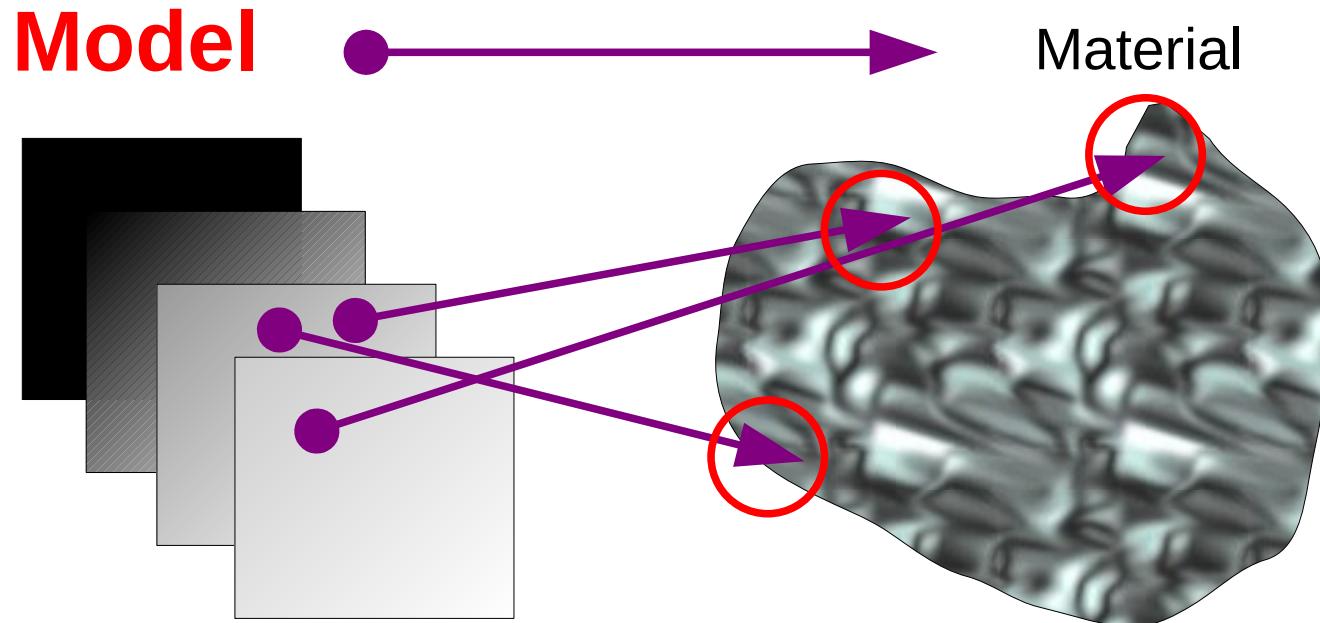


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R. M. Martin, Electronic Structure: Basic Theory and Practical Methods (Cambridge University Press, 2004)

$$v_{\text{xc}}(\mathbf{r}; [n]) = v_{\text{xc}}^m(\mathbf{r}; [n_{\mathbf{r}}^m])$$

“Connector”
???

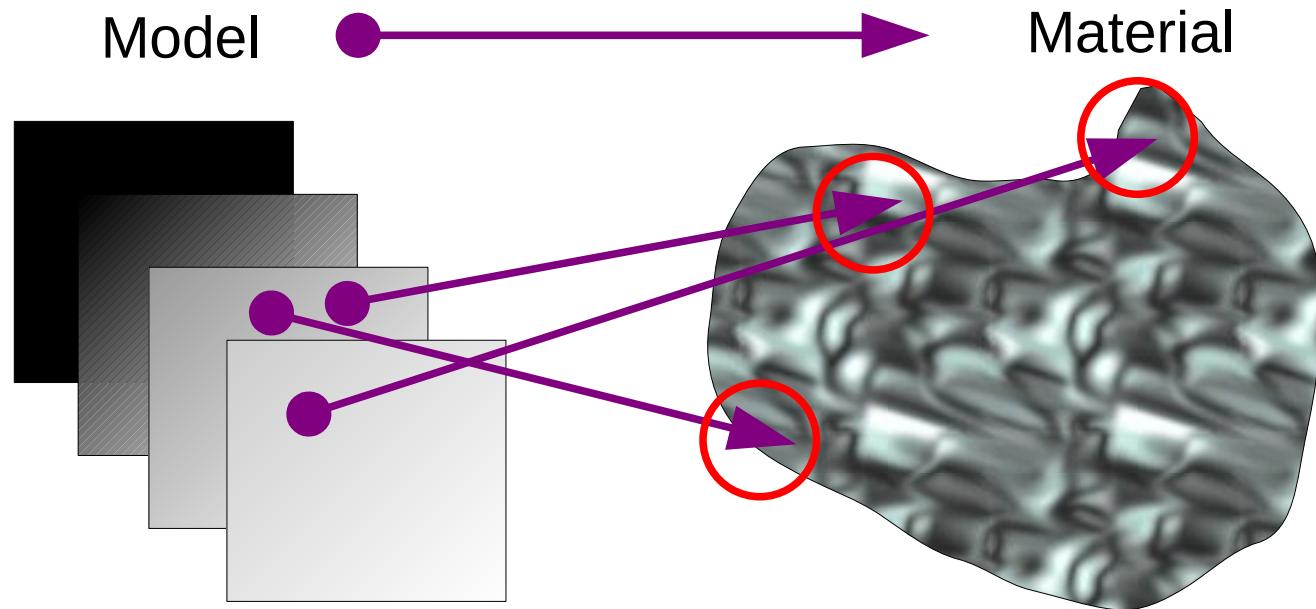


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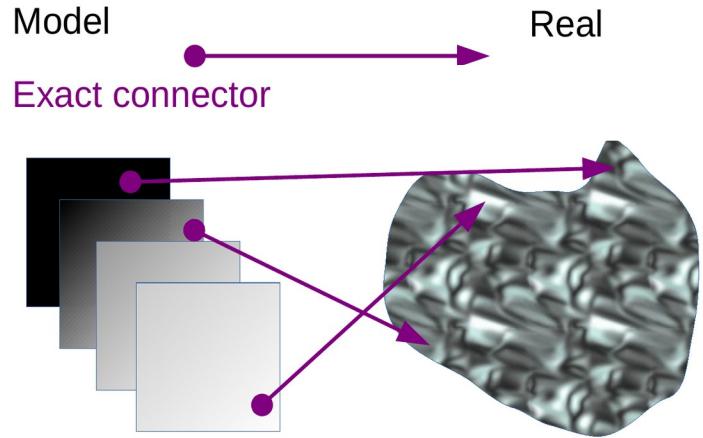
“Connector”

$$\Sigma(\mathbf{r}, \mathbf{r}', \omega; [G]) = \Sigma^m(\mathbf{r}, \mathbf{r}', \omega; [n_{\mathbf{rr}'\omega}^m])$$

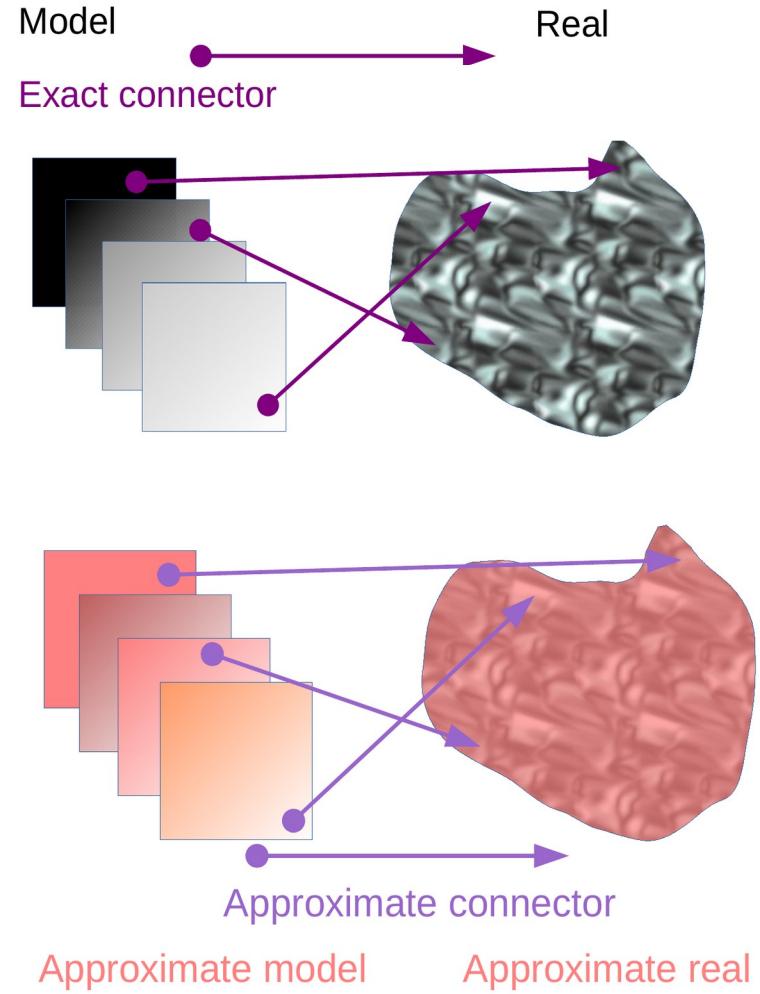
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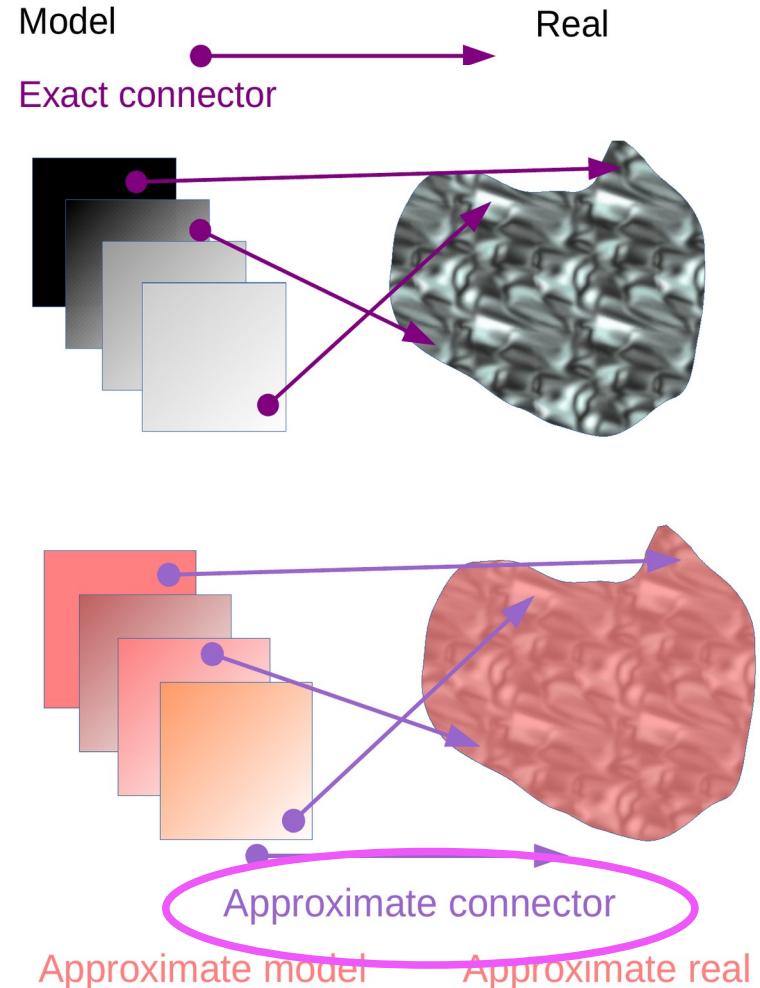


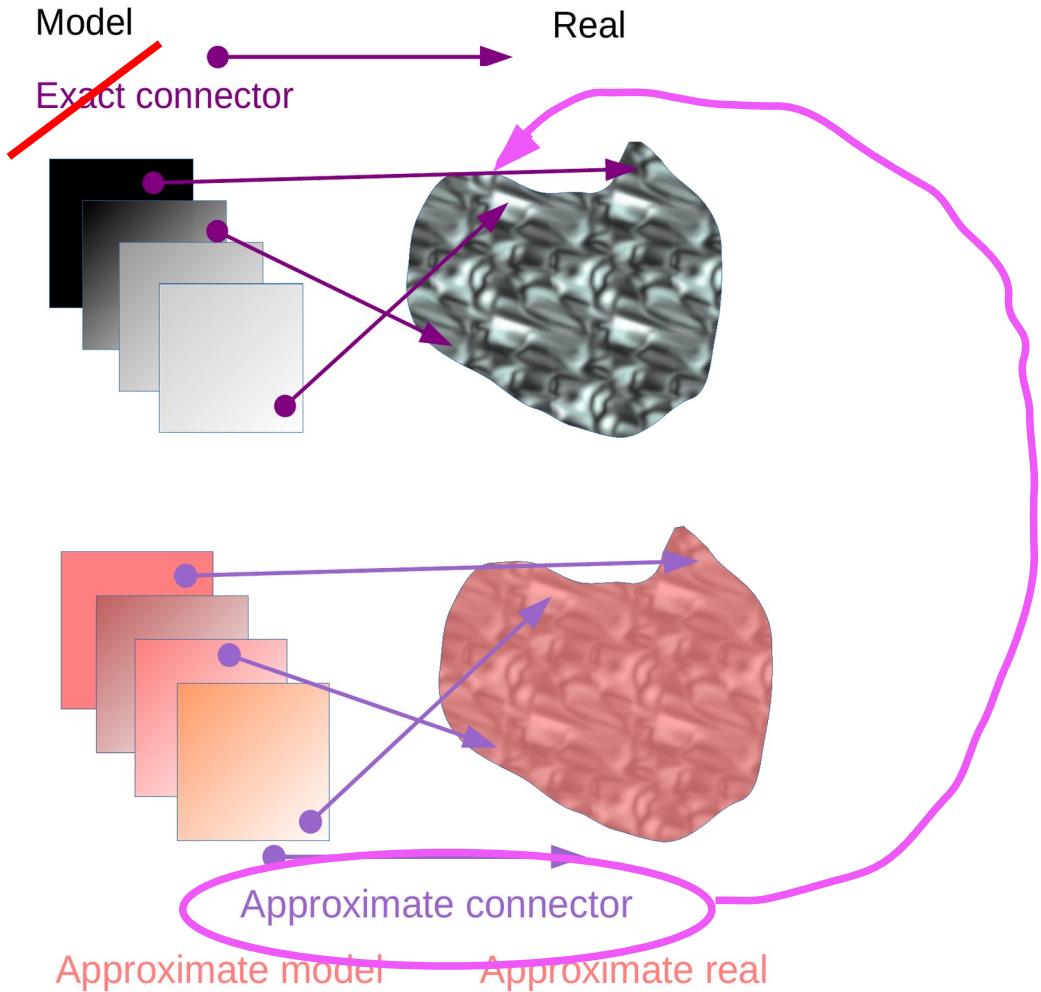
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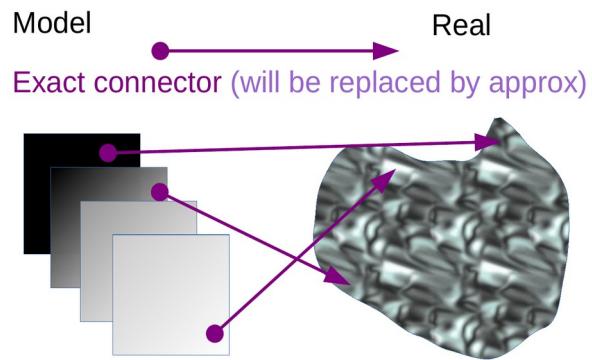
Approximation strategy







COT:



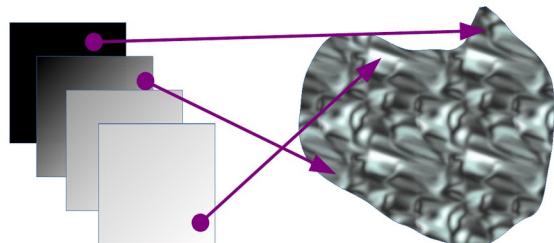
$$v_{\text{xc}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

$$n_{\mathbf{r}}^c = \left(v_{\text{xc}}^h \right)^{-1} \left(v_{\text{xc}}(\mathbf{r}, [n]) \right)$$

$$v_{\text{xc}}(\mathbf{r}, [n]) = ?$$

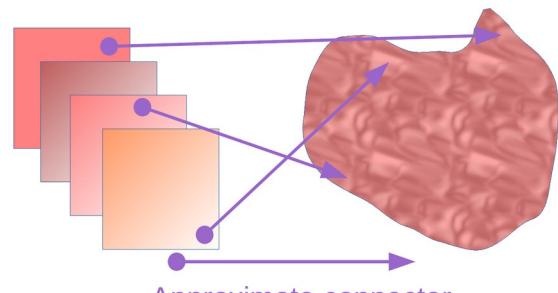
COT:

Model Real
Exact connector (will be replaced by approx)



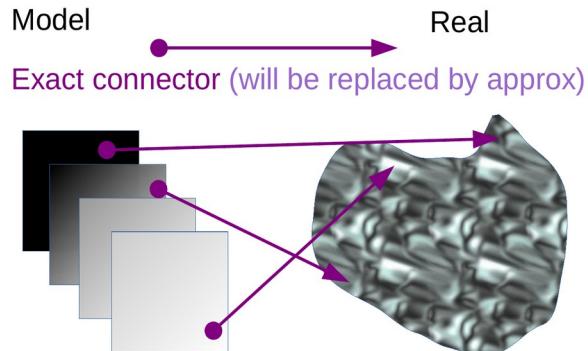
$$v_{\text{xc}}^{\text{approx}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

$$n_{\mathbf{r}}^c = \left(v_{\text{xc}}^h \right)^{-1} \left(v_{\text{xc}}(\mathbf{r}, [n]) \right)$$



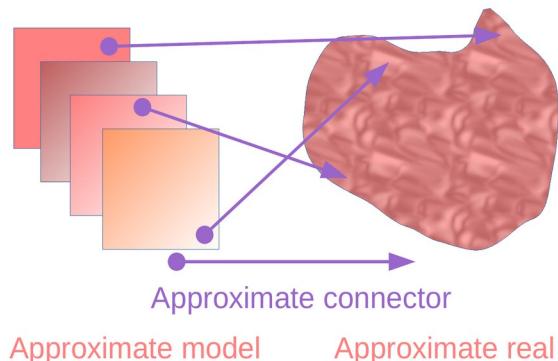
Approximate model Approximate real

COT:



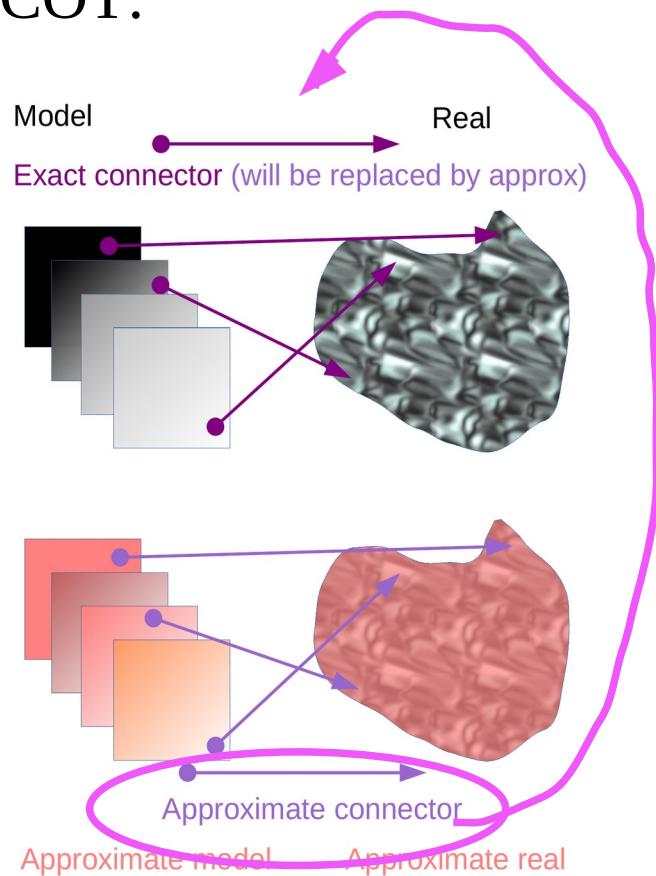
$$v_{\text{xc}}^{\text{approx}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

$$n_{\mathbf{r}}^c = (v_{\text{xc}}^h)^{-1}(v_{\text{xc}}(\mathbf{r}, [n]))$$



$$n_{\mathbf{r}}^{c,\text{approx}} = (v_{\text{xc}}^{h,\text{approx}})^{-1}(v_{\text{xc}}^{\text{approx}}(\mathbf{r}; [n]))$$

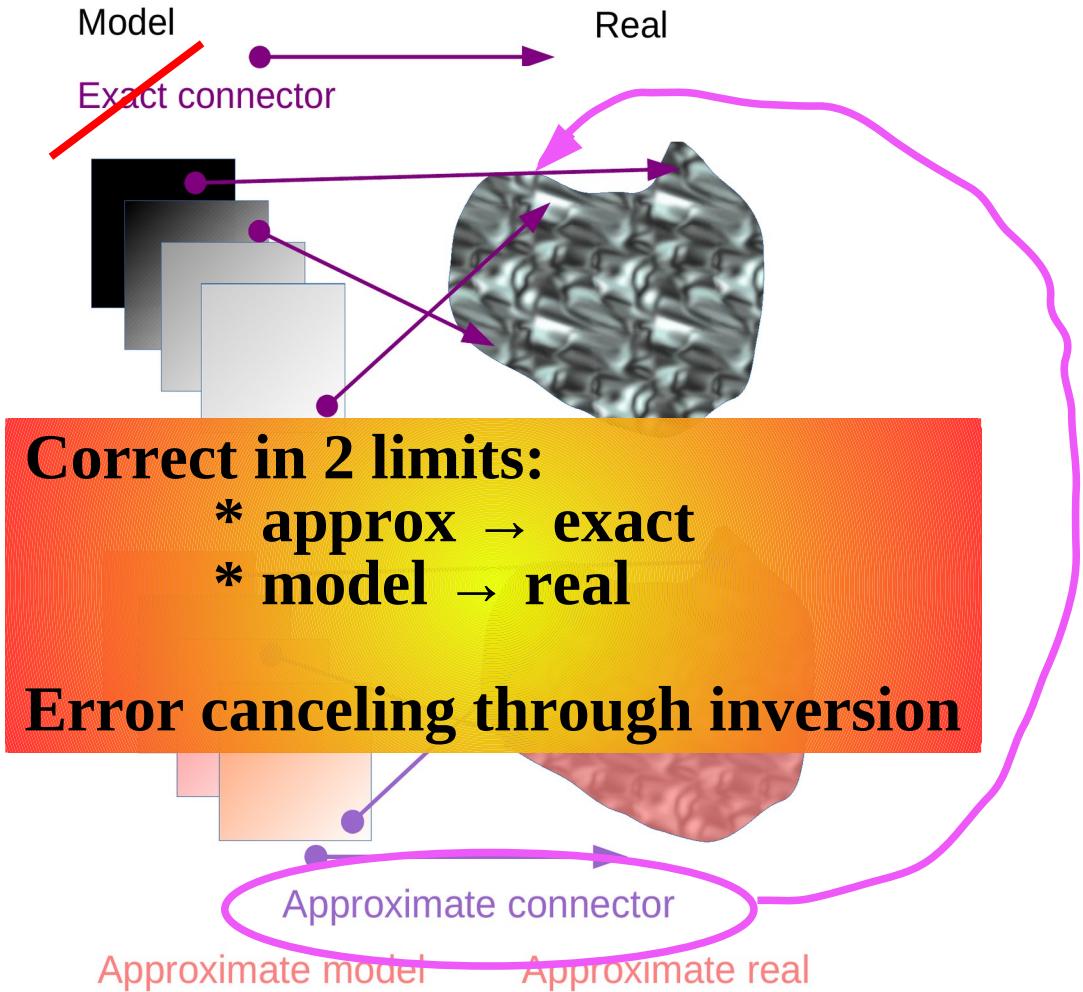
COT:



$$v_{\text{xc}}^{\text{approx}}(\mathbf{r}, [n]) = v_{\text{xc}}^h(n_{\mathbf{r}}^c)$$

$$v_{\text{xc}}^c(\mathbf{r}, [n]) = v_{\text{xc}}^h \left(n^h = n_{\mathbf{r}}^{c,\text{approx}}([n]) \right)$$

$$n_{\mathbf{r}}^{c,\text{approx}} = (v_{\text{xc}}^{h,\text{approx}})^{-1}(v_{\text{xc}}^{\text{approx}}(\mathbf{r}; [n]))$$



The connector imports knowledge from the model system

- Approximation already very good, model far from real: COT not useful
- Approximation rough, model reflects aspects of real: COT big gain

The connector imports knowledge from the model system

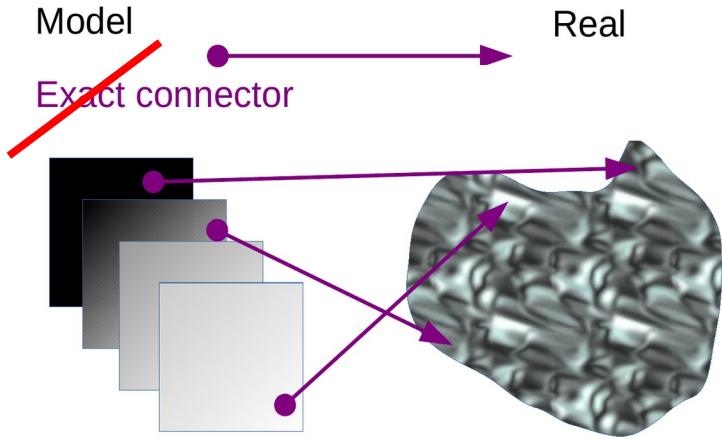
- Approximation already very good, model far from real: COT not useful
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KS-LDA exchange energy

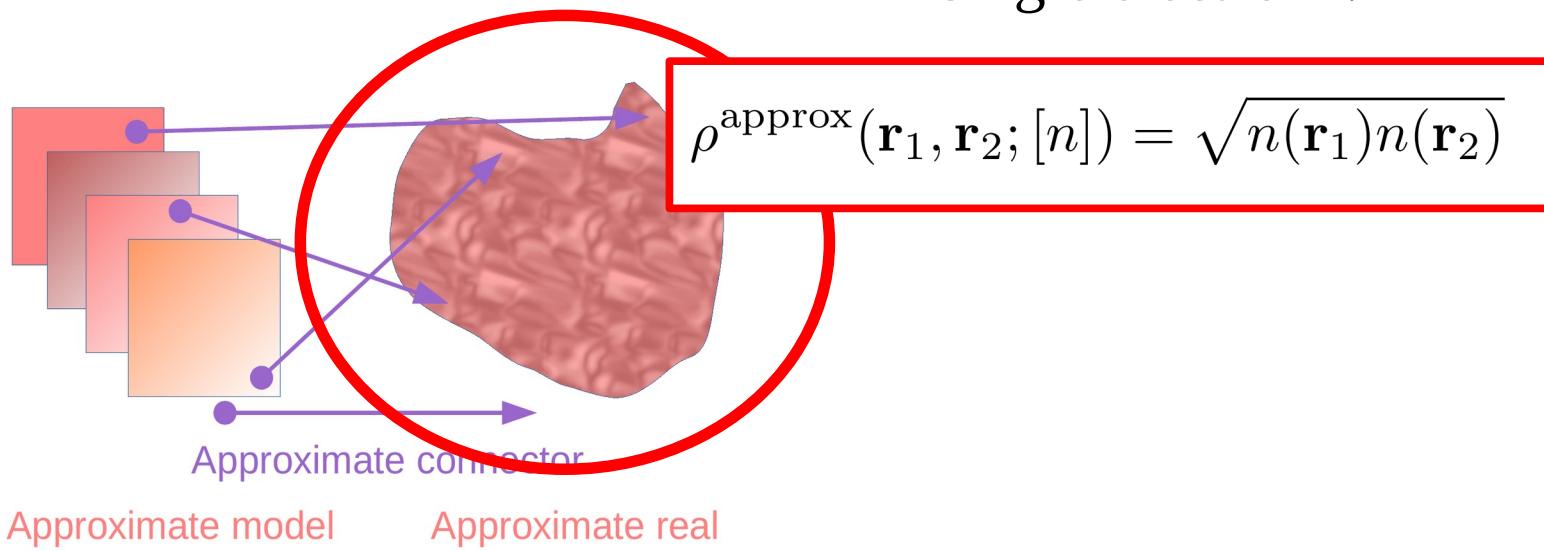
He

Si

Relative error in %



“single electron”:



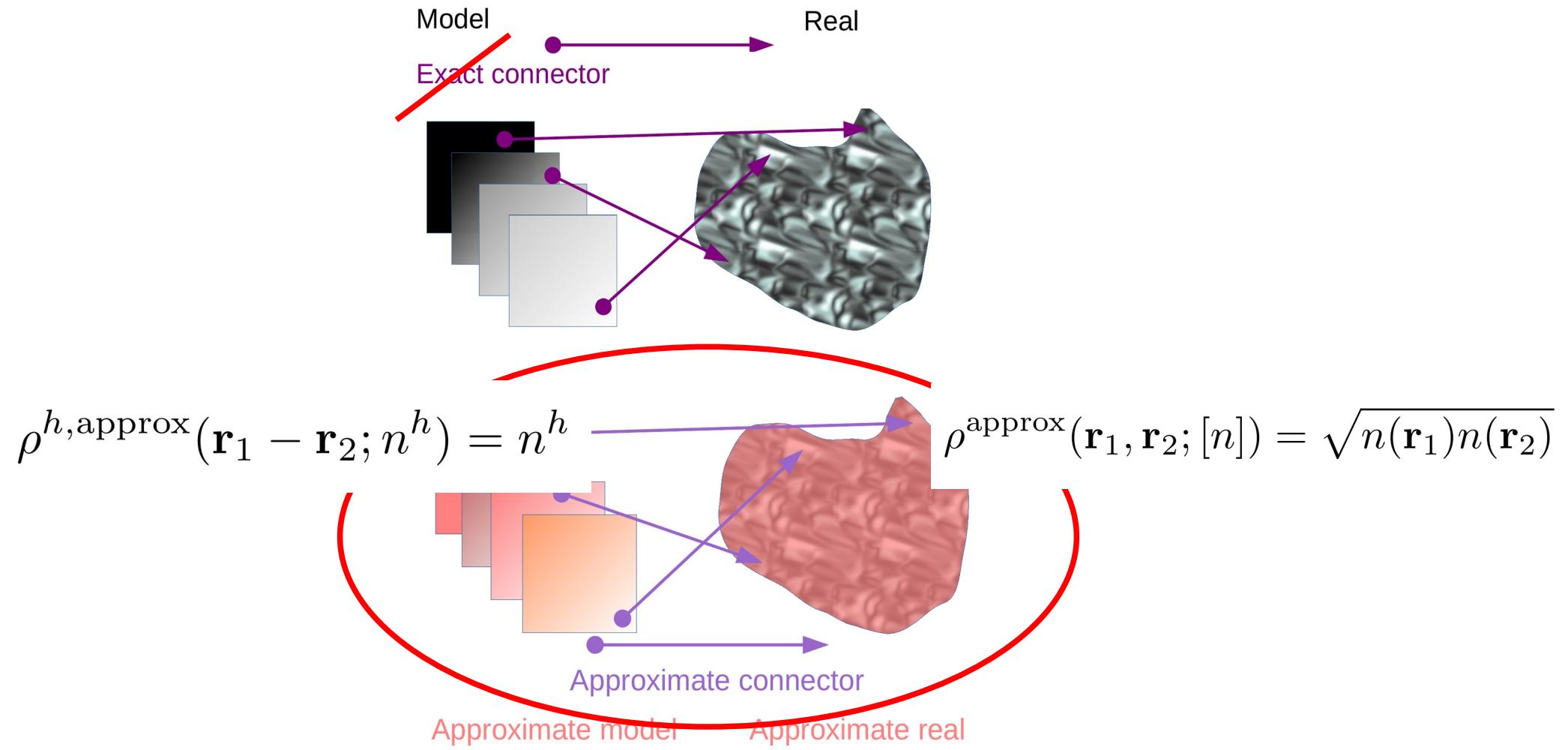
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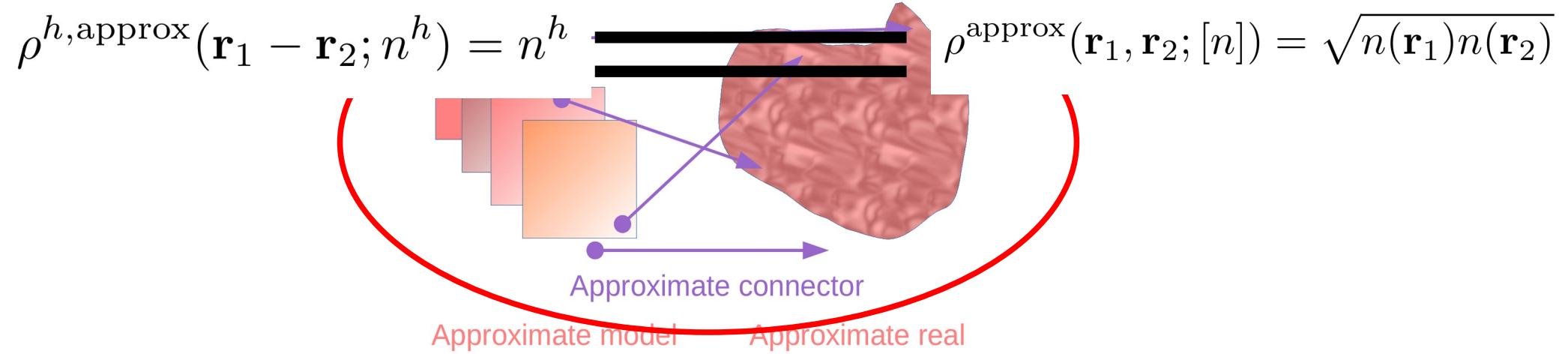
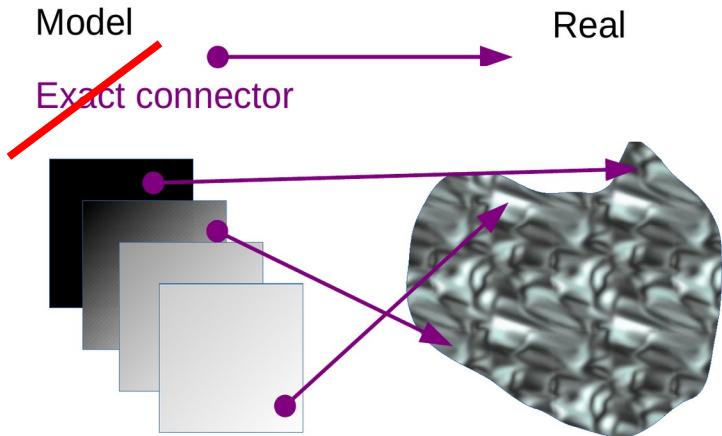
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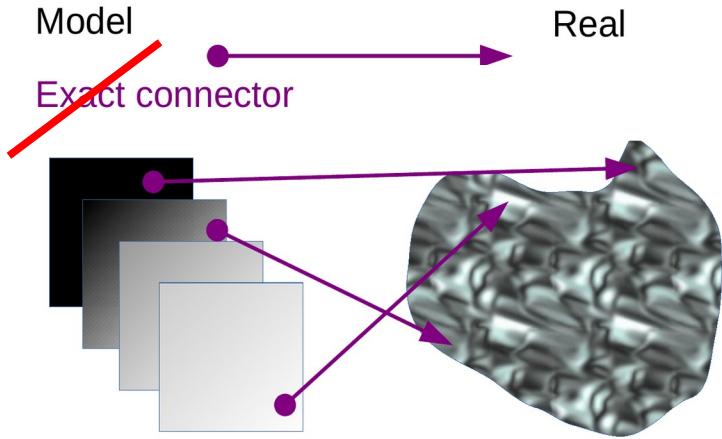
KS-LDA exchange energy	He	Si
Direct single-electron	167	575

Relative error in %

“single electron”: $\rho^{\text{approx}}(\mathbf{r}_1, \mathbf{r}_2; [n]) = \sqrt{n(\mathbf{r}_1)n(\mathbf{r}_2)}$







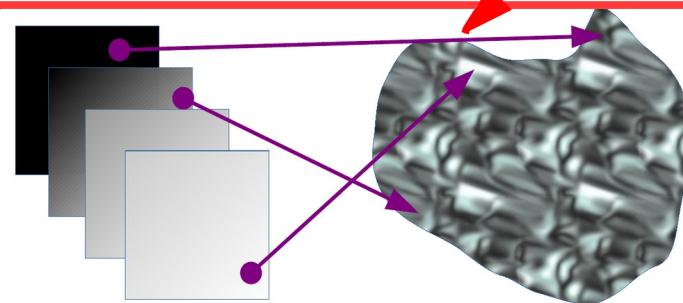
$$\rho^{h,\text{approx}}(\mathbf{r}_1 - \mathbf{r}_2; n^h) = n^h$$

$\rho^{\text{approx}}(\mathbf{r}_1, \mathbf{r}_2; [n]) = \sqrt{n(\mathbf{r}_1)n(\mathbf{r}_2)}$

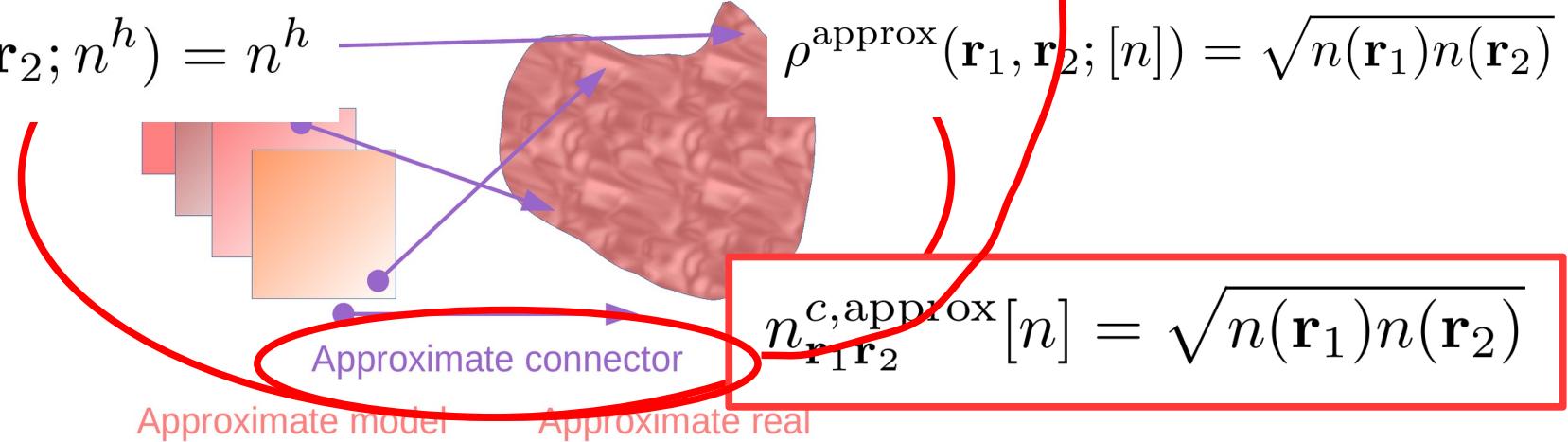
$n_{\mathbf{r}_1 \mathbf{r}_2}^{c,\text{approx}}[n] = \sqrt{n(\mathbf{r}_1)n(\mathbf{r}_2)}$

Approximate model
Approximate real

$$\rho^c(\mathbf{r}_1, \mathbf{r}_2; [n]) \approx \rho^h\left(\mathbf{r}_1 - \mathbf{r}_2; n^h = \sqrt{n(\mathbf{r}_1)n(\mathbf{r}_2)}\right)$$



$$\rho^{h,\text{approx}}(\mathbf{r}_1 - \mathbf{r}_2; n^h) = n^h \quad \rho^{\text{approx}}(\mathbf{r}_1, \mathbf{r}_2; [n]) = \sqrt{n(\mathbf{r}_1)n(\mathbf{r}_2)}$$



The connector imports knowledge from the model system

- Approximation already very good, model far from real: COT not useful
- Approximation rough, model reflects aspects of real: COT big gain

KS-LDA exchange energy	He	Si
Direct single-electron	167	575
COT single-electron	51	6

Relative error in %

The connector imports knowledge from the model system

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KS-LDA exchange energy	He	Si
Direct single-electron	167	575
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Relative error in %

A linear expansion connector for the KS xc potential

$$v_{\text{xc}}^{\text{approx}}(\mathbf{r}; [n]) = v_{\text{xc}}^h(n_0) + \int d\mathbf{r}'(n(\mathbf{r}') - n_0)f_{\text{xc}}(|\mathbf{r} - \mathbf{r}'|; n_0)$$

Linearization around some homogeneous density

Kohn, W. & Sham, L. J., Phys. Rev. 140, A1133 (1965)

Palummo, M., Onida, G., Del Sole, R., Corradini, M., Reining, L., Phys. Rev. B 60, 11329 (1999)

xc kernel known:

M. Corradini, R. Del Sole, G. Onida, and M. Palummo, Phys. Rev. B 57, 14569 (1998)

S. Moroni, D. M. Ceperley, and G. Senatore, PRL 75, 6 (1995)

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$$v_{\text{xc}}^{h,\text{approx}}(n^h) = v_{\text{xc}}^h(n_0) + (n^h - n_0)f_{\text{xc}}^h(n_0)$$

Linearization around some homogeneous density

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M. Corradini, R. Del Sole, G. Onida, and M. Palummo, Phys. Rev. B 57, 14569 (1998)
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A linear expansion connector for the KS xc potential

$$v_{\text{xc}}^{\text{approx}}(\mathbf{r}; [n]) = v_{\text{xc}}^h(n_0) + \int d\mathbf{r}' (n(\mathbf{r}') - n_0) f_{\text{xc}}(|\mathbf{r} - \mathbf{r}'|; n_0)$$

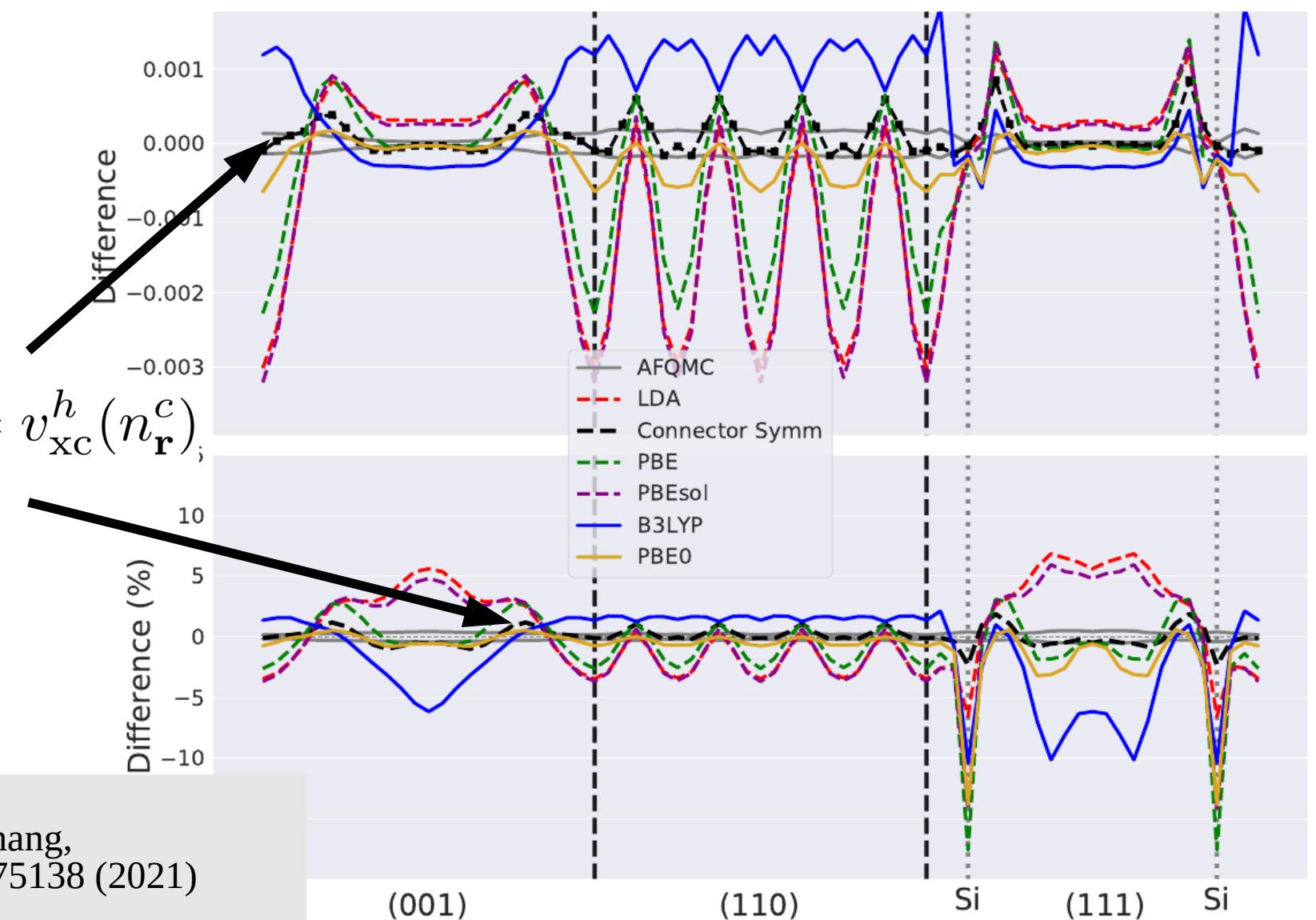
$$v_{\text{xc}}^{h,\text{approx}}(n^h) = v_{\text{xc}}^h(n_0) + (n^h - n_0) f_{\text{xc}}^h(n_0)$$

$$n_{\mathbf{r}}^{c,\text{approx}}([n]) = \frac{1}{f_{\text{xc}}^h(n_0)} \int d\mathbf{r}' n(\mathbf{r}') f_{\text{xc}}(|\mathbf{r} - \mathbf{r}'|; n_0)$$

xc kernel known:

M. Corradini, R. Del Sole, G. Onida, and M. Palummo, Phys. Rev. B 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore, PRL 75, 6 (1995)

Silicon,
density from
 $v_{xc}(\mathbf{r}, [n]) = v_{xc}^h(n_{\mathbf{r}}^c)$;



QMC benchmark:
Chen, Motta, Ma, Zhang,
Phys. Rev. B 103, 075138 (2021)

Silicon,
density from
 v_{xc}

HEG=good model for silicon

+ linear approx very good

→ BINGO at first attempt

Difference

-5
-10

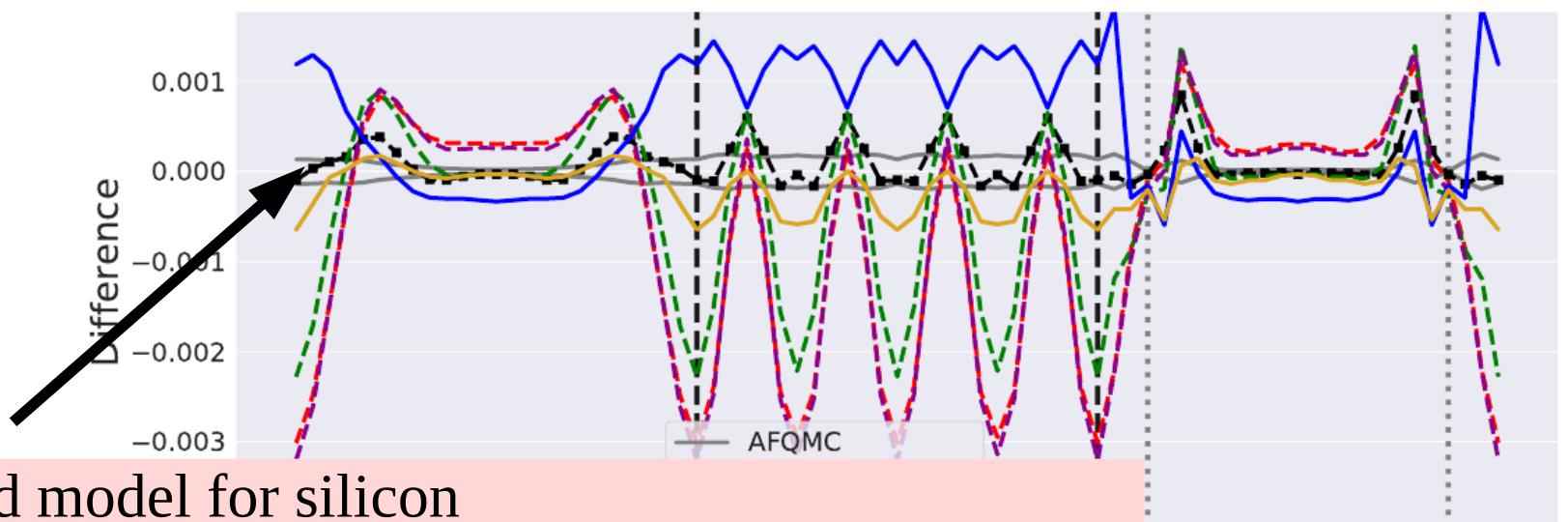
(001)

(110)

Si

(111)

Si



QMC benchmark:
Chen, Motta, Ma, Zhang,
Phys. Rev. B 103, 075138 (2021)

Sodium Chloride NaCl:

Approximation	MAE along the route (%)	MAE in 3D grid (%)
LDA	4.47	5.13
PBE	0.86	0.81
PBEsol	2.40	2.49
B3LYP	0.67	0.61
PBE0	1.61	1.30
Connector Symm	2.07	2.03

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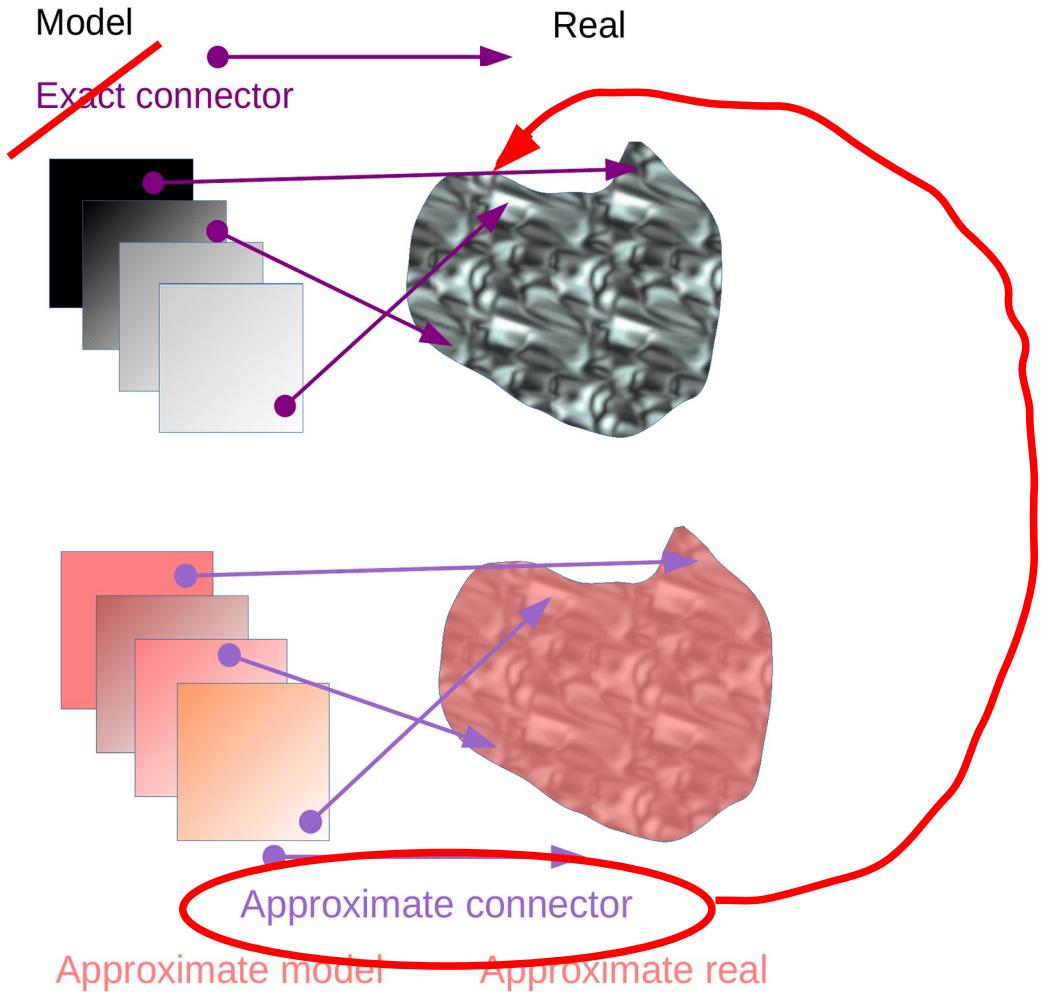
Sodium Chloride NaCl:

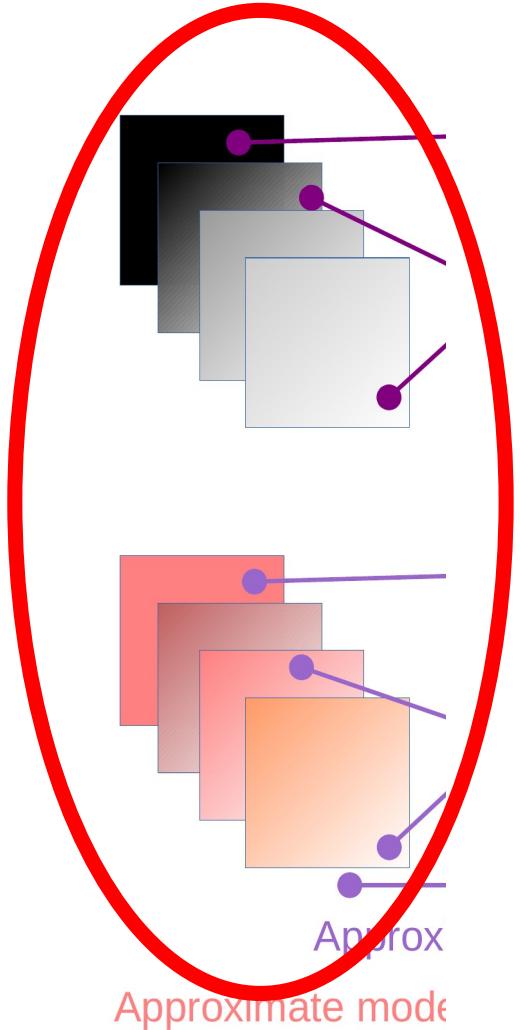
Approximation	MAE along the route (%)	MAE in 3D grid (%)
LDA	4.47	5.13
PBE	0.86	0.81

HEG = modest model for NaCl → improvement wrt LDA, but needs more work

B3LYP	0.67	0.61
PBE0	1.61	1.30
Connector Symm	2.07	2.03

QMC benchmark:
Chen, Motta, Ma, Zhang,
Phys. Rev. B 103, 075138 (2021)





Calculate the model

exactly

and with controlled approximations

in a *wide* parameter range

Methods, models and materials: Joining forces to deal with the many-body problem

- Functionals,
and strategies to find them
- The connector project,
or how to play Lego together
- The homogeneous electron gas,
trouble with our methods, and promising combinations
- Insert concerning MBPT+TDDFT,
the total energy
- A Christmas advocacy

Methods, models and materials: Joining forces to deal with the many-body problem

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**Spectroscopy
and screening in the HEG
in wide parameter range**

Methods, models and materials: Joining forces to deal with the many-body problem

- Functionals,
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Spectroscopy and screening in the HEG in wide parameter range



Jaakko Koskelo

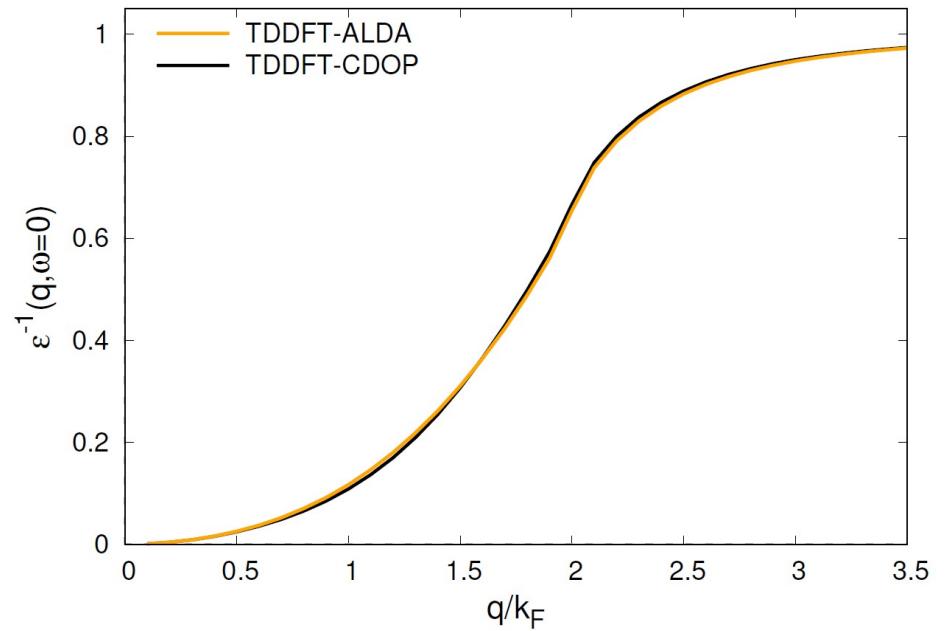


Matteo Gatti

M. Corradini, et al., PRB 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore,
PRL 75, 6 (1995)

HEG, rs=4

Static screening



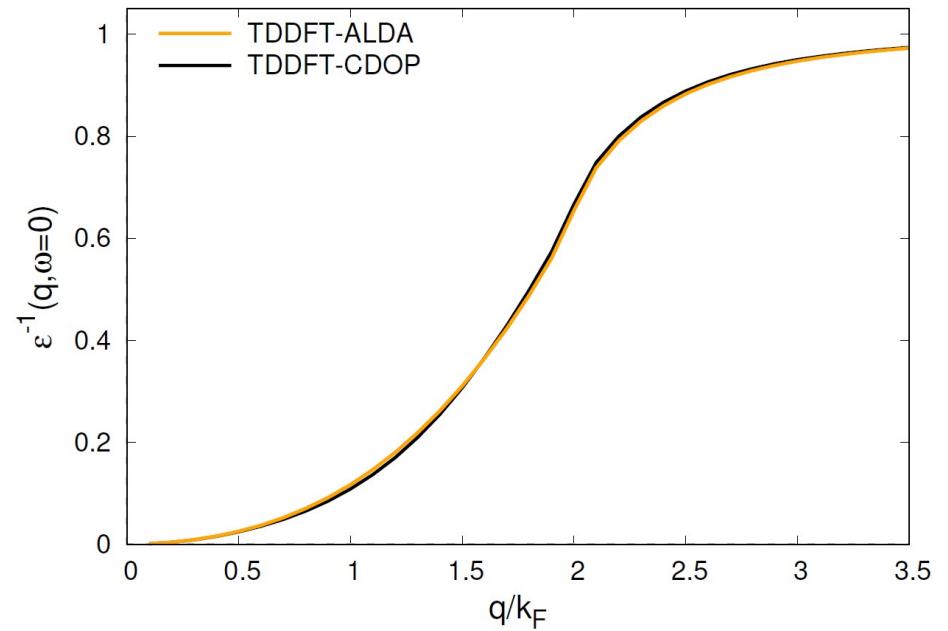
M. Corradini, et al., PRB 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore,
PRL 75, 6 (1995)

ALDA



HEG, rs=4

Static screening

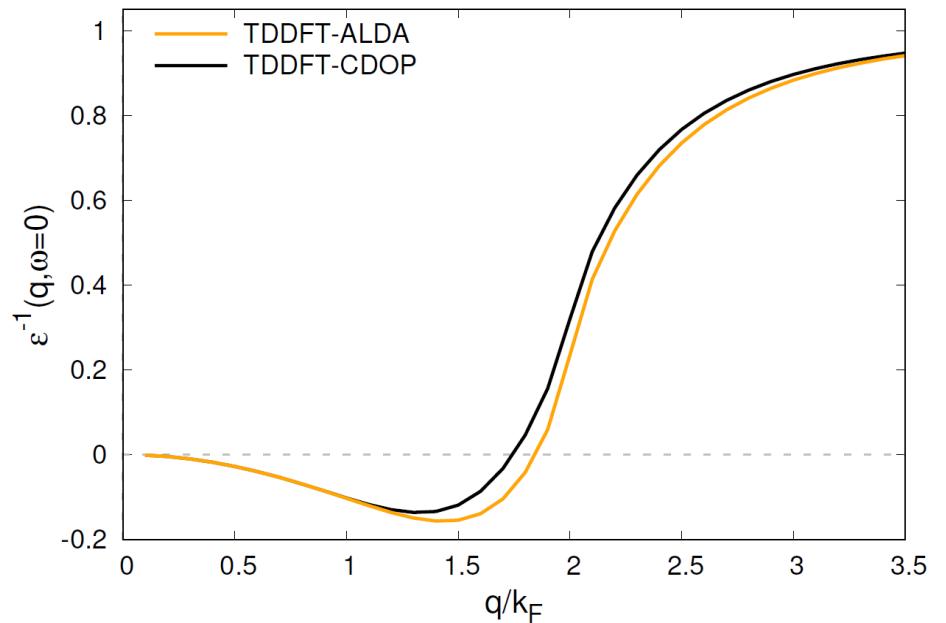
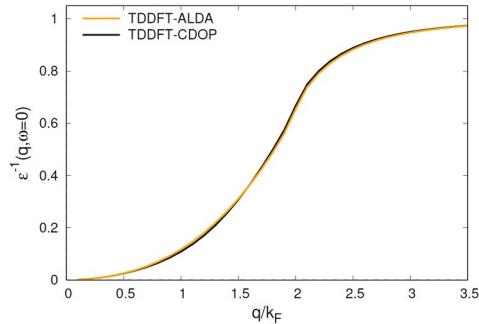


M. Corradini, et al., PRB 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore,
PRL 75, 6 (1995)

HEG, rs=8

Static screening

HEG, rs=4



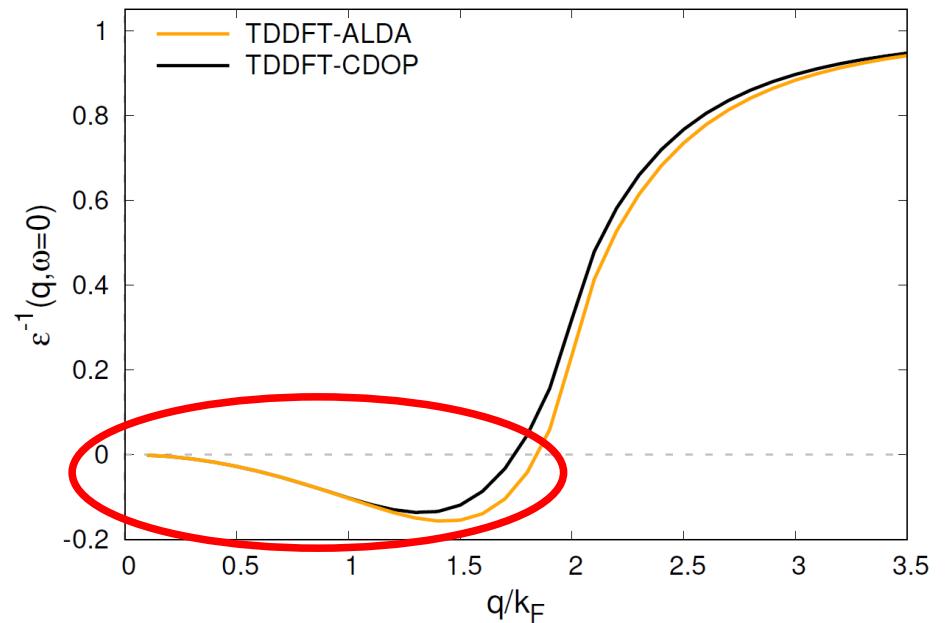
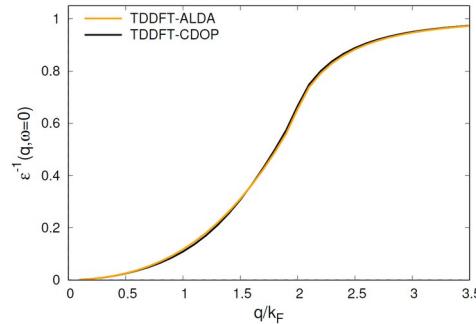
M. Corradini, et al., PRB 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore,
PRL 75, 6 (1995)

Negative static screening!!!

HEG, rs=8

Static screening

HEG, rs=4



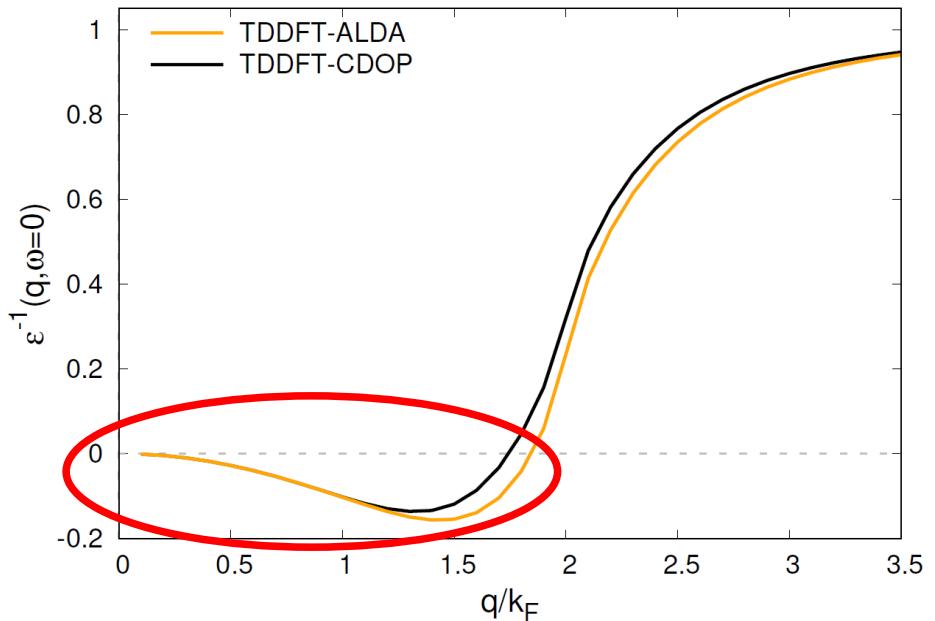
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Negative static screening!!!

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“Ghost plasmon”

Takayanagi and Lipparini, PRB 56, 4872 (1997)
Dolgov, Kirzhnits, and Maksimov, Rev. Mod. Phys. 53, 81 (1981)

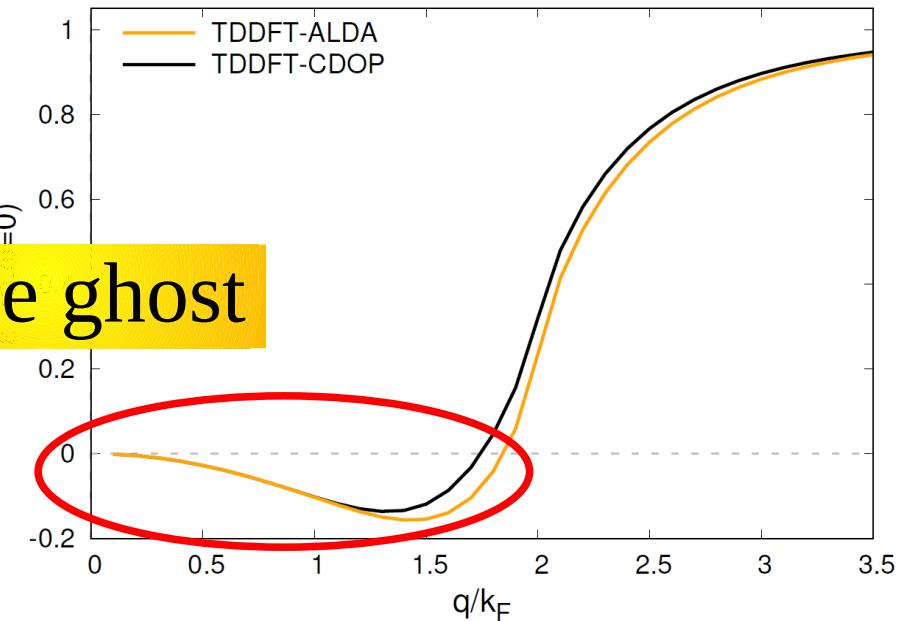


M. Corradini, et al., PRB 57, 14569 (1998)
S. Moroni, D. M. Ceperley, and G. Senatore,
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Negative static screening!!!

“Ghost plasmon”

Hunting the ghost



Takayanagi and Lipparini, PRB 56, 4872 (1997)
Dolgov, Kirzhnits, and Maksimov, Rev. Mod. Phys. 53, 81 (1981)

Is a ghost important?

$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega)v_{\text{ext}}(\omega)$$

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

Is a ghost important?

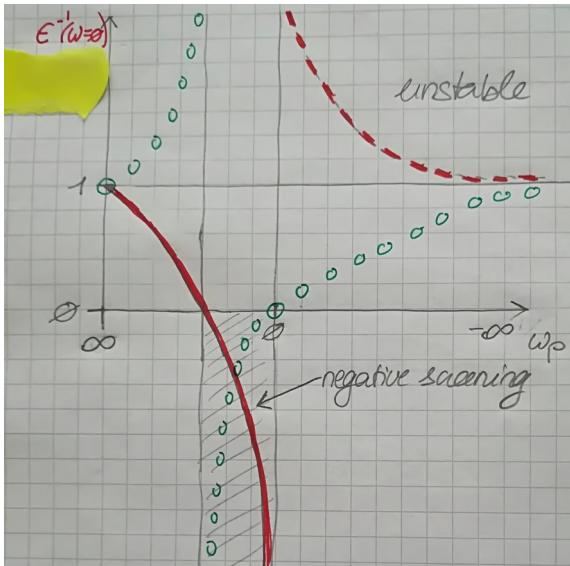
$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega)v_{\text{ext}}(\omega)$$

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

$$\chi(\omega) = a \frac{2\omega_p}{\omega^2 - \omega_p^2}$$

$$\epsilon^{-1}(\omega) = 1 + v_c a \frac{2\omega_p}{\omega^2 - \omega_p^2}$$

→ $\epsilon^{-1}(\omega = 0) = 1 - \frac{2v_c a}{\omega_p} < 0$ for $\omega_p < 2av_c$



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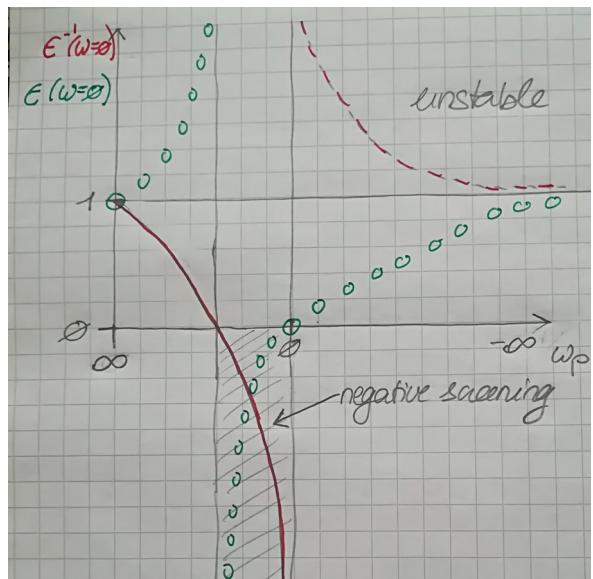
$$\epsilon^{-1}(\omega = 0) < 0 \rightarrow \epsilon(\omega = 0) < 0$$

→ $\epsilon(\omega) = \frac{\omega^2 - \omega_p^2}{\omega^2 - \omega_p^2 + 2av_c\omega_p}$

$$\epsilon = 1 - v_c P$$

$$\text{Pole at } \omega = \pm \sqrt{\omega_p^2 - 2av_c\omega_p}$$

Is a ghost important?



$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega)v_{\text{ext}}(\omega)$$

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

Is a ghost important?

$\chi(\omega)$ = Low energy excitation \rightarrow negative screening

Poles of P moving to zero \rightarrow ghost (imaginary) poles

Precursors for instability !

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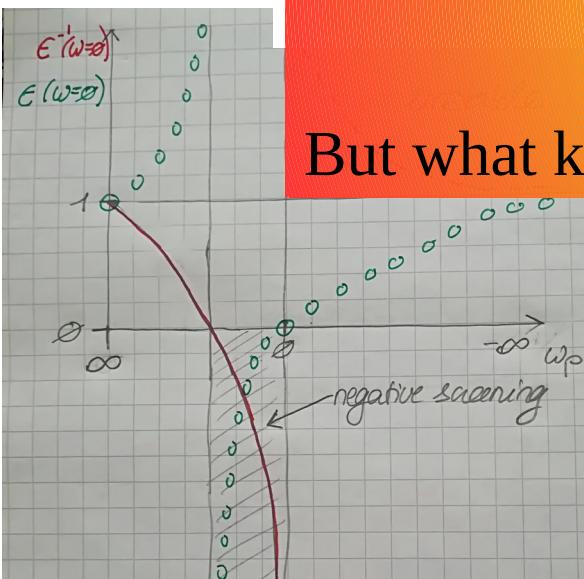
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But what kind of excitation is this?



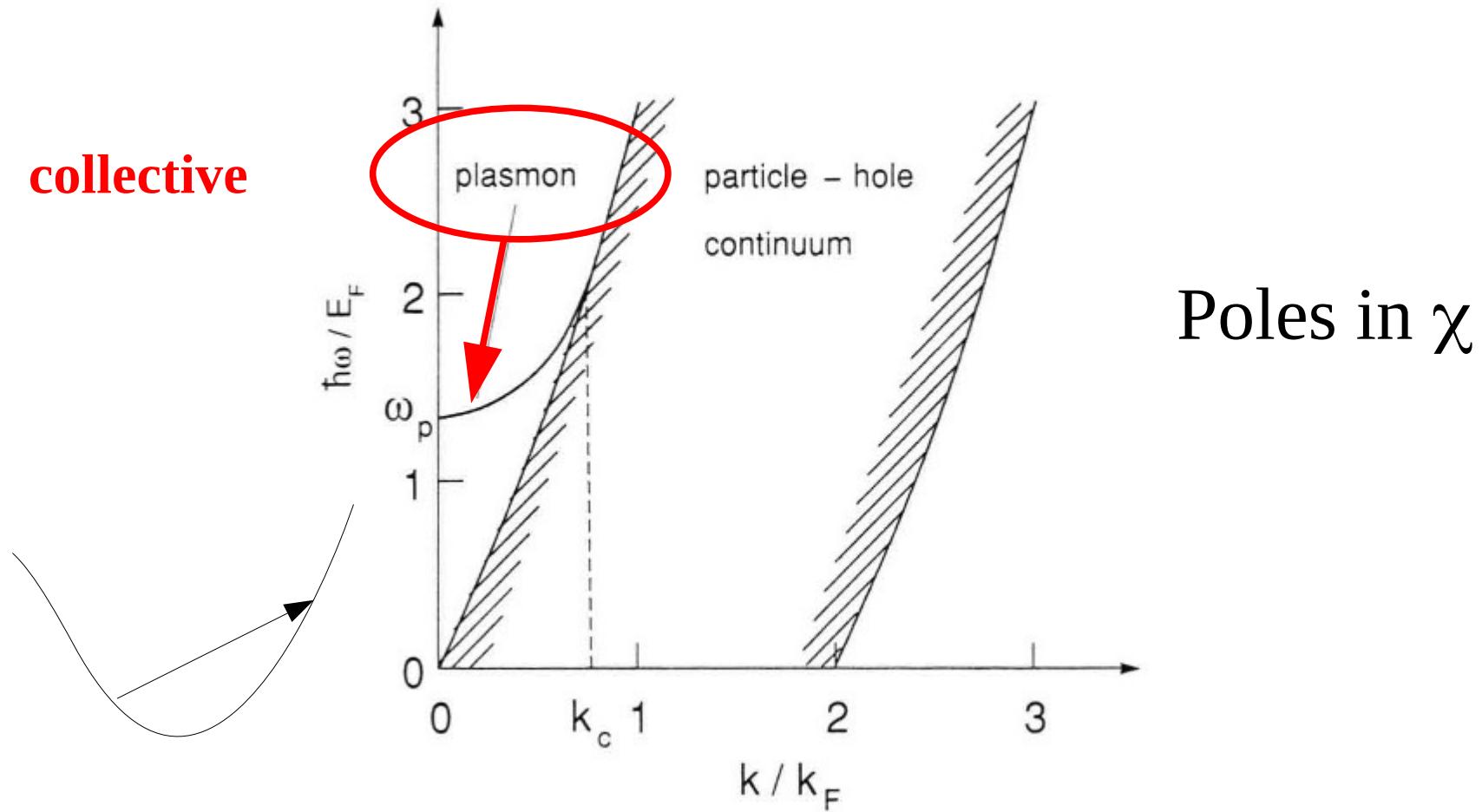
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Excitations in the homogeneous electron gas

collective



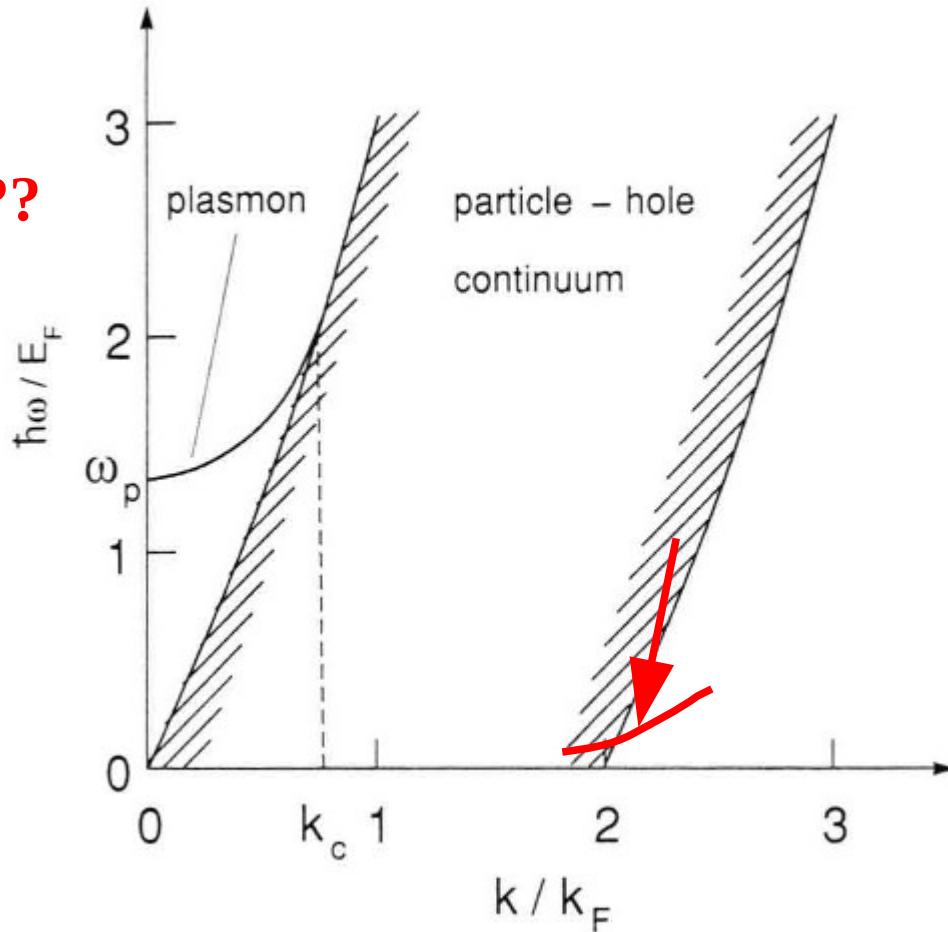
Poles in χ

from K. Sturm, "Dynamic Structure Factor: an Introduction", Zeitschrift für Naturforschung A (1993)

Excitations in the homogeneous electron gas

Collective???

Poles in χ



$$v_{\text{tot}}(\omega) = \epsilon^{-1}(\omega)v_{\text{ext}}(\omega)$$

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

Why should this be important?

$\chi(\omega)$ = Low energy excitation \rightarrow negative screening

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Precursors for instability !

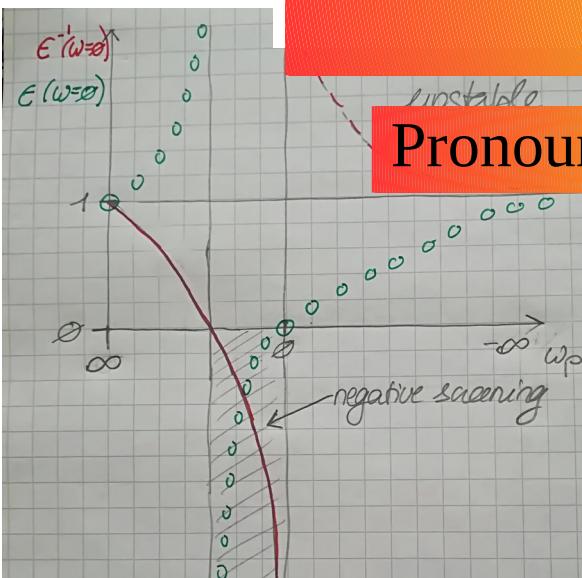
Pronounced low energy excitation = exciton?

$$\epsilon^{-1}(\omega=0) < 0 \quad \epsilon(\omega=0) < 0$$

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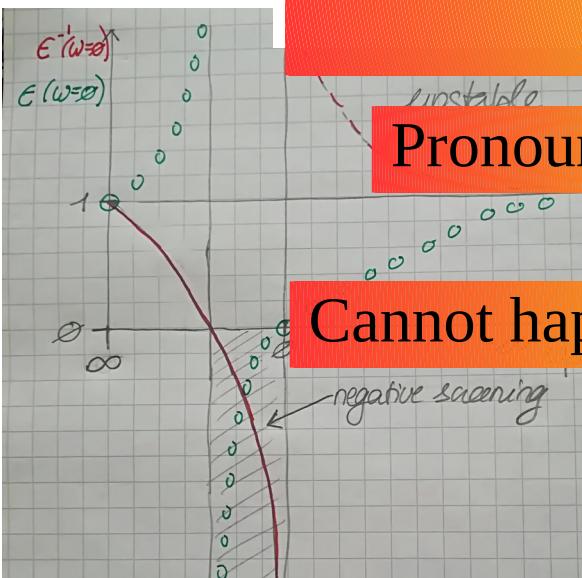
Pronounced low energy excitation = exciton?

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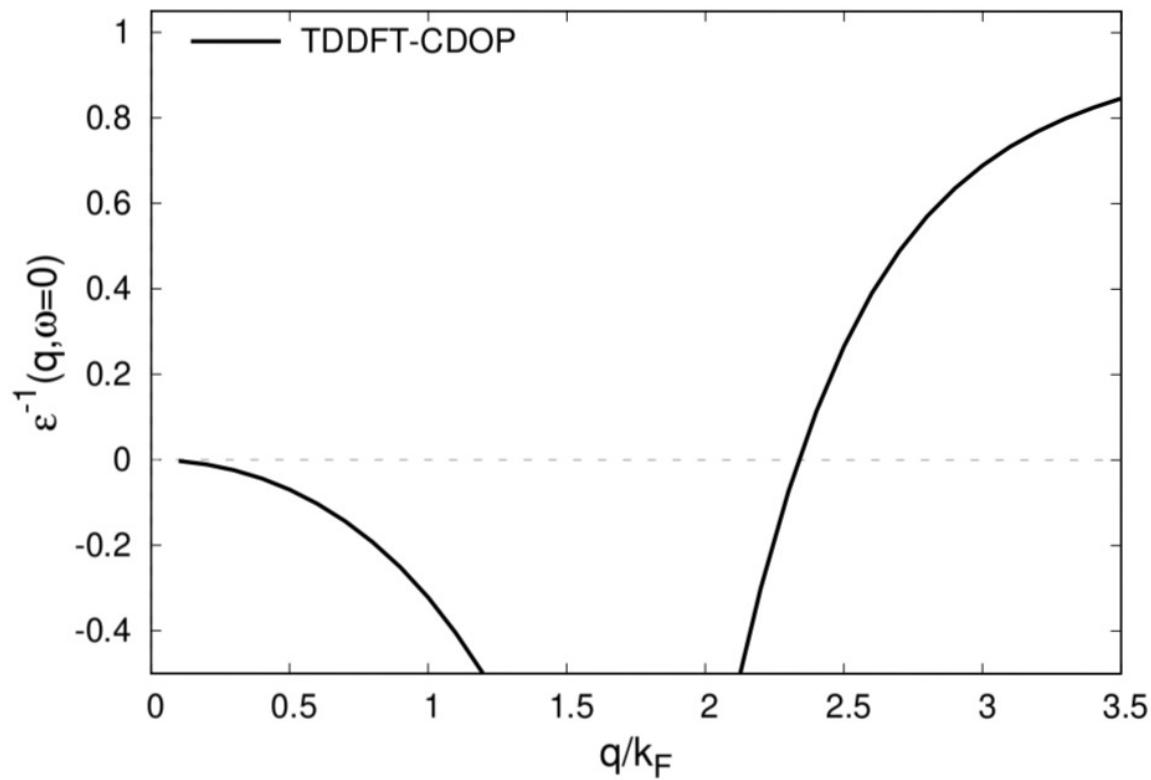
Cannot happen with classical electrostatics (the RPA)!!!

$$\epsilon = 1 - v_c P$$

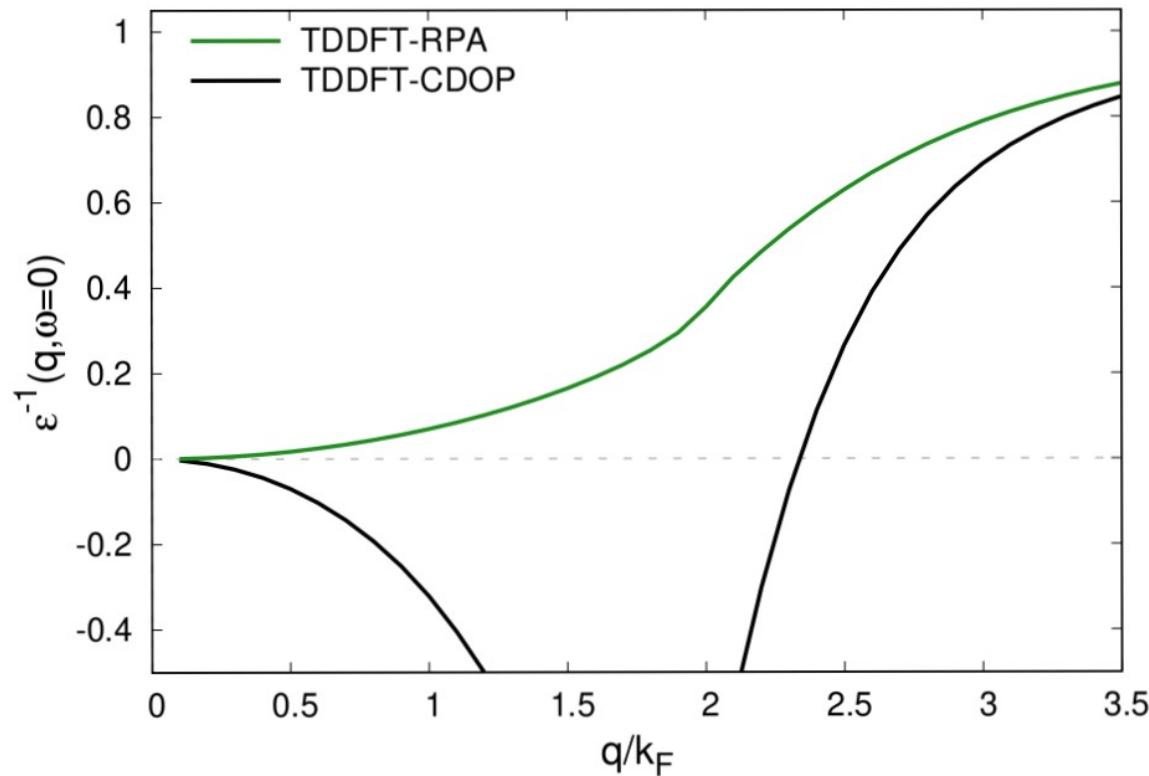
$$\text{Pole at } \omega = \pm \sqrt{\omega_p^2 - 2av_c\omega_p}$$



$r_s=22$

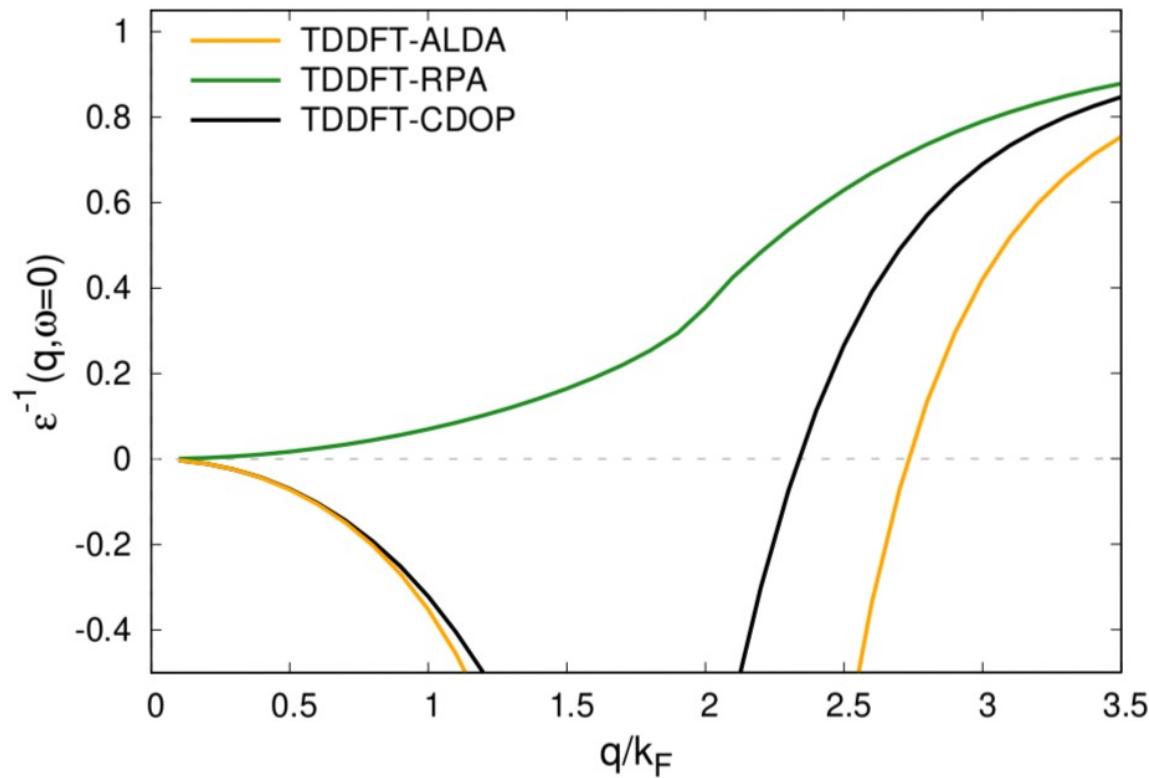


$r_s=22$



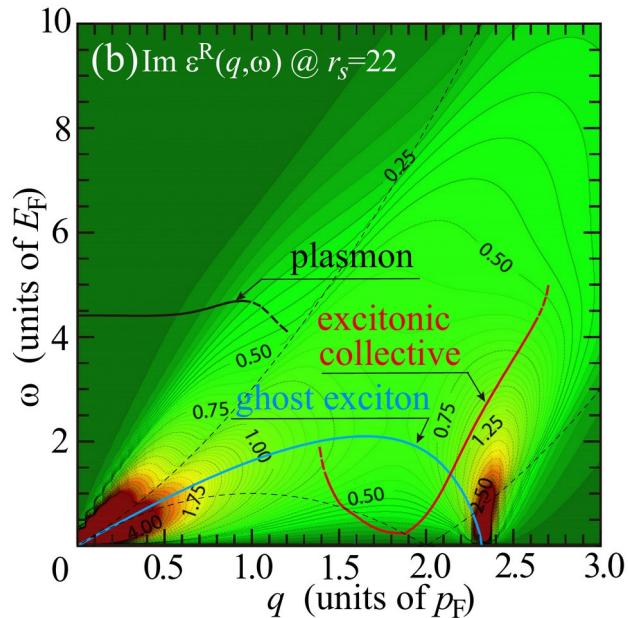
Short-range physics?

$r_s=22$



Intuitively: excitons screened out in the HEG!!!

But at low density.....



Y. Takada, PRB 94, 245106 (2016)

See also: Takayanagi&Lipparini, PRB 56, 4872 (1997)

Panholzer, Gatti, Reining, Phys. Rev. Lett. 120, 166402 (2018)

K. Chen and K. Haule, Nature Communications 10, 3725 (2019)

T. Dornheim, S. Groth, and M. Bonitz, Physics Reports 744, 1 (2018)

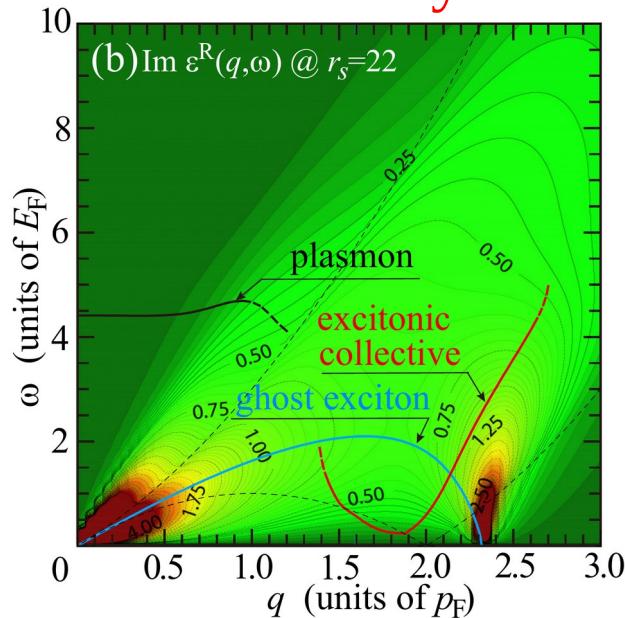
T. Dornheim, S. Groth, J. Vorberger, and M. Bonitz, Phys. Rev. Lett. 121, 255001 (2018)

S. Groth, T. Dornheim, and J. Vorberger, Phys. Rev. B 99, 235122 (2019)

Intuitively: excitons screened out in the HEG!!!

But at low density..... Does the Bethe Salpeter equation (with our approx.) yield low energy and ghost modes?

If yes, what is their nature?



Y. Takada, PRB 94, 245106 (2016)

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Panholzer, Gatti, Reining, Phys. Rev. Lett. 120, 166402 (2018)

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S. Groth, T. Dornheim, and J. Vorberger, Phys. Rev. B 99, 235122 (2019)

$$f_{\text{xc}}(q, \omega) \xrightarrow{\text{TDDFT}} \epsilon^{\text{out}}(q, \omega)$$

$$L = \underline{\quad} + \underline{\quad} \begin{matrix} \frac{\delta \Sigma}{\delta G} \\ L \end{matrix}$$

GW

W is input

The electron-hole BSE

$$\left. \begin{array}{l} \epsilon^{\text{in}}(q, \omega) \rightarrow \Sigma = iG W^{\text{in}} : \text{e-e repulsion} \\ \epsilon^{\text{in}}(q, \omega = 0) \rightarrow -W^{\text{in}} : \text{e-h attraction} \end{array} \right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q, \omega)$$

Alternative: $f_{\text{xc}}(q, \omega) \xrightarrow{\text{TDDFT}} \epsilon^{\text{out}}(q, \omega)$

The electron-hole BSE

$$\left. \begin{array}{l} \epsilon^{\text{in}}(q, \omega) \rightarrow \Sigma = iG W^{\text{in}} : \text{e-e repulsion} \\ \epsilon^{\text{in}}(q, \omega = 0) \rightarrow -W^{\text{in}} : \text{e-h attraction} \end{array} \right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q, \omega)$$

Alternative: $f_{\text{xc}}(q, \omega) \xrightarrow{\text{TDDFT}} \epsilon^{\text{out}}(q, \omega)$

Strong screening \rightarrow we do not expect excitons!

The electron-hole BSE

$$\left. \begin{array}{l} \epsilon^{\text{Screening}} \text{ is perfect in the HEG - e-e repulsion} \\ \epsilon^{\text{out}}(q, \omega = 0) \rightarrow -W : \text{e-h attraction} \end{array} \right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q, \omega)$$

Alternative: $f_{\text{xc}}(q, \omega) \xrightarrow{\text{TDDFT}} \epsilon^{\text{out}}(q, \omega)$

Strong screening \rightarrow we do not expect excitons!

The electron-hole BSE

ϵ Screening is perfect in the HEG - e-e repulsion
 ϵ at long distances and long times! e-h attraction

$\left. \begin{array}{l} \text{e-e repulsion} \\ \text{e-h attraction} \end{array} \right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q, \omega)$

Alternative: $f_{\text{xc}}(q, \omega) \xrightarrow{\text{TDDFT}} \epsilon^{\text{out}}(q, \omega)$

Strong screening \rightarrow we do not expect excitons!

The electron-hole BSE

• Screening is perfect in the HEG -
at long distances and long times!

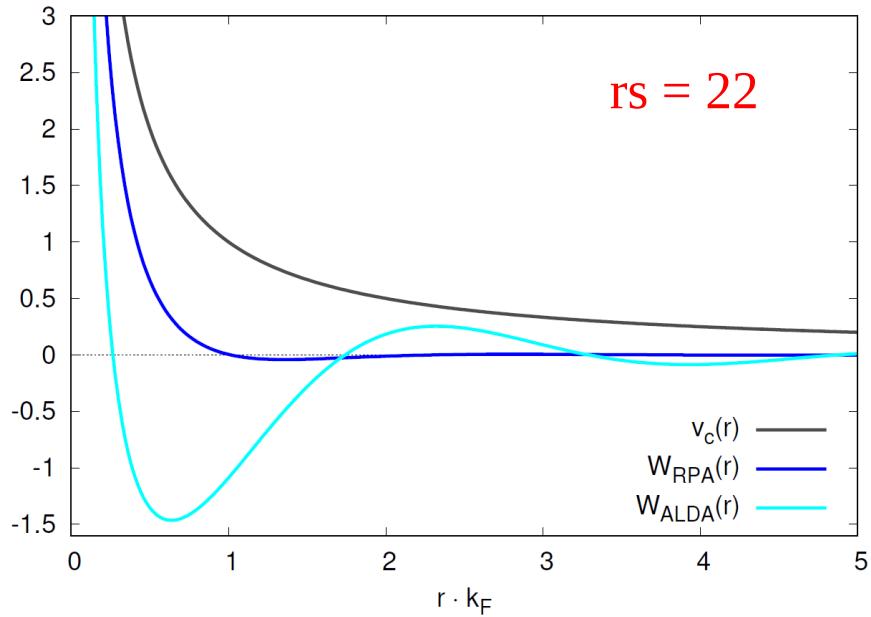
All Our input screening is more sophisticated (spatially)

$$\xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q, \omega)$$

$$\longrightarrow \epsilon^{\text{out}}(q, \omega)$$

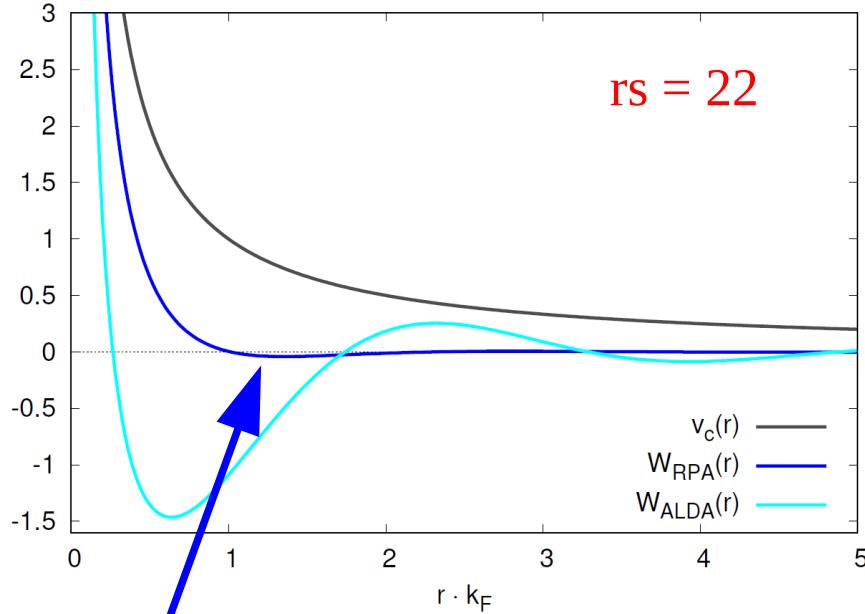
Strong screening \rightarrow we do not expect excitons!

Screened interaction in real space



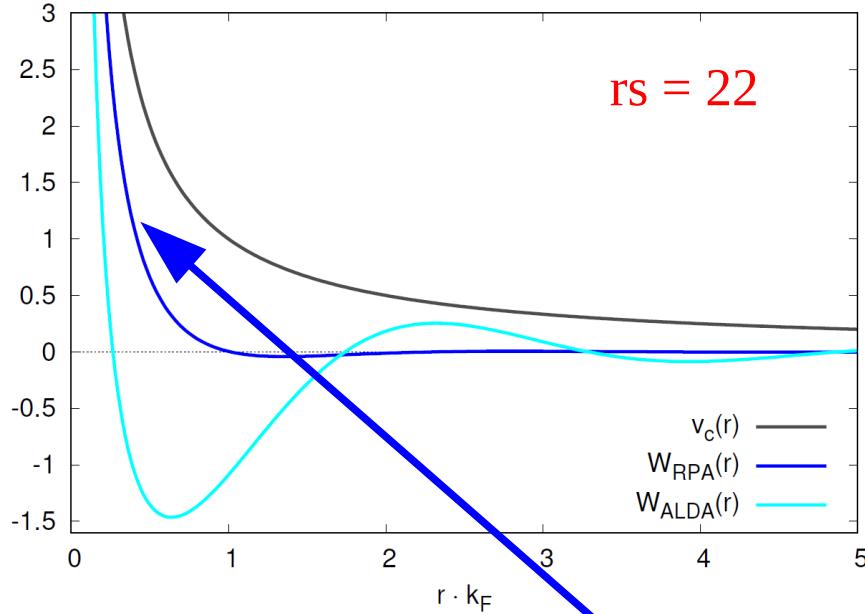
→ RPA screened interaction is indeed short ranged

Screened interaction in real space



- RPA screened interaction is indeed short ranged
- It has even negative regions (nothing to do with negative $\epsilon(q)$)

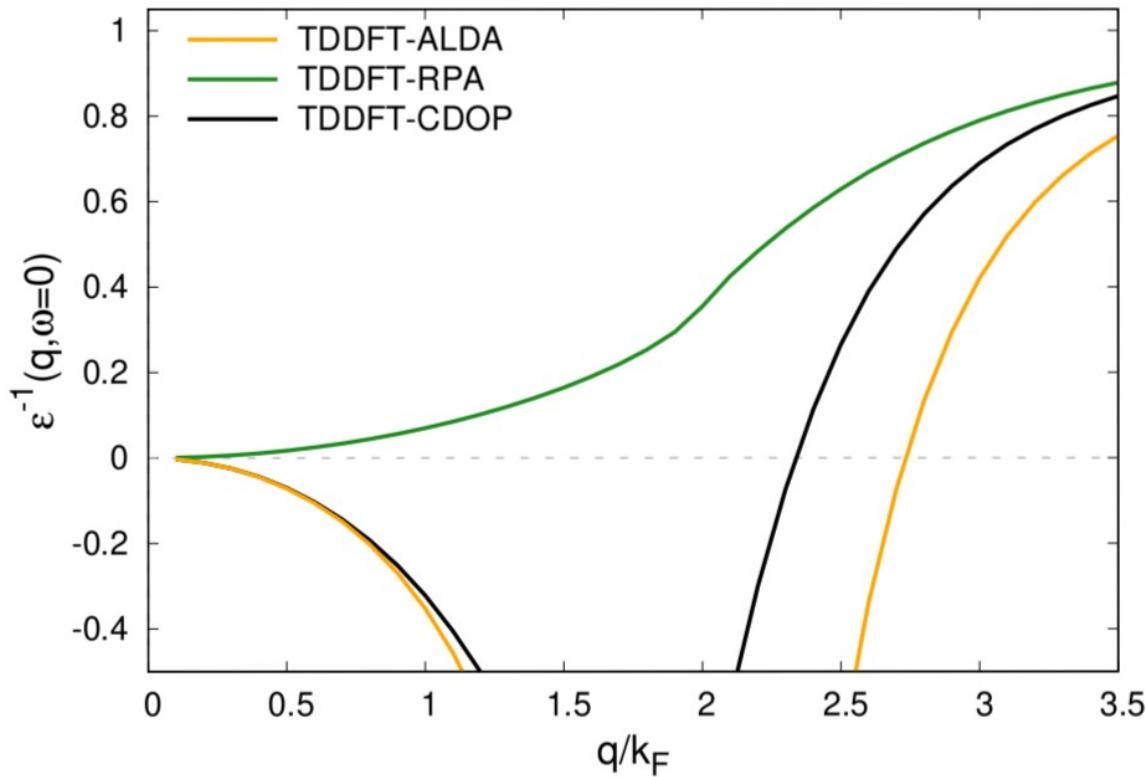
Screened interaction in real space



- RPA screened interaction is indeed short ranged
- It has even negative regions (nothing to do with negative $\epsilon(q)$)
- But there is still substantial interaction at short distances

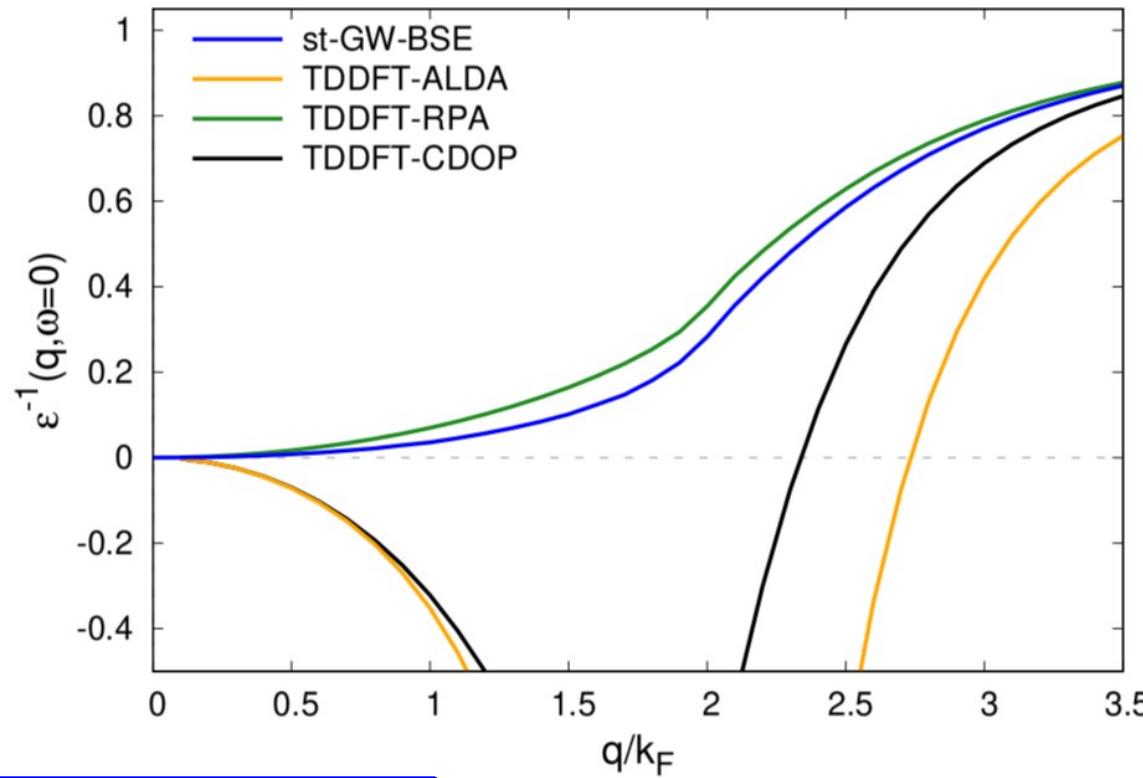
Short-range physics?

$r_s=22$



Short-range physics?

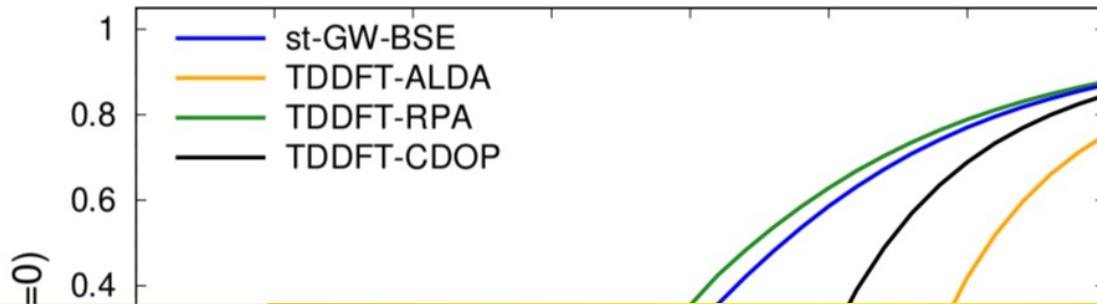
$r_s=22$



BSE with $\epsilon^{in} = \epsilon^{RPA}$

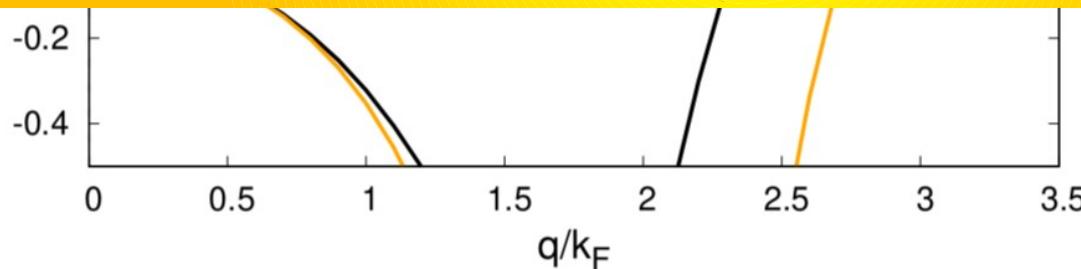
Short-range physics?

$r_s=22$



Screening is not perfect at shorter distances, even in the RPA

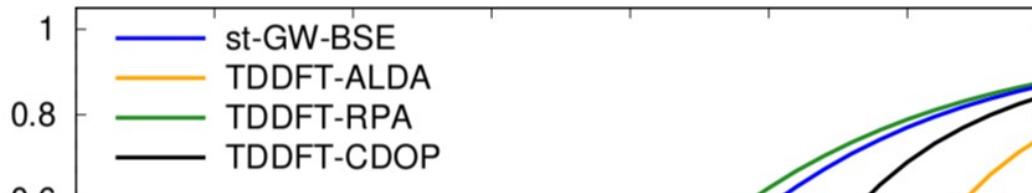
But the e-h attraction is by far not strong enough



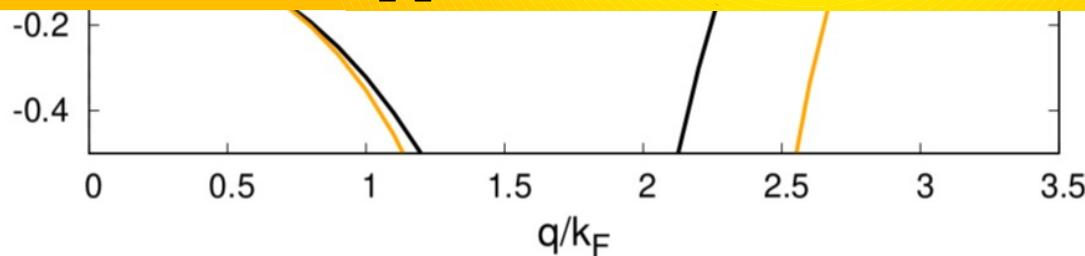
BSE with $\epsilon^{in} = \epsilon^{RPA}$

Short-range physics?

$r_s=22$



- Lousy “BSE” results in low density HEG
- Effective screening should be weaker
- Beyond current approximations: vertex corrections

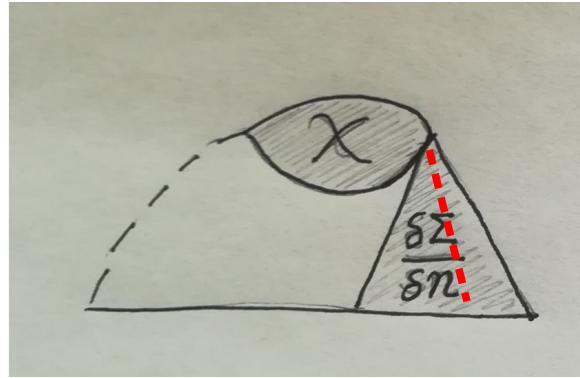


BSE with $\epsilon^{in} = \epsilon^{RPA}$

$$L = \underline{\quad} + \underline{\quad} \begin{matrix} \frac{\delta \Sigma}{\delta G} \\ L \end{matrix}$$

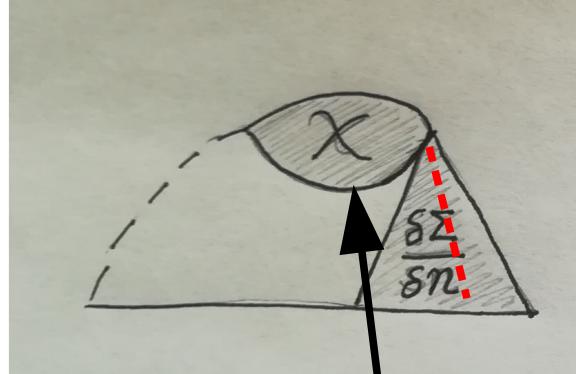
Beyond GW

Correlation self-energy:



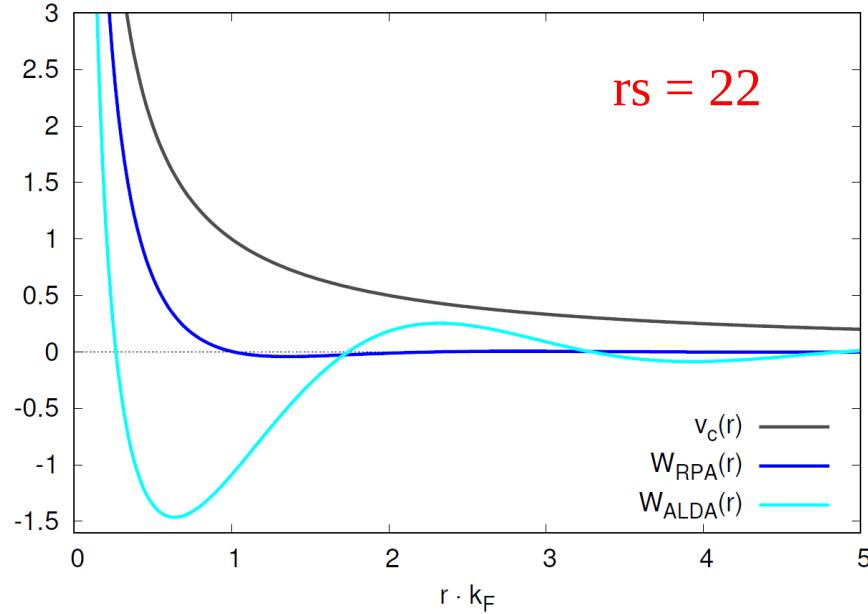
GW

Correlation self-energy:



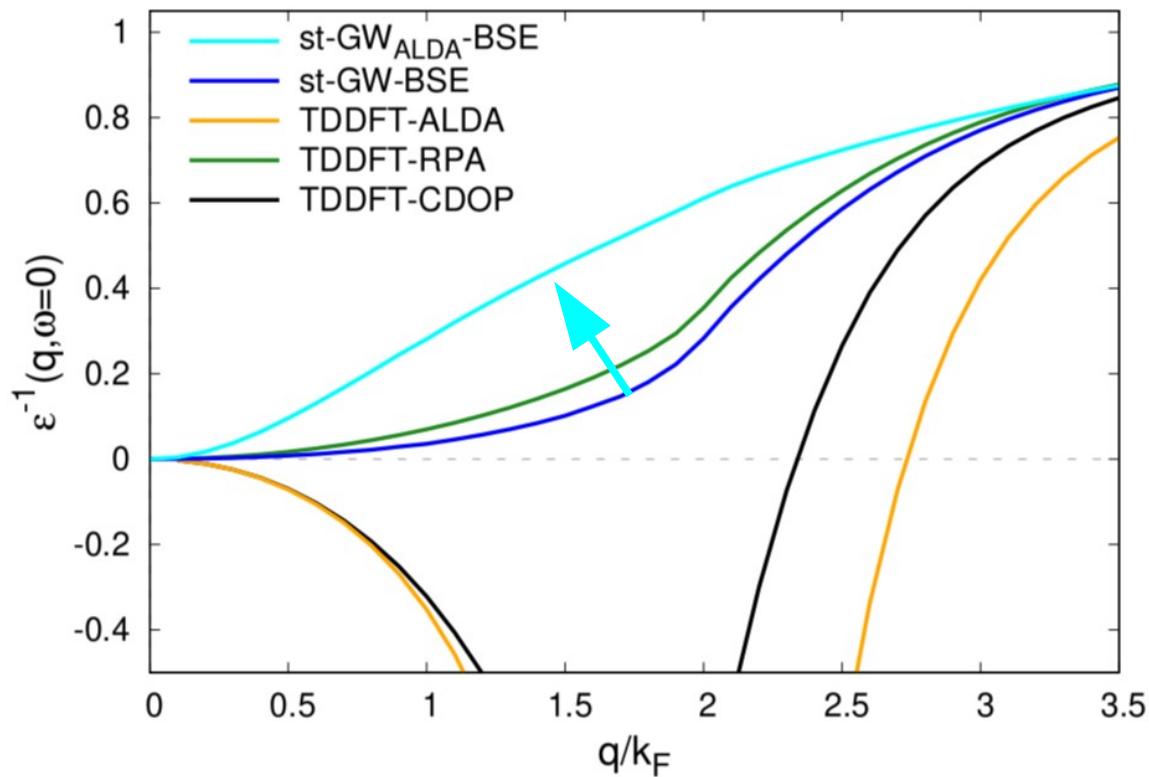
Beyond RPA: ALDA

Screened interaction in real space

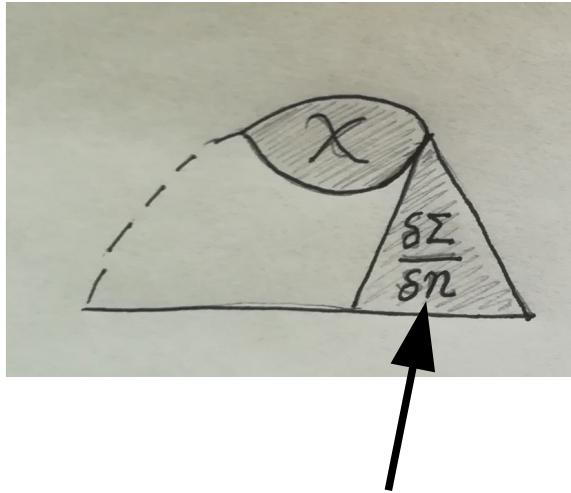


- RPA screened interaction is indeed short ranged
- ALDA oscillates more, large regions of negative $\epsilon(q)$
- But very much reduced interaction at short distances

Include xc effects in χ via TDDFT

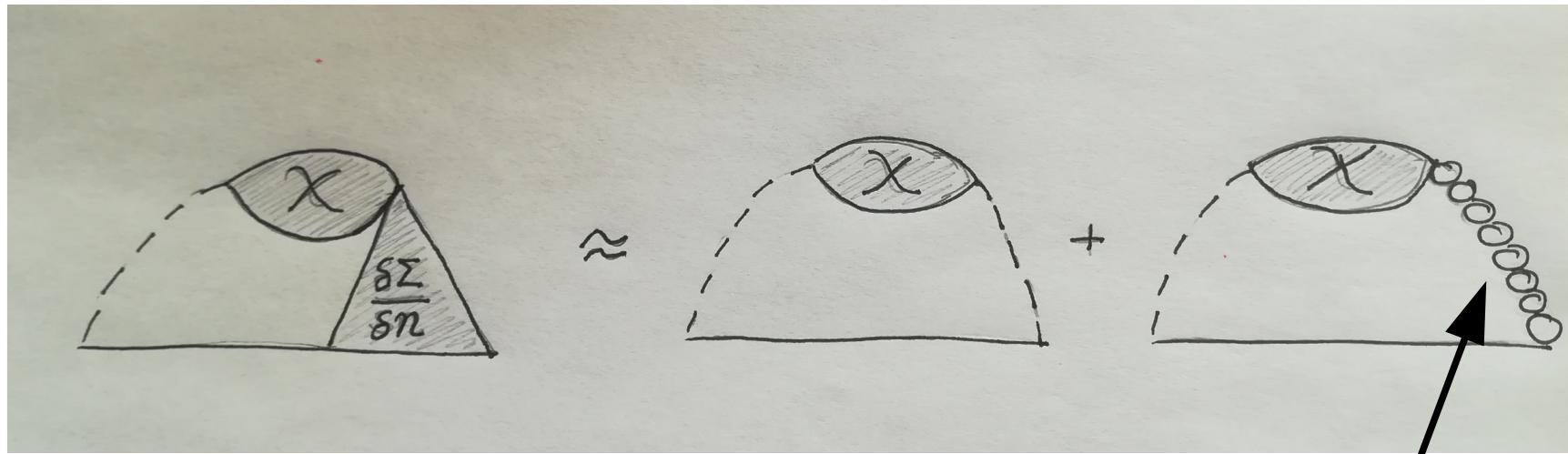


Correlation self-energy:

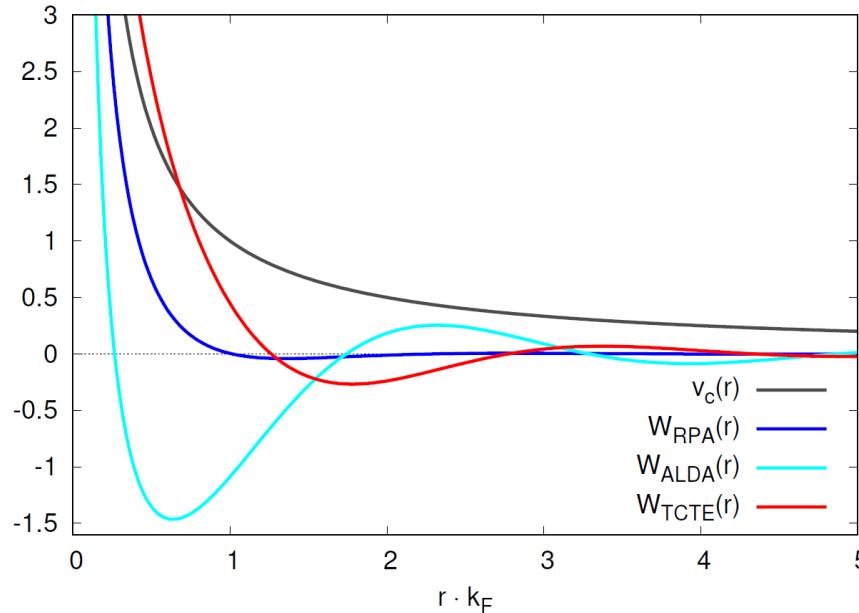


Beyond Hartree: derivative of xc self-energy

Correlation self-energy:



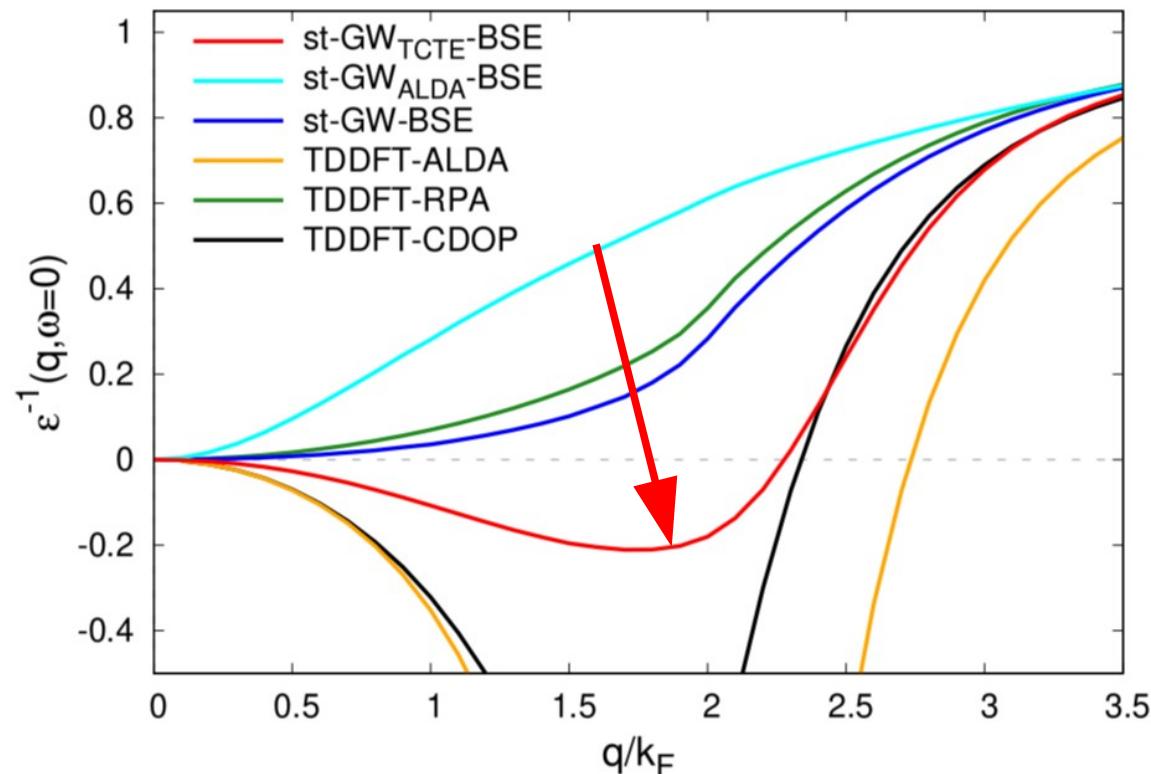
$$i \frac{\delta\Sigma_{xc}}{\delta G} \rightarrow \frac{\delta v_{xc}}{\delta n} = f_{xc}$$



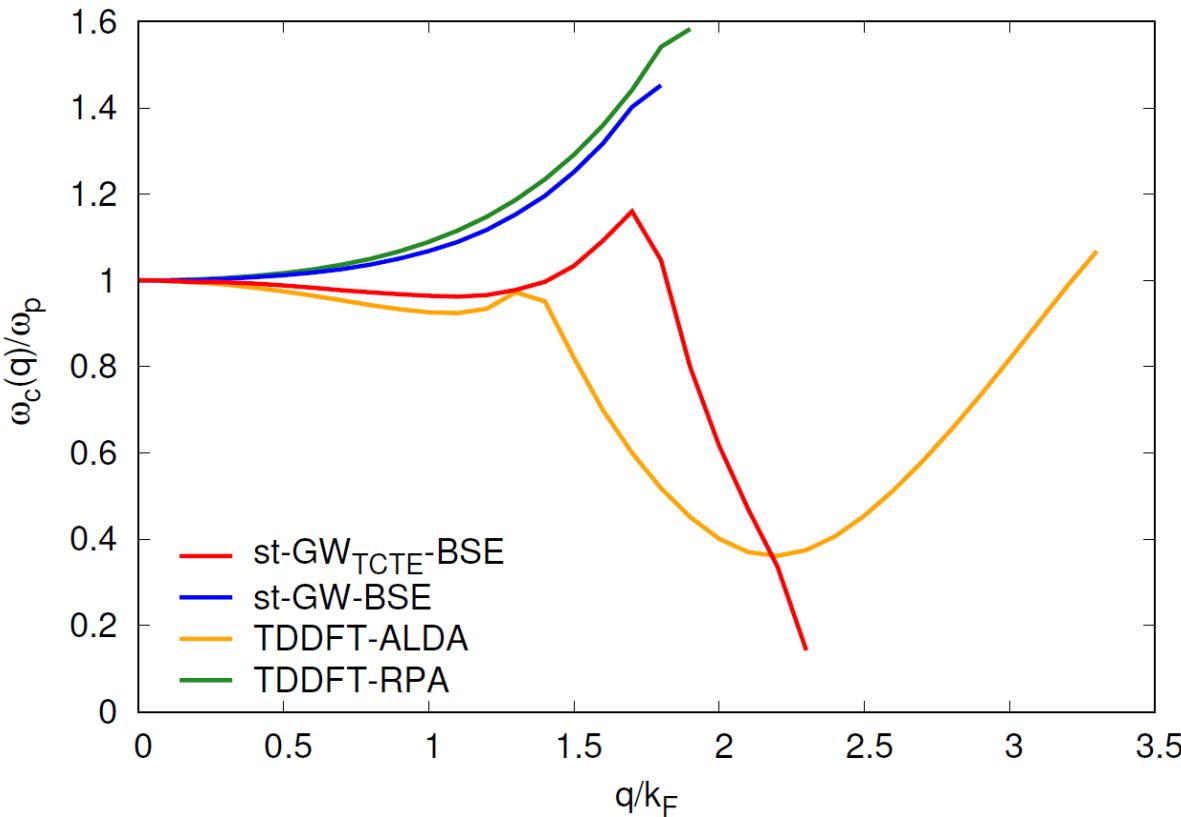
- RPA screened interaction is indeed short ranged
- ALDA oscillates more
- TCTE interaction oscillates less,
but strongly enhanced interaction at short distances

Include xc effects in χ via TDDFT

Approx. xc effects in Σ via TDDFT



Collective modes: $\text{Re } \epsilon(q, \omega_c(q)) = 0$



The electron-hole BSE as 2-particle problem

$$H_{\text{exc}} \Psi_\lambda(\mathbf{r}_h, \mathbf{r}_e) = E_\lambda \Psi_\lambda(\mathbf{r}_h, \mathbf{r}_e)$$



Intensities

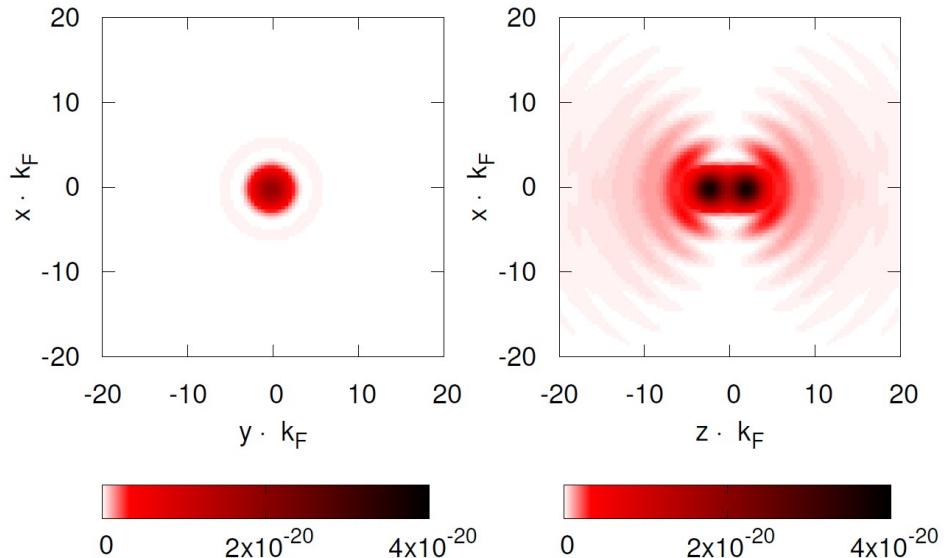
Excitation energies

$$\left. \begin{array}{l} \epsilon^{\text{in}}(q, \omega) \rightarrow \Sigma = iG W^{\text{in}} : \text{ e-e repulsion} \\ \epsilon^{\text{in}}(q, \omega = 0) \rightarrow -W^{\text{in}} : \text{ e-h attraction} \end{array} \right\} \xrightarrow{\text{BSE}} \epsilon^{\text{out}}(q, \omega)$$

Alternative: $f_{\text{xc}}(q, \omega) \xrightarrow{\text{TDDFT}} \epsilon^{\text{out}}(q, \omega)$

$q=0.001 k_F$ along z
(c)

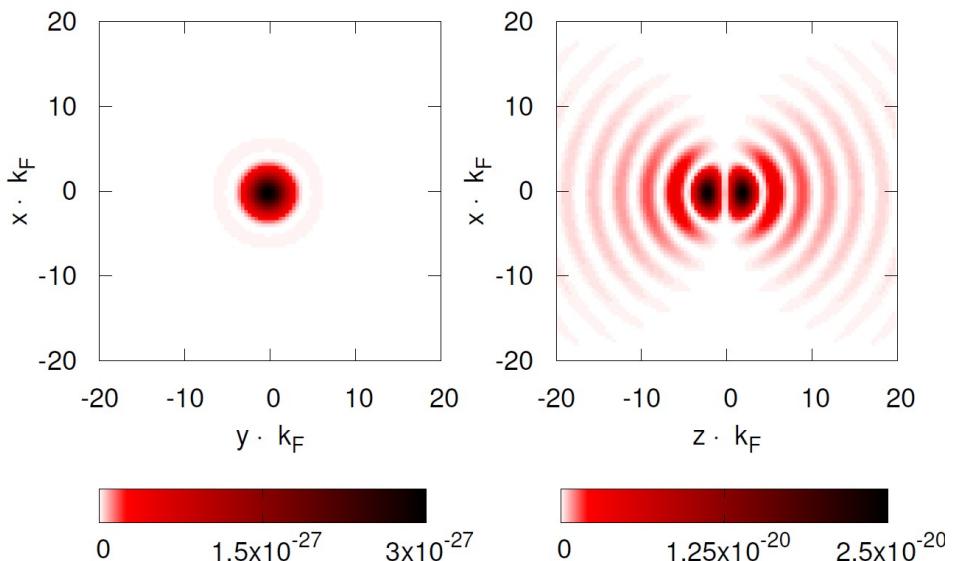
Poles of P



Sum of a couple of imaginary ghost poles

Plasmon

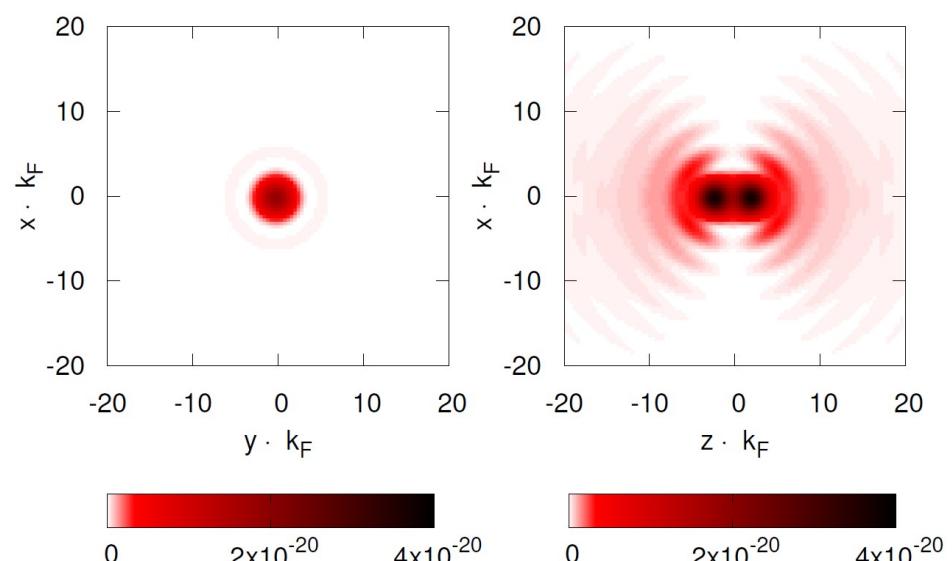
(a)



$q=0.001 k_F$ along z

Poles of P

(c)

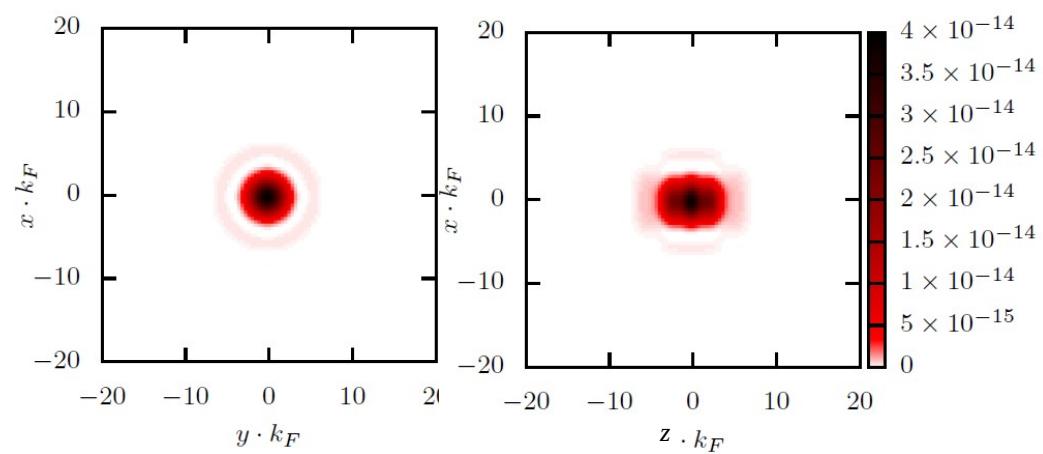
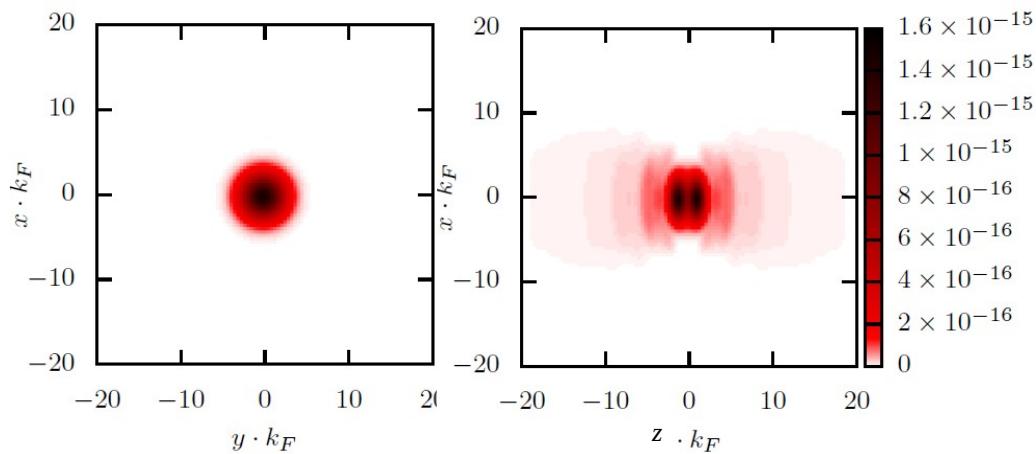


Sum of a couple of imaginary ghost poles

Plasmon

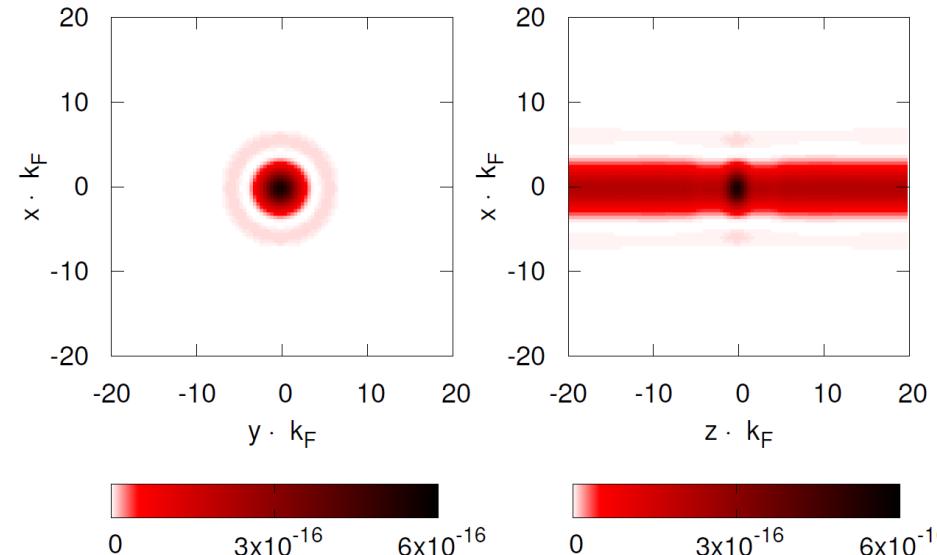
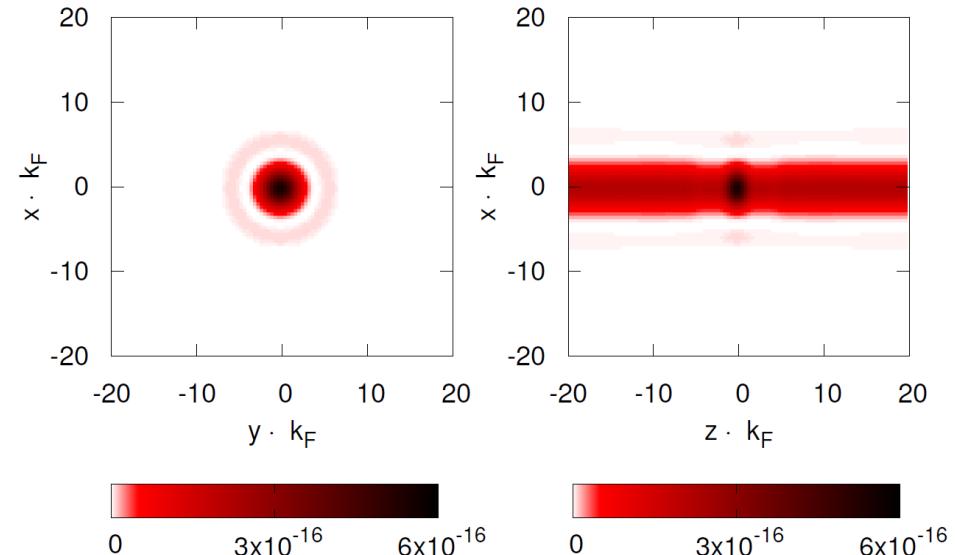
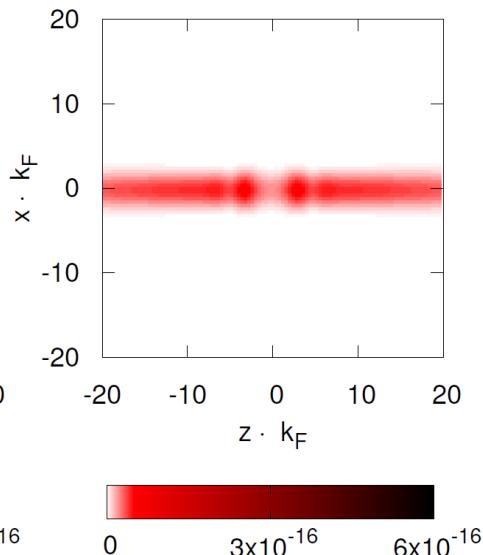
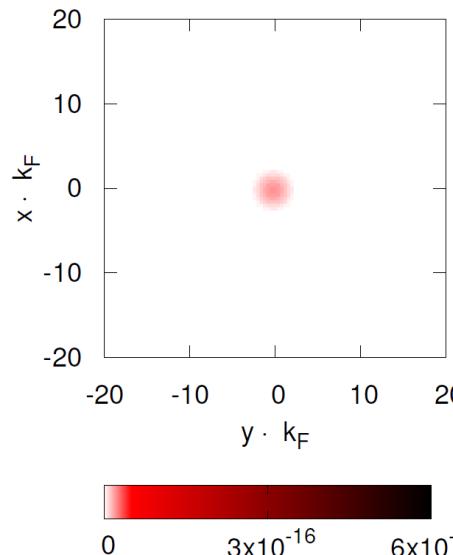
$q=1.8 k_F$ along z

Poles of P



Sum of a couple of imaginary ghost poles

Poles of χ

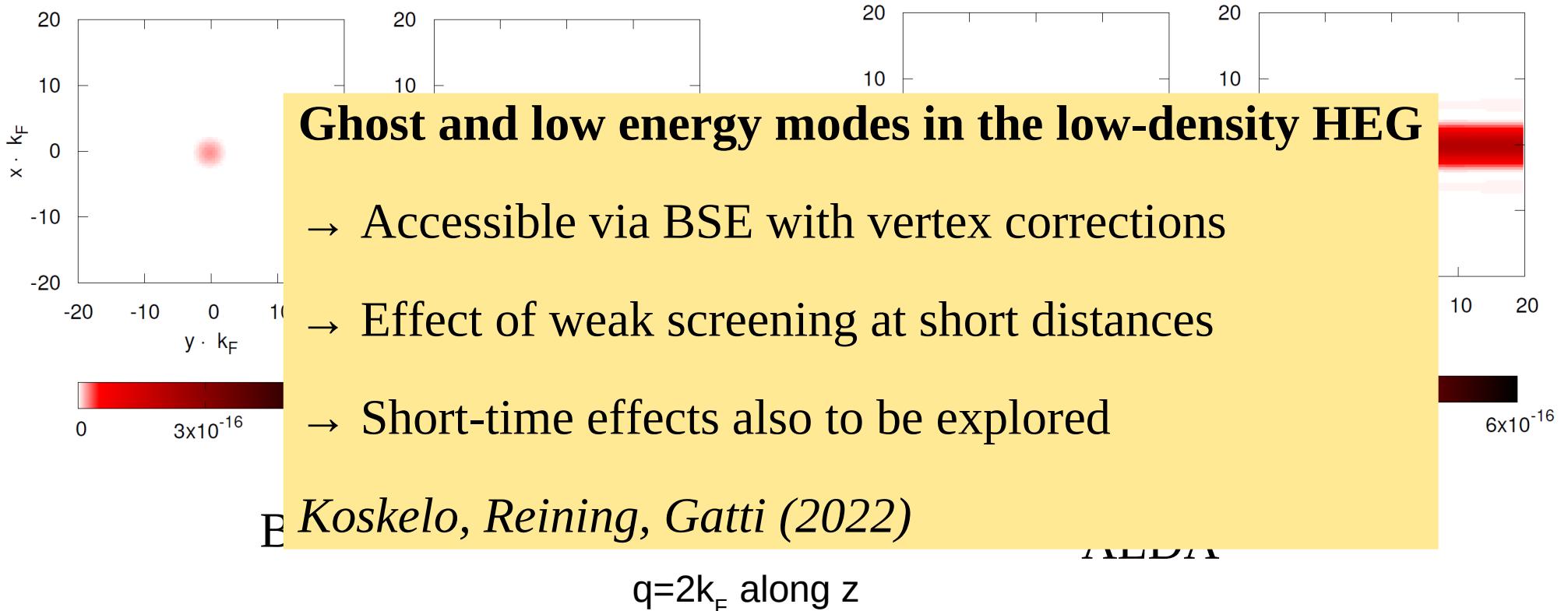


BSE+vertex

$q=2k_F$ along z

ALDA

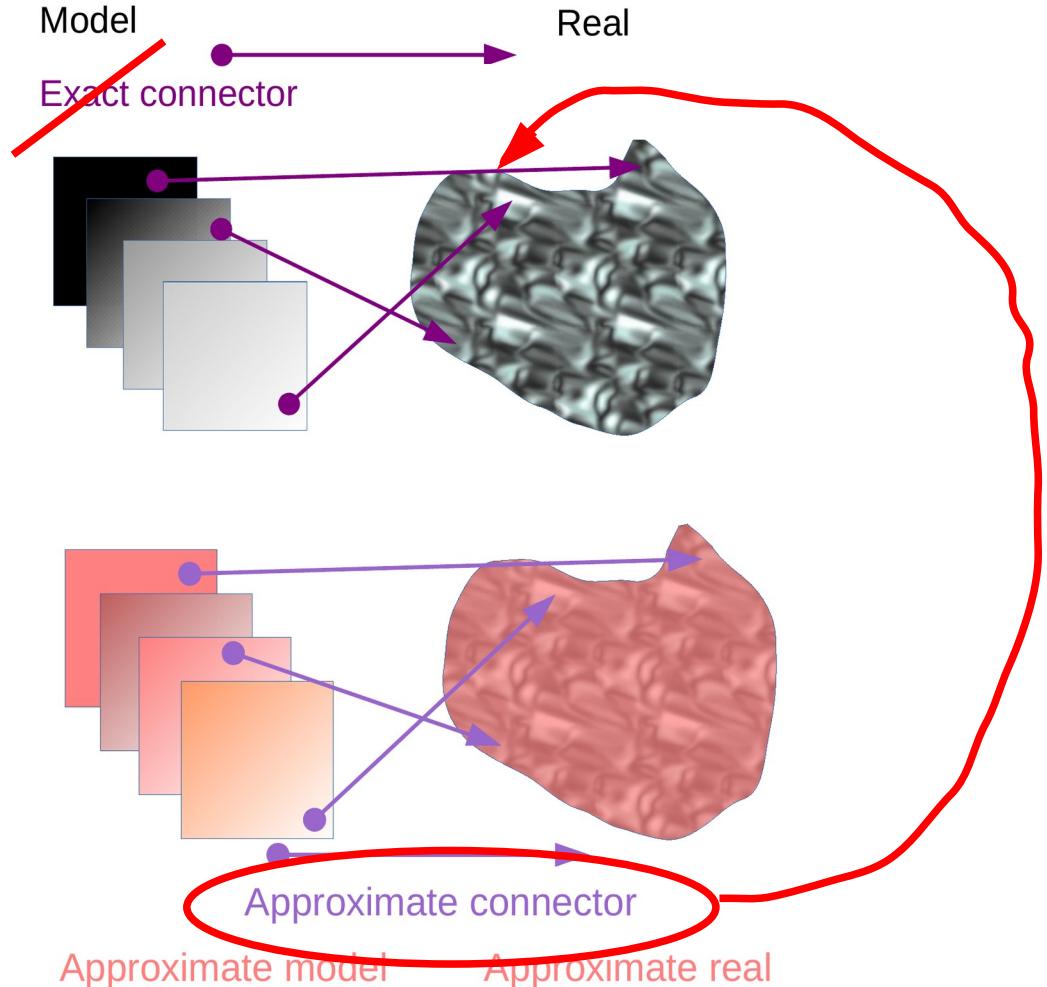
Poles of χ



Methods, models and materials: Joining forces to deal with the many-body problem

- Functionals,
and strategies to find them
- The connector project,
or how to play Lego together
- The homogeneous electron gas,
trouble with our methods, and promising combinations
- Insert concerning MBPT+TDDFT,
the total energy
- A Christmas advocacy

“More work”:



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- Explore observables
- Explore different approximations

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- Explore different approximations
- **More flexible model systems (inhomogeneous)**
- **Complete model data base with ML**
- **New ways to merge methods**

“More work”:

- Explore **Work once**
- Explore different approximations
- More **Store** → **Model systems (inhomogeneous)**
- Complete model data base with **ML**
- **Share**

“More work”:

- Explore once
- Explore different approximations
- More iterations → Store → Model systems (inhomogeneous)
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- Share

Methods, models and materials: Joining forces to deal with the many-body problem

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