

# Orbital-dependent functionals - from the optimized effective potential to generalized Kohn-Sham theory

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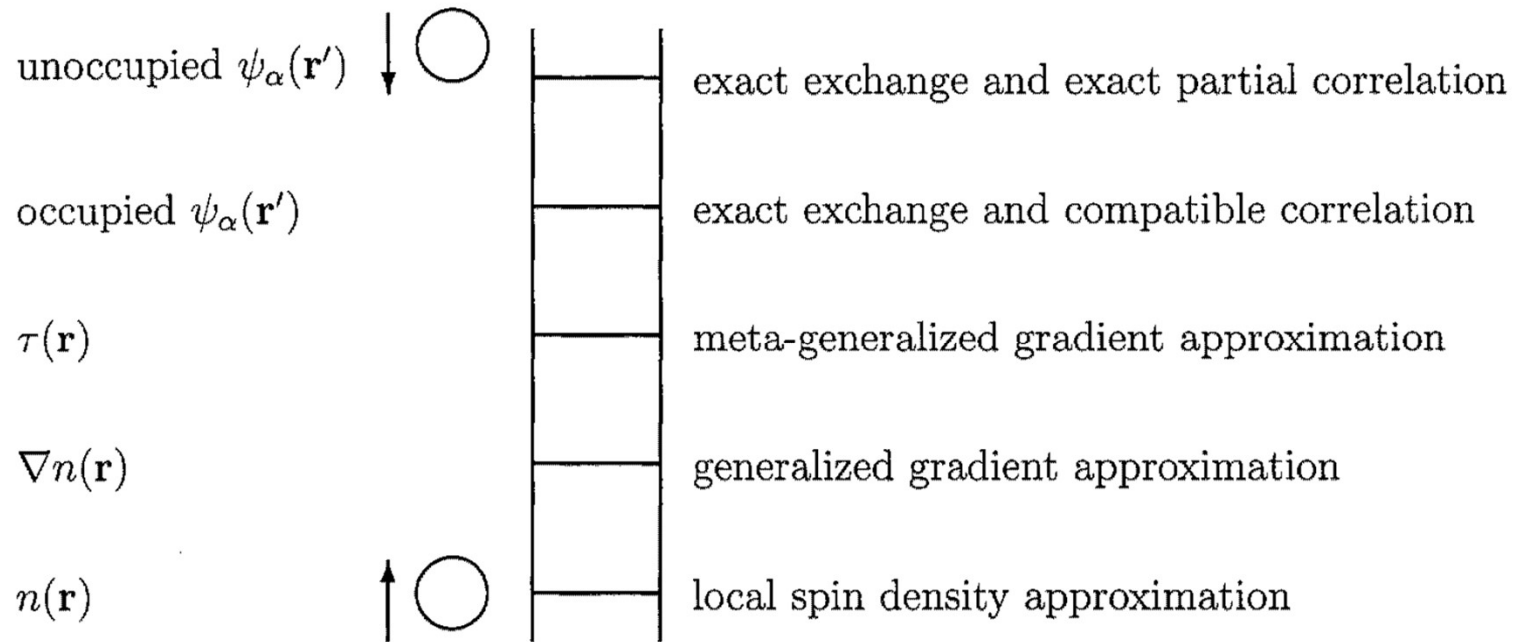
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Workshop on Theoretical Chemistry, Austria, March 2020

# Motivation: “Jacob’s ladder”

Chemical Accuracy



Hartree World

**Perdew and Schmidt, AIP Conference Proceedings 577, 1 (2001)**

## An important example: Exact exchange

$$E_x \equiv -\frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \sum_{i,j=1}^{N_\sigma} \iint d^3\vec{r} d^3\vec{r}' \frac{\varphi_{i\sigma}^*(\vec{r})\varphi_{i\sigma}(\vec{r}')\varphi_{j\sigma}^*(\vec{r}')\varphi_{j\sigma}(\vec{r})}{|\vec{r} - \vec{r}'|}$$

### Advantages:

- One more ingredient treated exactly
- 1-e self-interaction eliminated
- Natural derivative discontinuity

## Exact exchange within DFT

$$E_x^{ex} \equiv -\frac{1}{2} \sum_{\sigma=\uparrow,\downarrow} \sum_{i,j=1}^{N_\sigma} \iint d^3\vec{r} d^3\vec{r}' \frac{\varphi_{i\sigma}^*(\vec{r}) \varphi_{j\sigma}^*(\vec{r}') \varphi_{j\sigma}(\vec{r}) \varphi_{i\sigma}(\vec{r}')}{|\vec{r} - \vec{r}'|}$$

...but

**Orbital dependence. Density dependence implicit.**

$$V_{xc\Box}(\vec{r}) = \frac{\delta E_{xc}[n(\vec{r})]}{\delta n(\vec{r})} = ?$$

# First foray into the problem

## A Variational Approach to the Unipotential Many-Electron Problem

R. T. SHARP AND G. K. HORTON  
 University of Alberta, Edmonton, Canada  
 (Received January 26, 1953)

SLATER<sup>1</sup> has pointed out the advantage of an approximate solution of the many-electron problem in which all the electrons move in the same potential field. He gave an *ad hoc* formula for constructing such a potential by averaging the Hartree-Fock potentials<sup>2</sup> of the various electrons in a certain way. For the exchange part of the potential, he gave

$$\frac{\sum_{i,j} \psi_j(\mathbf{r}_1)\psi_i^*(\mathbf{r}_1) \int d\tau_2 \psi_j^*(\mathbf{r}_2)\psi_i(\mathbf{r}_2)/r_{12}}{[\sum_i \psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_1)]}$$

Slater's work suggests the following variational problem. Find that potential, the same for all the electrons, such that when it, and consequently the wave functions, are given a small variation, the energy of the system remains stationary. A Slater determinant constructed from the one-electron wave functions is used as the wave function of the system.

The potential which fulfills this prescription turns out to be

$$V(\mathbf{r}_1) = V_n(\mathbf{r}_1) + \sum_k \int d\tau_2 \frac{\psi_k^*(\mathbf{r}_2)\psi_k(\mathbf{r}_2)}{r_{12}} - W(\mathbf{r}_1), \quad (1)$$

where the exchange potential  $W(\mathbf{r})$  is the solution of the integral equation

$$\int d\tau_1 W(\mathbf{r}_1) \sum_{i \neq \alpha} \frac{\psi_i(\mathbf{r}_1)\psi_\alpha^*(\mathbf{r}_1)\psi_\alpha(\mathbf{r})\psi_i^*(\mathbf{r})}{E_i - E_\alpha} = \sum_{i,j} \sum_{\alpha \neq i} \int d\tau_i \frac{\psi_\alpha^*(\mathbf{r}_1)\psi_j(\mathbf{r}_1)}{E_i - E_\alpha} \int d\tau_2 \frac{\psi_j^*(\mathbf{r}_2)\psi_i(\mathbf{r}_2)}{r_{12}} \psi_\alpha(\mathbf{r})\psi_i^*(\mathbf{r}). \quad (2)$$

Here  $V_n(\mathbf{r})$  represents the external field acting on the electrons. The  $\psi$ 's are the solutions of the Schrödinger equation:

$$-\frac{1}{2}\nabla^2\psi_\beta(\mathbf{r}) + V(\mathbf{r})\psi_\beta(\mathbf{r}) = E_\beta\psi_\beta(\mathbf{r}). \quad (3)$$

Greek subscripts refer to all bound solutions of Eq. (3). Roman subscripts refer to occupied levels only. Hartree units<sup>3</sup> are used throughout.

The integral equation (2) can be solved approximately if  $E_\alpha$  is replaced by a suitable average value  $E_{0i}$ . The approximate solution<sup>4</sup> is

$$W(\mathbf{r}_1) = \frac{\sum_{i,j} \frac{\psi_j(\mathbf{r}_1)\psi_i^*(\mathbf{r}_1)}{E_i - E_{0i}} \int d\tau_2 \frac{\psi_j^*(\mathbf{r}_2)\psi_i(\mathbf{r}_2)}{r_{12}}}{\left(\sum_i \frac{\psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_1)}{E_i - E_{0i}}\right)}. \quad (4)$$

Slater's result is obtained from Eq. (4) by making the further approximation that all the  $E_i - E_{0i}$  are equal.

Equation (4) is being applied to the quadrivalent state of the carbon atom.

<sup>1</sup> J. C. Slater, *Phys. Rev.* **81**, 385 (1951).

<sup>2</sup> Actually the potentials averaged differ from the Hartree-Fock potentials in that they are evaluated using Slater wave functions.

<sup>3</sup> Hartree, *Proc. Roy. Soc. (London)* **141**, 282 (1933).

<sup>4</sup> After replacing  $E_\alpha$  by  $E_{0i}$ , the summations over  $\alpha$  are allowed to include  $\alpha = i$ . This implies adding to both sides of the equation terms which would be equal if the Fock exchange potential did not differ from Eq. (4).

Sharp & Horton, *Phys. Rev.* **90**, 317 (1953)

# First Numerical solutions

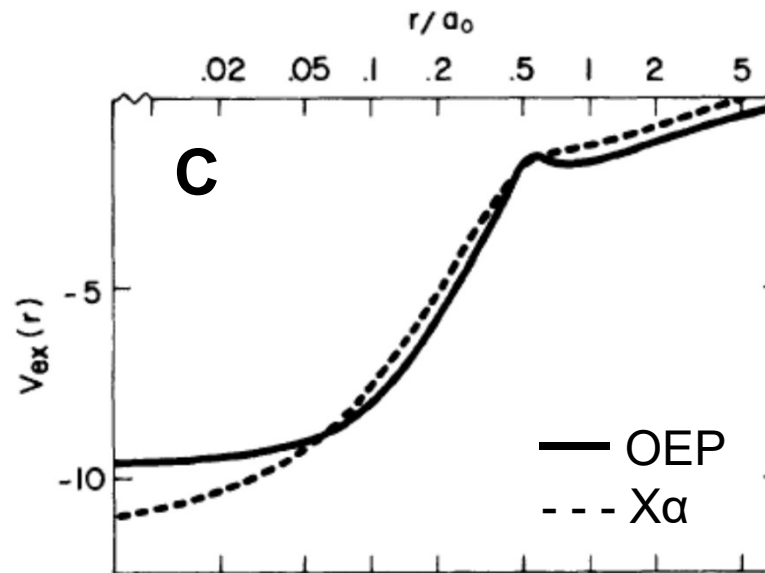
## Optimized effective atomic central potential\* *Phys. Rev. A* 14, 36 (1976)

James D. Talman and William F. Shadwick

*Department of Applied Mathematics, University of Western Ontario, London, Ontario, Canada N6A 5B9*

(Received 13 November 1975; revised manuscript received 24 February 1976)

A self-consistent set of equations is derived for an atomic central potential such that the energy given by the orbitals for the potential is minimized. It is shown that this effective potential behaves like  $-e^2/r$  for large  $r$  values. The equations have been solved for carbon, neon, and aluminum, and the resulting total energies exceed the Hartree-Fock total energies by less than 0.005%. The theory leads to an effective, local, central exchange potential analogous to the  $X\alpha$  potential.



The optimized effective potential  
is the Kohn-Sham potential!

Sahni, Gruenebaum, Perdew, Phys. Rev. B. 26, 4731 (1982)

**Simple plausibility argument**  
[Kümmel & Kronik, Rev. Mod. Phys. 80, 3 (2008)]

**OEP condition:**  $\delta E_{\text{tot}} / \delta v_{\text{KS}}(\vec{r}) = 0$

$$0 = \frac{\delta E_{\text{tot}}}{\delta v_{\text{KS}}(\vec{r})} = \int \frac{\delta E_{\text{tot}}}{\delta n(\vec{r}')} \frac{\delta n(\vec{r}')}{\delta v_{\text{KS}}(\vec{r})} d^3 r'$$

**Kohn-Sham response function (invertible!):**

$$\chi_{\text{KS}}(\vec{r}, \vec{r}') = \delta n(\vec{r}) / \delta v_{\text{KS}}(\vec{r}')$$

**Therefore:**  $0 = \delta E_{\text{tot}} / \delta n(\vec{r})$

## The optimized effective potential: A modern DFT perspective

$$\begin{aligned}
 v_{\text{xc},\sigma}(\vec{r}) &= \frac{\delta E_{\text{xc}}[\{\varphi_{j,\tau}\}]}{\delta n_{\sigma}(\vec{r})} \\
 &= \sum_{\alpha=\uparrow,\downarrow} \sum_{i=1}^{N_{\alpha}} \int \frac{\delta E_{\text{xc}}[\{\varphi_{j,\tau}\}]}{\delta \varphi_{i,\alpha}(\vec{r}')} \frac{\delta \varphi_{i,\alpha}(\vec{r}')}{\delta n_{\sigma}(\vec{r})} d^3 r' + \text{c.c.} \\
 &= \sum_{\alpha,\beta=\uparrow,\downarrow} \sum_{i=1}^{N_{\sigma}} \int \int \frac{\delta E_{\text{xc}}[\{\varphi_{j,\tau}\}]}{\delta \varphi_{i,\alpha}(\vec{r}')} \frac{\delta \varphi_{i,\alpha}(\vec{r}')}{\delta v_{\text{KS},\beta}(\vec{r}'')} \\
 &\quad \times \frac{\delta v_{\text{KS},\beta}(\vec{r}'')}{\delta n_{\sigma}(\vec{r})} d^3 r' d^3 r'' + \text{c.c.},
 \end{aligned}$$

Grabo, Kreibich, and Gross, *Mol. Eng.* **7**, 20 (1997); Engel, in *A primer in DFT* (2003)  
Kümmel & Kronik, *Rev. Mod. Phys.* **80**, 3 (2008)



## The optimized effective potential: A modern DFT perspective (2)

**Second term  
(1<sup>st</sup> order pert. Theory)**

$$\frac{\delta\varphi_{i,\alpha}(\vec{r}')}{\delta v_{\text{KS},\sigma}(\vec{r})} = \delta_{\alpha,\sigma} \sum_{\substack{j=1 \\ j \neq i}}^{\infty} \frac{\varphi_{j,\sigma}(\vec{r}')\varphi_{j,\sigma}^*(\vec{r})}{\varepsilon_{i,\sigma} - \varepsilon_{j,\sigma}} \varphi_{i,\sigma}(\vec{r})$$

**Inverse of  
third term**

$$\chi_{\text{KS},\sigma\beta}(\vec{r},\vec{r}') = \delta_{\sigma,\beta} \frac{\delta n_{\sigma}(\vec{r})}{\delta v_{\text{KS},\beta}(\vec{r}')}.$$

**Pert. Theory  
again**

$$\chi_{\text{KS},\sigma}(\vec{r},\vec{r}') = \sum_{k=1}^{N_{\sigma}} \sum_{\substack{j=1 \\ j \neq i}}^{\infty} \frac{\varphi_{k,\sigma}^*(\vec{r})\varphi_{k,\sigma}(\vec{r}')\varphi_{j,\sigma}(\vec{r})\varphi_{j,\sigma}^*(\vec{r}')}{\varepsilon_{k,\sigma} - \varepsilon_{j,\sigma}} + \text{c.c.}$$

## The OEP equation

$$\sum_{i=1}^{N_\sigma} \int \varphi_{i,\sigma}^*(\vec{r}') [v_{xc,\sigma}(\vec{r}') - u_{xci,\sigma}(\vec{r}')] \\ \times G_{KS i,\sigma}(\vec{r}', \vec{r}) \varphi_{i,\sigma}(\vec{r}) d^3 r' + \text{c.c.} = 0$$

**where**

$$G_{KS i,\sigma}(\vec{r}', \vec{r}) = \sum_{\substack{j=1 \\ j \neq i}}^{\infty} \frac{\varphi_{j,\sigma}(\vec{r}') \varphi_{j,\sigma}^*(\vec{r})}{\varepsilon_{i,\sigma} - \varepsilon_{j,\sigma}} \quad u_{xci,\sigma}(\vec{r}) = \frac{1}{\varphi_{i,\sigma}^*(\vec{r})} \frac{\delta E_{xc}[\{\varphi_{j,\tau}\}]}{\delta \varphi_{i,\sigma}(\vec{r})}$$

# The OEP equation

## Pros

**Applies to *any* orbital-dependent functional!**

**Fully and rigorously within the Kohn-Sham formalism**

## Cons

***Nasty* integro-differential equation**

**Rarely solved exactly**

**Typically within KLI approx.**

**= constant numerator in the Green function**

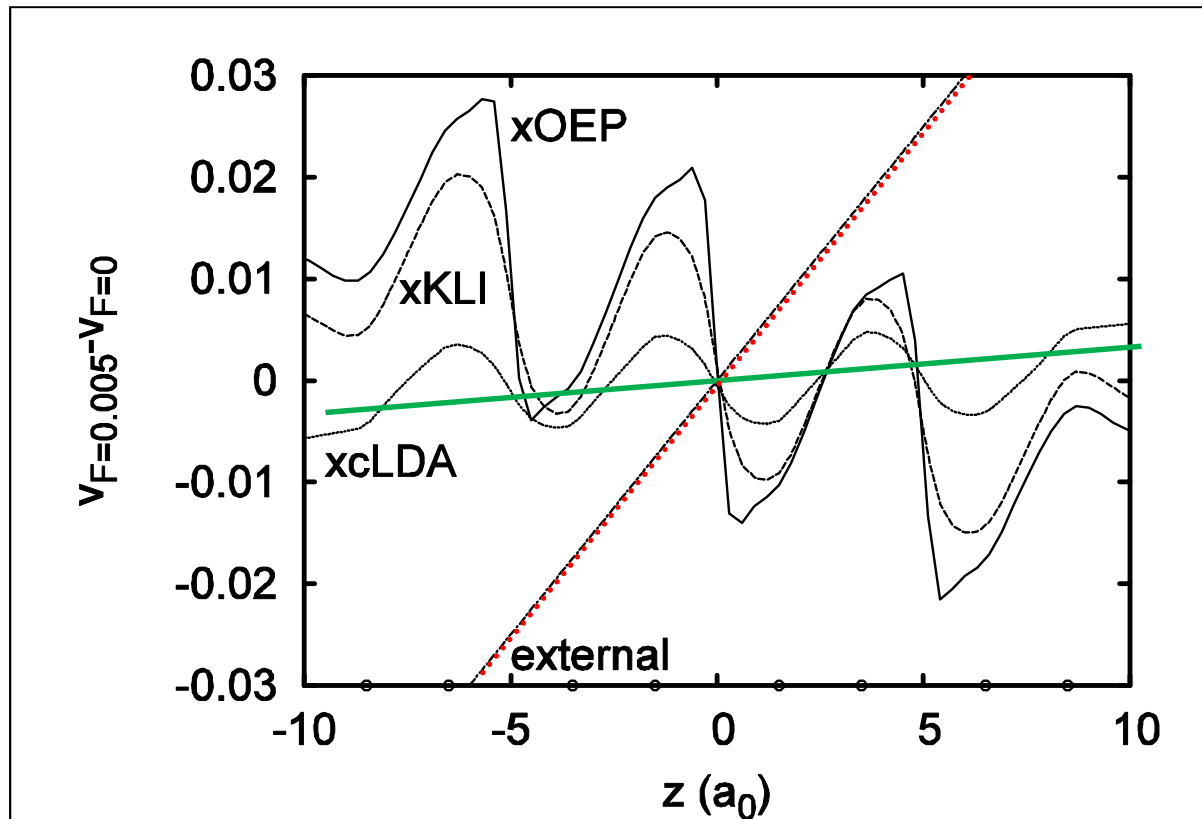
# xOEP for (hyper-)polarizability of hydrogen chain!



method	$\alpha$ [a.u.]	$\gamma$ [a.u.]
“exact”	124	179,000
HF	138	147,000
LDA	211	$1.27 \times 10^6$
xKLI	157	277,000
xOEP	138	144,000



# Field Counteracting behavior



**LDA – follows the field (via density)**  
**xKLI, xOEP – counteract the field**

**Kümmel, Kronik, and Perdew, *Phys. Rev. Lett.* 93, 213002 (2004).**

Do we really have to use the OEP equation to do theoretically rigorous work with any explicitly orbital-dependent functional?

# Consider hybrid functionals

$$E_{xc}^{\text{hyb}}[n] = aE_x^{\text{exact}}[n] + (1-a)E_x^{\text{app}}[n] + E_c^{\text{app}}[n]$$

a - Fraction of exact (Fock) exchange  
app = usually GGA, sometimes meta-GGA

**Becke, J. Chem. Phys. 98, 5648 (1993)**

Can be solved using OEP, but practically almost never is. Instead:

$$\left( -\frac{1}{2}\nabla^2 + V_{ion}(r) + V_H([n];r) + a\hat{V}_F + (1-a)v_x^{sl}([n];r) + v_c^{sl}([n];r) \right) \phi_i(r) = \varepsilon_i \phi_i(r)$$

- Hence the name “hybrid” ...
- Just “mix and match” of Hartree-Fock and Kohn-Sham?
- Uncontrolled approximation to Kohn-Sham theory?

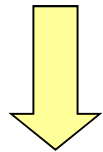
# Finding $V_{KS}$

## Model system

$$"E_{KS}" = \min_n \left\{ T_s[n] + \int V_{KS}(\vec{r}) n(\vec{r}) dr \right\}$$

$$T_s[n] = \text{Non-interacting kinetic energy}$$

$$\min_{\{\psi_i\} \rightarrow n} \sum_{\text{occupied states}} \langle \psi_i(r) | -\frac{\nabla^2}{2} | \psi_i(r) \rangle$$



$$\delta \left\{ T_s[n] + \int V_{KS}(\vec{r}) n(\vec{r}) dr - \mu \int n(\vec{r}) dr \right\} = 0$$

$$\frac{\delta T_s[n]}{\delta n(\vec{r})} + V_{KS}(\vec{r}) = \mu$$

## Real System

$$E_{gs} = \min_n \left\{ T_s[n] + \int V_{ext}(\vec{r}) n(\vec{r}) dr + E_H[n] + E_{xc}[n] \right\} \leftarrow \text{"everything else"}$$

$$E_H = \frac{1}{2} \iint \frac{n(r)n(r')}{|r-r'|} dr dr' \quad \text{Classical Coulomb energy}$$



$$\frac{\delta T_s[n]}{\delta n(\vec{r})} + V_{ext}(\vec{r}) + \frac{\delta E_H[n]}{\delta n(\vec{r})} + \frac{\delta E_{xc}[n]}{\delta n(\vec{r})} = \mu$$



## Generalized Kohn-Sham theory

Seidl, Goerling, Vogl, Majevski, Levy, Phys. Rev. B 53, 3764 (1996).

**Can we map the density to a *partially interacting* model system that can still be represented by a single Slater determinant!**

$$\hat{O}^S[\{\phi_i\}]\phi_j + \hat{v}_{\text{eff}}\phi_j = \varepsilon_j\phi_j$$

## Generalized Kohn-Sham theory


Seidl, Goerling, Vogl, Majevski, Levy, Phys. Rev. B 53, 3764 (1996).

**Define a density functional based on a functional of the Slater-determinant**

$$F^S[\rho] = \min_{\Phi \rightarrow \rho(\mathbf{r})} S[\Phi] = \min_{\{\phi_i\} \rightarrow \rho(\mathbf{r})} S[\{\phi_i\}].$$

**Hohenberg-Kohn:**

$$E_0[v] = \min_{\rho(\mathbf{r}) \rightarrow N} \left\{ F^S[\rho] + R^S[\rho] + \int d\mathbf{r} v(\mathbf{r}) \rho(\mathbf{r}) \right\}$$


$$F_{\text{HK}}$$

## Generalized Kohn-Sham theory – real system

$$\begin{aligned} E_0[v] &= \min_{\rho(\mathbf{r}) \rightarrow N} \left\{ F^S[\rho] + R^S[\rho] + \int d\mathbf{r} v(\mathbf{r}) \rho(\mathbf{r}) \right\} \\ &= \min_{\rho(\mathbf{r}) \rightarrow N} \left\{ \min_{\Phi \rightarrow \rho(\mathbf{r})} S[\Phi] + R^S[\rho] + \int d\mathbf{r} v(\mathbf{r}) \rho(\mathbf{r}) \right\} \\ &= \min_{\Phi \rightarrow N} \left\{ S[\Phi] + R^S[\rho[\Phi]] + \int d\mathbf{r} v(\mathbf{r}) \rho([\Phi]; \mathbf{r}) \right\} \\ &= \min_{\{\phi_i\} \rightarrow N} \left\{ S[\{\phi_i\}] + R^S[\rho[\{\phi_i\}]] + \int d\mathbf{r} v(\mathbf{r}) \rho([\{\phi_i\}]; \mathbf{r}) \right\} \end{aligned}$$

## Generalized Kohn-Sham theory: Constrained minimization leads to model system

$$\hat{O}^S[\{\phi_i\}]\phi_j + \hat{v}_R\phi_j + \hat{v}\phi_j = \varepsilon_j\phi_j$$

where  $v_R(\mathbf{r}) = \frac{\delta R^S[\rho]}{\delta \rho(\mathbf{r})}$

**Conclusion:**

$$v_{\text{eff}}(\mathbf{r}) = v(\mathbf{r}) + v_R(\mathbf{r})$$

## Generalized Kohn-Sham theory: Important Examples

$$S[\Phi] = \langle \Phi | \hat{T} | \Phi \rangle \quad \longrightarrow \quad \text{Kohn-Sham}$$

$$S[\Phi] = \langle \Phi | \hat{T} + \hat{V}_{ee} | \Phi \rangle \quad \longrightarrow \quad \text{Hartree-Fock-} \\ \text{Kohn-Sham}$$

$$-\frac{1}{2} \nabla^2 \phi_i(\mathbf{r}) + v(\mathbf{r}) \phi_i(\mathbf{r}) + u([\rho]; \mathbf{r}) \phi_i(\mathbf{r})$$

$$- \int d\mathbf{r}' v_x^{\text{NL}}(\mathbf{r}, \mathbf{r}') \phi_i(\mathbf{r}') + v_c^{\text{HF}}([\rho]; \mathbf{r}) \phi_i(\mathbf{r}) = \varepsilon_i \phi_i$$

Hartree-Fock is just a special case!

# Generalized Kohn-Sham theory in action: hybrid functionals

## Exact Hybrid Functional Theory

$$S[\Phi_\alpha] = \langle \Phi_\alpha | \hat{T} + \alpha \hat{W} | \Phi_\alpha \rangle \quad \hat{O}^S[\{\phi_j\}] = -\frac{1}{2}\nabla^2 + \alpha \hat{V}_F + \alpha V_H([n]; \mathbf{r})$$

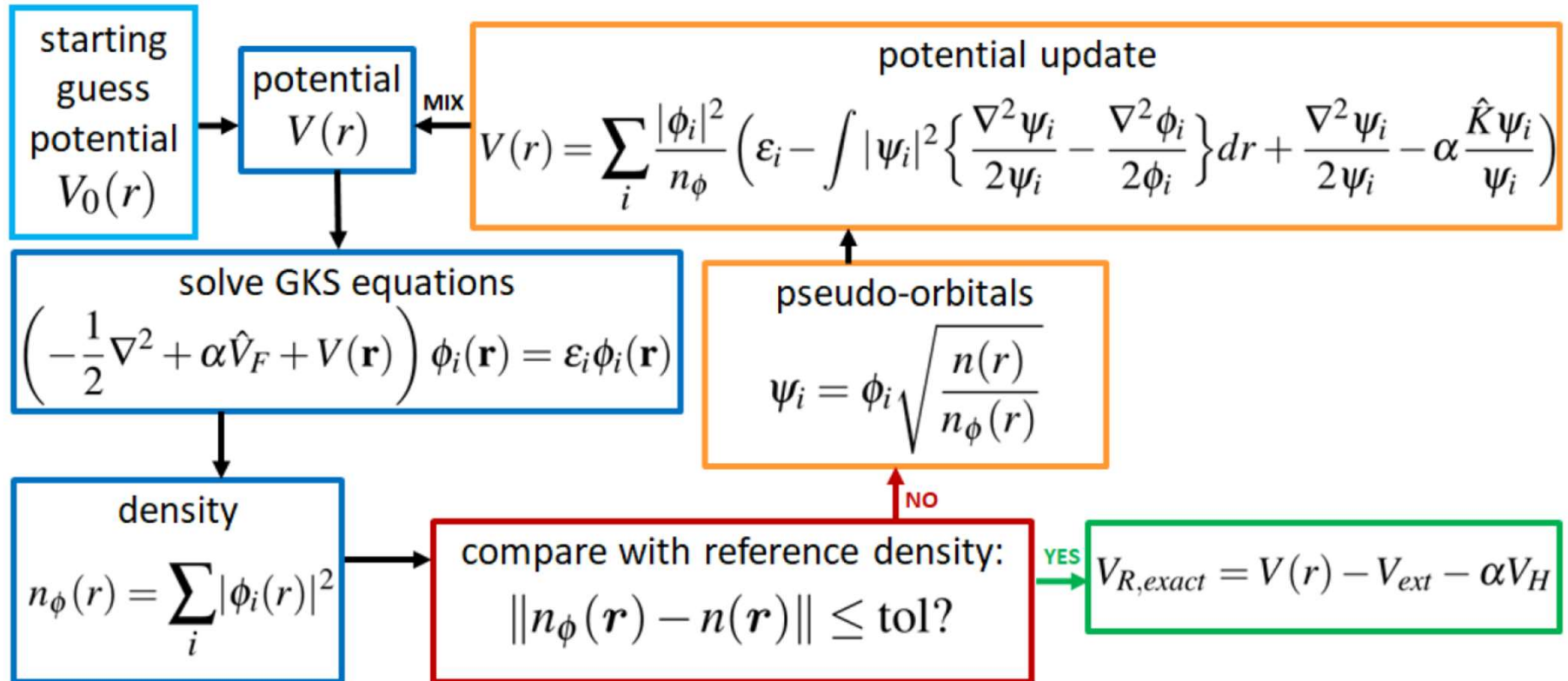
$$\left( -\frac{1}{2}\nabla^2 + V_{ext}(\mathbf{r}) + \alpha \hat{V}_F + \alpha V_H([n]; \mathbf{r}) + V_R([n]; \mathbf{r}) \right) \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

## Approximate Hybrid Functional Theory

$$V_R^\alpha([n]; \mathbf{r}) = (1 - \alpha)V_H([n]; \mathbf{r}) + (1 - \alpha)V_{x,sl}([n]; \mathbf{r}) + V_{c,sl}([n]; \mathbf{r})$$

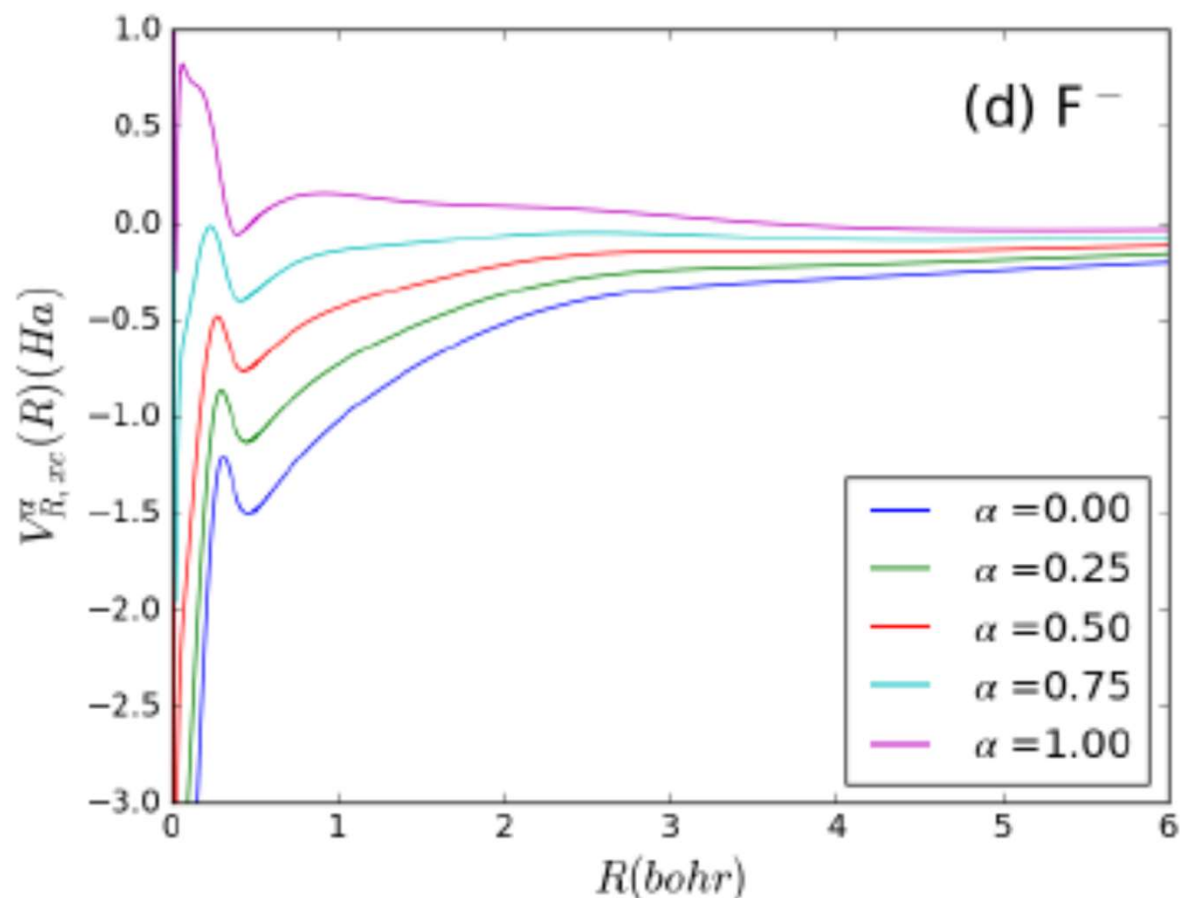
Görling, Levy, J. Chem. Phys. 106, 2675 (1997)

# Generalized Kohn-Sham theory in action: hybrid functionals



Garrick, Natan, Gould, Kronik, ChemRxiv (2019).

# Exact Generalized Kohn-Sham theory in action: The case of a hybrid functional



Garrick, Natan, Gould, Kronik, ChemRxiv (2019).



# Time-dependent GKS

	DFT	TDDFT
Kohn-Sham	Kohn & Sham 1965	Runge & Gross 1984
Generalized Kohn-Sham	Seidl et al. 1996	Baer & Kronik 2018

**Caveat: watch out for the continuity equation!  
Especially in meta-GGAs**

**[see Bates and Furche, J. Chem. Phys. 137, 164105 (2012)]**

GKS is as rigorous as OEP!

Beyond computational cost,  
are there reasons to  
prefer GKS to OEP?

# Piecewise linearity in DFT: Exact results from ensemble arguments

Fractional no. of electrons:

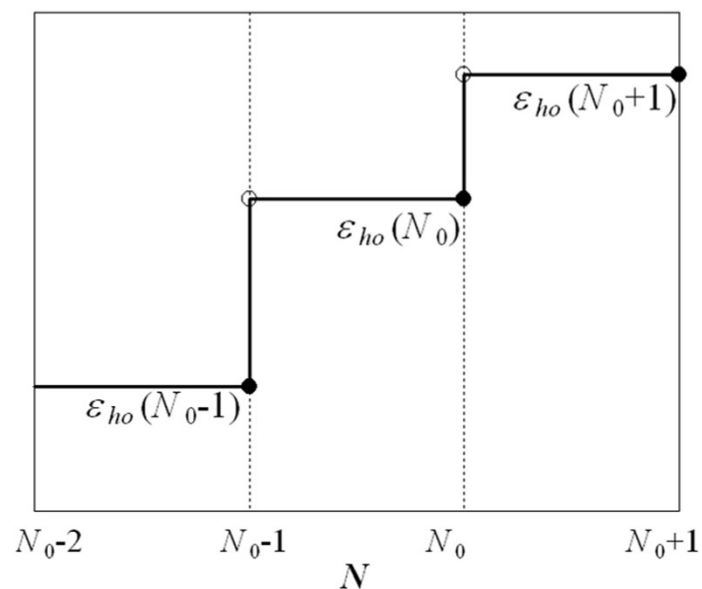
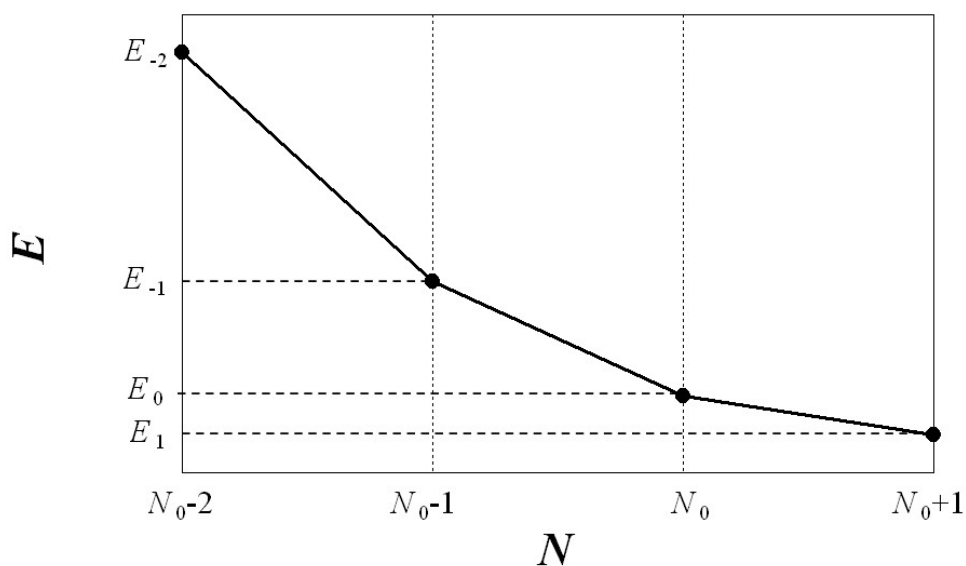
$$N = N_0 + \alpha$$

- Piecewise-linearity

$$E(N) = (1 - \alpha)E_0 + \alpha E_1$$

- The IP theorem

$$\varepsilon_{ho}(N) = -I(N_0) =: E_0 - E_{-1}$$



Perdew, Parr, Levy, Balduz, PRL **49**, 1691 (1982); Yang, Zhang, Ayers, PRL **84**, 5172 (2000).

Janak, PRB **18**, 7165 (1978); Levy, Perdew, Sahni, PRA **30**, 2745 (1984).

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# The Kohn-Sham equation

$$\left( \underbrace{-\frac{1}{2}\nabla^2}_{\text{kinetic}} + \underbrace{V_{ion}}_{\text{ion-e}} + \underbrace{V_{Hartree}}_{\text{e-e}} + \underbrace{V_{xc}}_{\text{many body}} \right) \psi_i(r) = E_i \psi_i(r)$$

$$\rho(r) = \sum_{\text{occupied states}} |\psi_i(r)|^2$$

$$V_{xc}([\rho]; r) = \frac{\delta E_{xc}[\rho]}{\delta \rho}$$

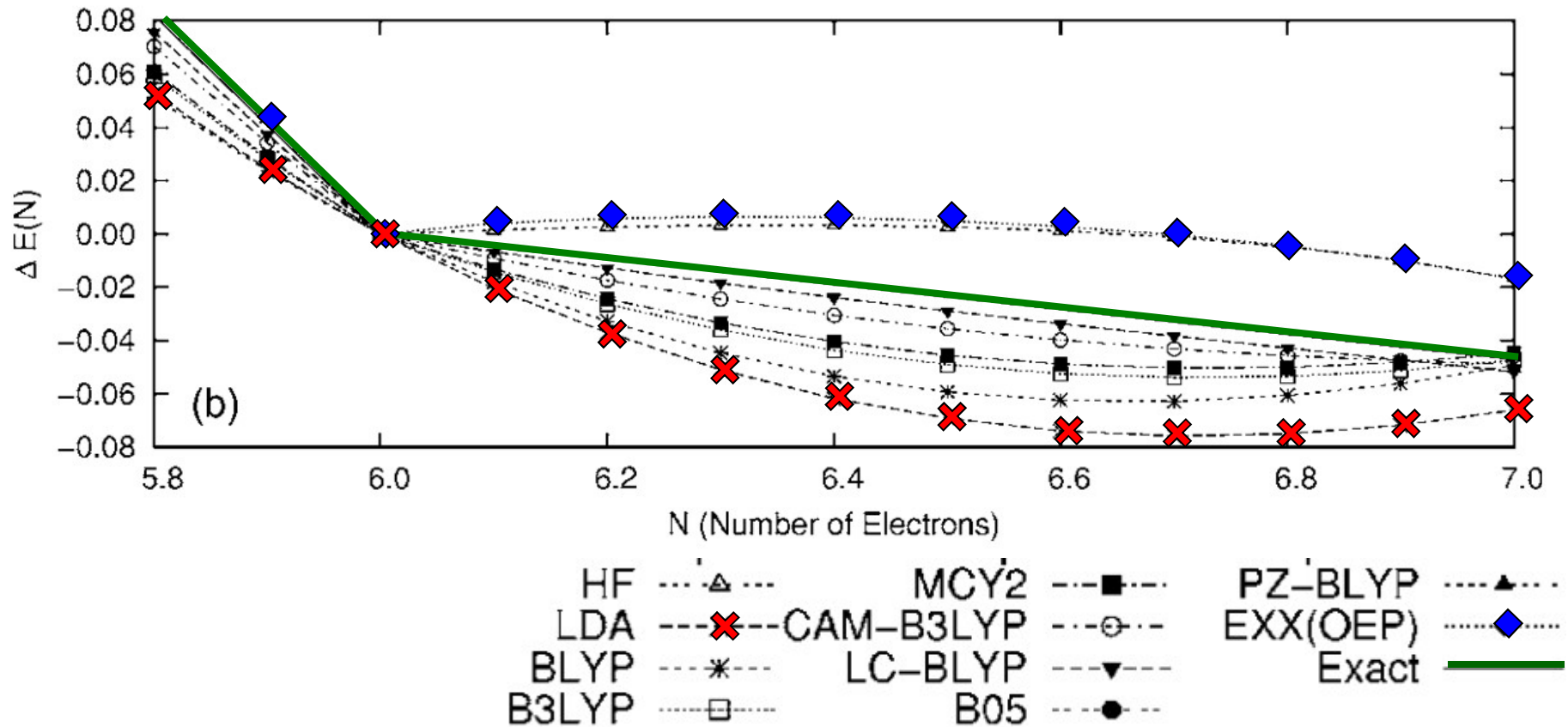
***$V_{xc}$  may “jump” by a spatially uniform constant across the integer point. A derivative discontinuity!***

**Confirmed by calculations:**

**Godby, Schlüter, Sham, Phys. Rev. Lett. 56, 2415 (1986);**

**Chan, J. Chem. Phys. 110, 4710 (1999); Allen and Tozer, Mol. Phys. 100, 433 (2002).**

# Performance of various functionals

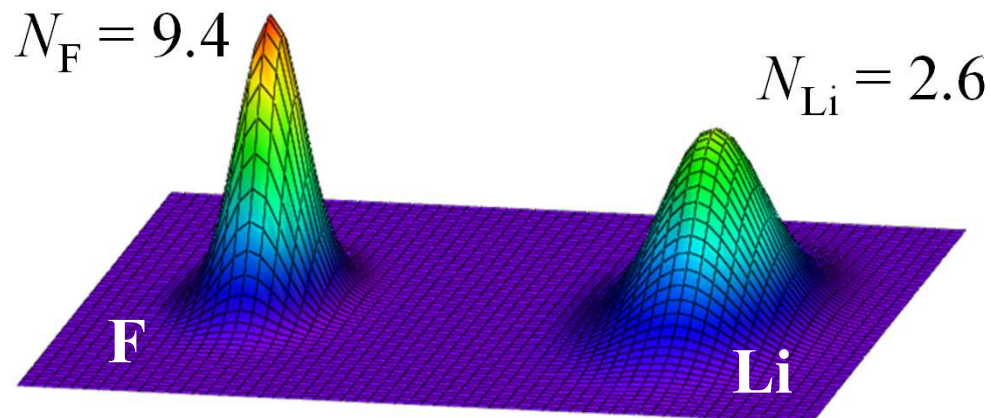


**Note ensemble theory caveat!**

**Kraisler & Kronik Phys. Rev. Lett. 110, 126403 (2013).**

# Fractional Dissociation Problem

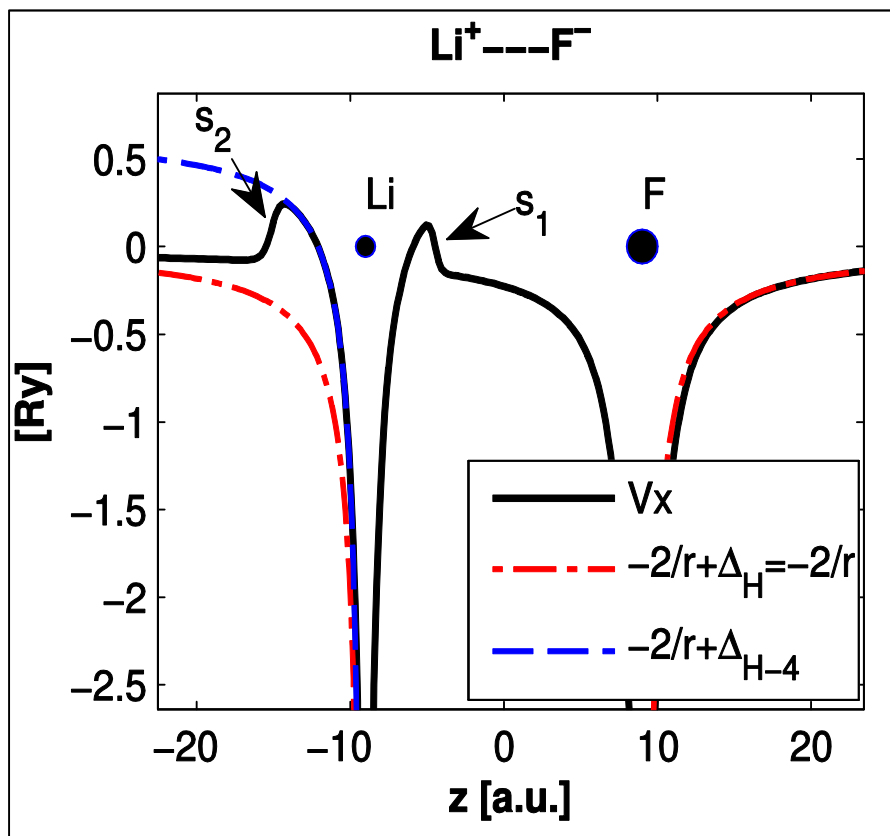
- Consider a stretched diatomic molecule  $A \dots B$  (e.g. Li...F)



schematic electron density of a stretched diatomic molecule

- *Principle of integer preference*: dissociation into fragments with integer no. of e<sup>-</sup>'s:  $N_A^0$  and  $N_B^0$  (unless special symmetry exists)
  - not obeyed by many xc approximations
  - spurious fractional dissociation:  $\text{Li}^{+0.4} \dots \text{F}^{-0.4}$
- Relevant for many charge-transfer cases
  - ▶ J. P. Perdew *et al.* PRL **49**, 1691 (1982)
  - ▶ J. P. Perdew, Adv. Quantum Chem. **21**, 113 (1990)
  - ▶ A. Ruzsinszky, J. Chem. Phys. **126**, 104102 (2007)

# Derivative discontinuity observed directly in exact-exchange DFT



Makmal, Kümmel, Kronik, *Phys. Rev. A* **83**, 062512 (2011).

See also: Fuks, Rubio, Maitra, *Phys. Rev. A* **83**, 042501 (2011).

Hodgson, Kraisler, Schild, Gross, *J. Phys. Chem. Lett.* **8**, 5974 (2017).

# Mind the gap

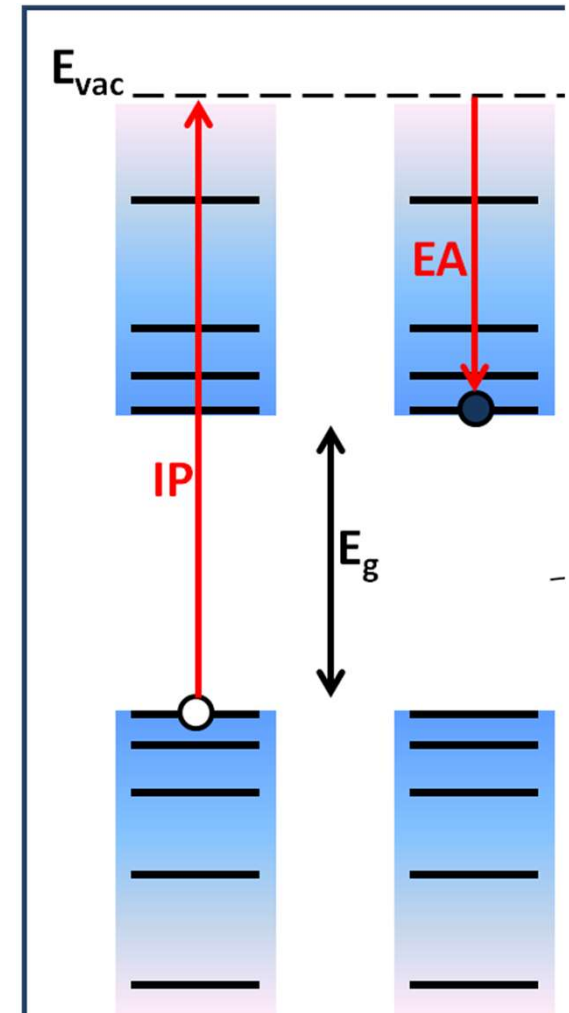
The Kohn-Sham gap underestimates the real gap

$$E_g = I - A = \epsilon_{KS}^{LUMO} - \epsilon_{KS}^{HOMO} + \Delta_{xc}$$

Perdew and Levy, *PRL* 1983;  
Sham and Schlüter, *PRL* 1983

derivative  
discontinuity!

**Kohn-Sham eigenvalues do not mimic  
the quasi-particle picture  
even in principle!**





## Generalized Kohn-Sham theory

$$\left( \hat{O}_S[\{\varphi_j\}] + V_{ion}(r) + v_R([n]; r) \right) \varphi_i(r) = \varepsilon_i \varphi_i(r)$$

**Derivative discontinuity problem possibly mitigated, perhaps even eliminated, by non-local operator!!**

# Conclusions

- Orbital-dependent exchange-correlation functionals are useful
- They can be handled rigorously within Kohn-Sham theory using the OEP approach.
- They can accommodate non-multiplicative potentials rigorously via the GKS scheme.
- Each approach has pros and cons