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Kohn-Sham density functional theory for strong-interacting systems

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Outline

- The exact strong-interacting limit (SCE) of DFT as an approximation for the exchange-correlation energy
- Self-consistent KS SCE results for model quantum wires and quantum dots
- Generalization to open systems with fluctuating particle number
- Chemistry
- Monge-Kantorovich formulation of the SCE functional

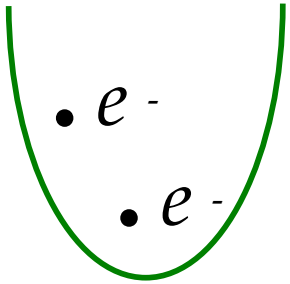
Kohn-Sham DFT and strong correlation

Example: two electrons (singlet) in 1D harmonic confinement

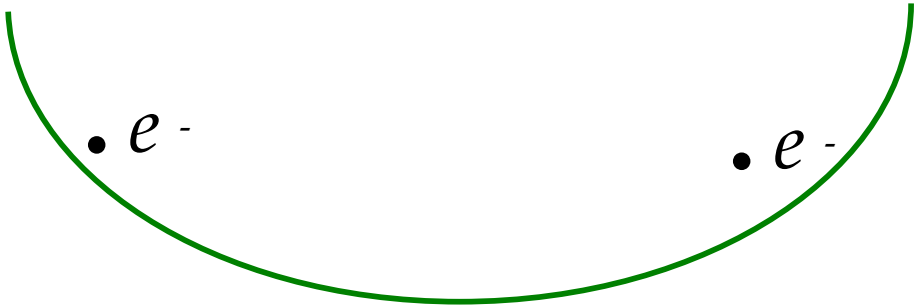
$$v_{\rm ext}(x) = \frac{1}{2}\omega^2 x^2 \qquad \omega = \frac{4}{L^2}$$

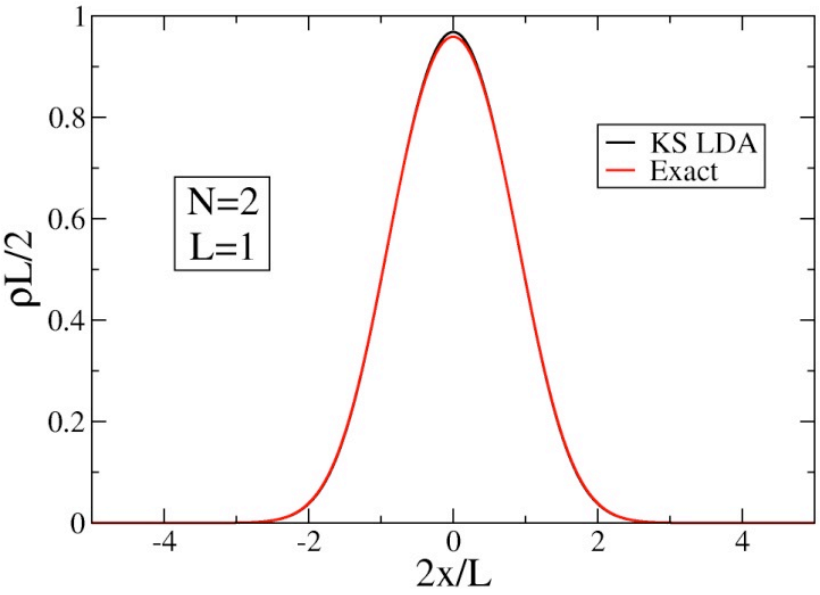
L: effective length

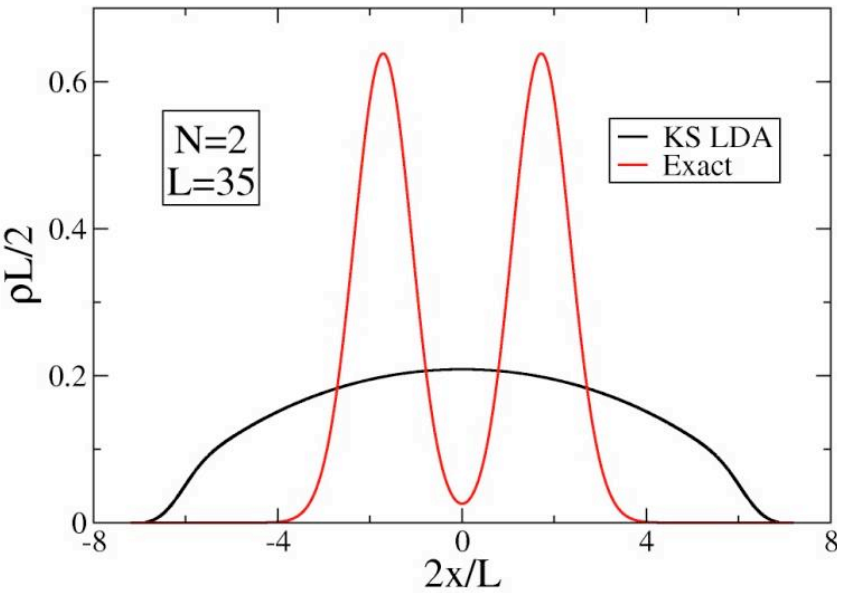
weak correlation (small *L*)



Strong correlation (large *L*)





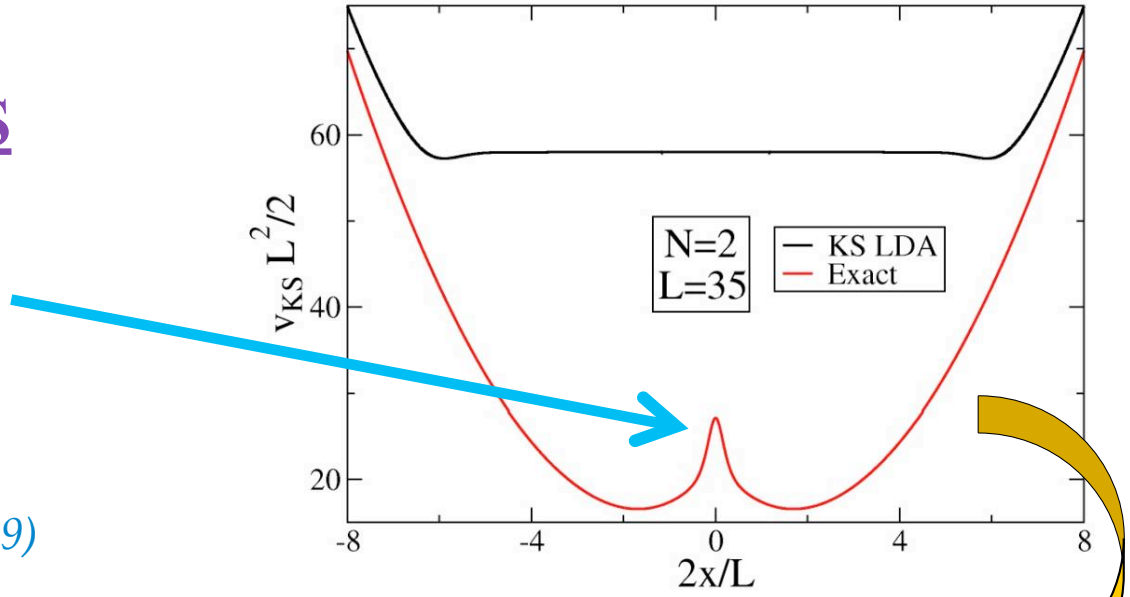


Kohn-Sham DFT and strong correlation

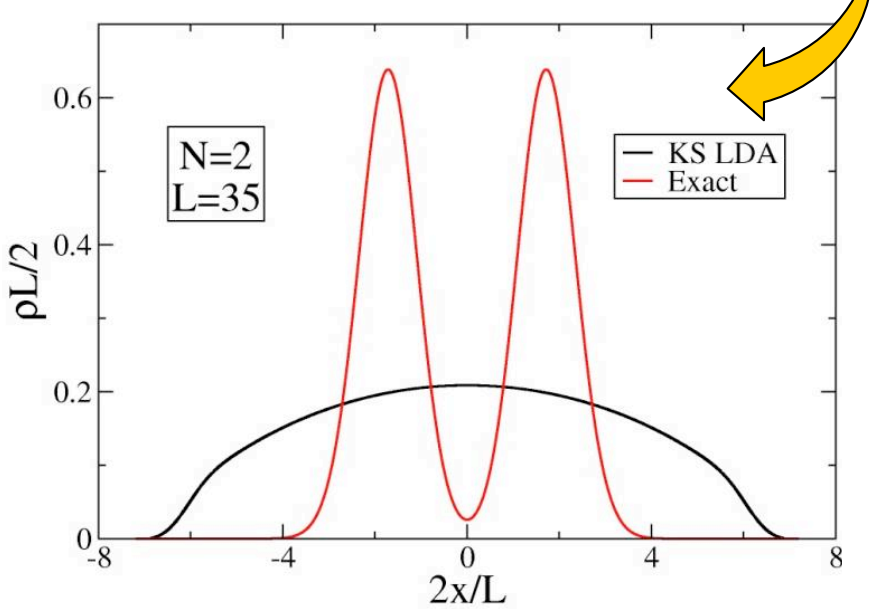
Kohn-Sham potential:

"Bump" in the exact KS potential: localization

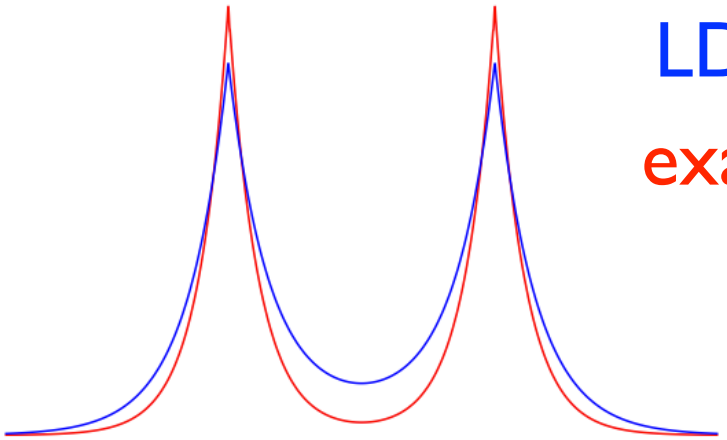
- *Buijse, Baerends & Snijders Phys. Rev. A* ***40****, 4190 (1989)*
- *Helbig, Tokatly & Rubio, J. Chem. Phys.* ***131****, 224105 (2009)*



The "bump" is missing in the KS LDA potential: delocalized density



Stretched bond, e.g. H_2 molecule



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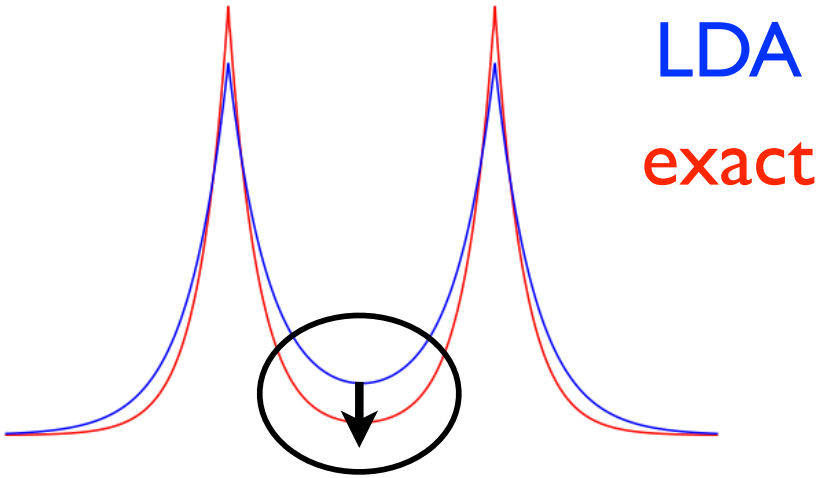

exact KS potential localizes more:
"bump" in the midpoint

- *Buijse, Baerends & Snijders Phys. Rev. A* ***40****, 4190 (1989)*
- *Helbig, Tokatly & Rubio, J. Chem. Phys.* ***131****, 224105 (2009)*

Unrestricted KS & strong correlation...

- Like UHF, UKS can mimic strong correlation (not always!)
- Often better energies, but wrong characterizations of several properties
- Formally not well founded
- Huge literature: controversial, wrong interpretation, etc...
- Crucial for: transition metals, Mott insulators, bond breaking, nanostructures,...

Exchange-correlation from the strong-interaction limit of DFT:

The "bumps" in the KS potential from the right physics (no spin/spatial-symmetry breaking)

Hohenberg-Kohn functional

Kohn-Sham DFT:

$$F[\rho] = \min_{\Psi \to \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle = \min_{\Psi \to \rho} \langle \Psi | \hat{T} | \Psi \rangle + E_{\mathrm{Hartree}}[\rho] + E_{\mathrm{xc}}[\rho]$$

Hohenberg-Kohn functional

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$$F[\rho] = \min_{\Psi \to \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle = \underbrace{\min_{\Psi \to \rho} \langle \Psi | \hat{T} | \Psi \rangle}_{T_s[\rho]\ \text{(known)}} + \underbrace{E_{\text{Hartree}}[\rho]}_{\text{(known)}} + \underbrace{E_{\text{xc}}[\rho]}_{\text{(unknown)}}$$

Hohenberg-Kohn functional

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$$v_{\text{Hartree}}[\rho] = \frac{\delta E_{\text{Hartree}}[\rho]}{\delta \rho}$$

$$v_{\text{xc}}[\rho] = \frac{\delta E_{\text{xc}}[\rho]}{\delta \rho}$$

Kohn-Sham equations:

$$\left(-\frac{1}{2}\nabla^2 + v_{\text{KS}}[\rho](\mathbf{r}) \right) \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

$$v_{\text{KS}}[\rho] = v_{\text{ext}}[\rho] + v_{\text{Hartree}}[\rho] + v_{\text{xc}}[\rho]$$

$$\rho(\mathbf{r}) = \sum_i |\phi_i(\mathbf{r})|^2$$

Hohenberg-Kohn functional

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Our approach:

$$\approx \min_{\Psi\to\rho}\langle\Psi|\hat{T}|\Psi\rangle + \min_{\Psi\to\rho}\langle\Psi|\hat{V}_{ee}|\Psi\rangle$$

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Our approach:

$$\approx \underbrace{\min_{\Psi\to\rho}\langle\Psi|\hat{T}|\Psi\rangle}_{T_s[\rho]} + \underbrace{\min_{\Psi\to\rho}\langle\Psi|\hat{V}_{ee}|\Psi\rangle}_{V_{ee}^{SCE}[\rho]}$$

***Strictly-correlated-electrons (SCE) DFT*:**

- *M. Seidl, PRA **60**, 4387 (1999)*
- *M. Seidl, P. Gori-Giorgi and A. Savin, PRA **75**, 042511 (2007)*
- *P.Gori-Giorgi, G.Vignale and M. Seidl, JCTC **5**, 743 (2009)*
- *P. Gori-Giorgi, M. Seidl, and G. Vignale, PRL **103**, 166402 (2009).*

e-e interaction energy of system with *zero kinetic energy* and density ρ (SCE reference system)

Hohenberg-Kohn functional

Kohn-Sham DFT:

$$F[\rho] = \min_{\Psi\to\rho}\langle\Psi|\hat{T}+\hat{V}_{ee}|\Psi\rangle = \min_{\Psi\to\rho}\langle\Psi|\hat{T}|\Psi\rangle + E_{\mathrm{Hartree}}[\rho] + E_{\mathrm{xc}}[\rho]$$

Our approach:

$$\approx \min_{\Psi\to\rho}\langle\Psi|\hat{T}|\Psi\rangle + \underbrace{\min_{\Psi\to\rho}\langle\Psi|\hat{V}_{ee}|\Psi\rangle}_{V_{ee}^{\mathrm{SCE}}[\rho]}$$

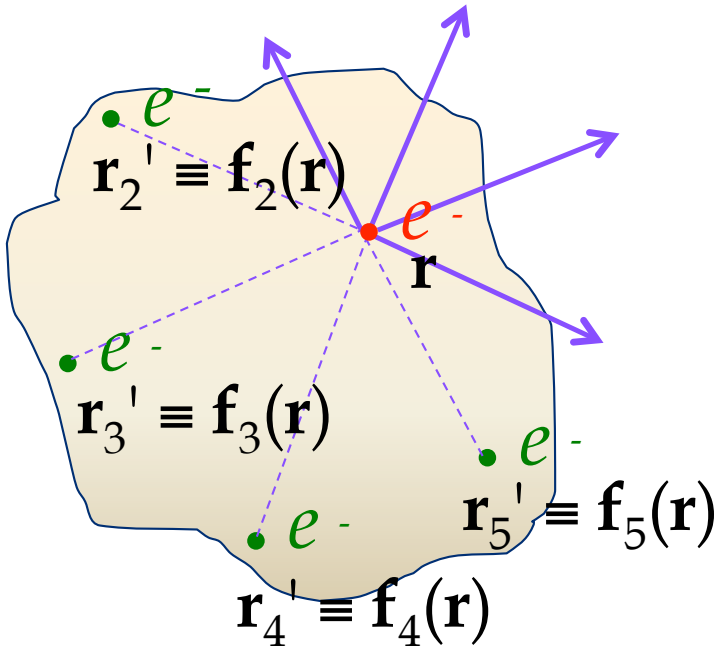
$$v_{\mathrm{SCE}}[\rho] \simeq v_{\mathrm{Hartree}}[\rho] + v_{\mathrm{xc}}[\rho]$$

$$\left(-\frac{1}{2}\nabla^2 + v_{\mathrm{KS}}[\rho](\mathbf{r})\right)\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$$

$$v_{\mathrm{KS}}[\rho] = v_{\mathrm{ext}}[\rho] + v_{\mathrm{SCE}}[\rho]$$

$$v_{\mathrm{SCE}}[\rho] = \frac{\delta V_{ee}^{SCE}[\rho]}{\delta\rho}$$

Strictly-interacting-electrons (SCE) DFT



The SCE reference system:

- For a given smooth density $\rho(\mathbf{r})$:

$$\rho(\mathbf{f}_i(\mathbf{r}))d\mathbf{f}_i(\mathbf{r}) = \rho(\mathbf{r})d\mathbf{r} \qquad (1)$$

- A <u>local one-body potential</u> can be defined:

$$-\nabla v_{\mathrm{SCE}}[\rho](\mathbf{r}) = \mathbf{F}_{\mathrm{Coul}}(\mathbf{r}) = \sum_{\mathbf{i}=\mathbf{2}}^{\mathbf{N}} \frac{\mathbf{r} - \mathbf{f_i}[\rho](\mathbf{r})}{|\mathbf{r} - \mathbf{f_i}[\rho](\mathbf{r})|^{\mathbf{3}}} \qquad (2)$$

KS-SCE approach:

1-Integrate (1) to obtain the co-motion functions $\mathbf{f}_i(\mathbf{r})$

2-Integrate (2) to obtain the potential $v_{\mathrm{SCE}}(\mathbf{r})$

3-Approximate the Hxc potential of KS DFT with $v_{\mathrm{SCE}}(\mathbf{r})$

$$v_{\mathrm{SCE}}[\rho] \simeq v_{\mathrm{Hartree}}[\rho] + v_{\mathrm{xc}}[\rho]$$

$$\rho(\mathbf{f}_i(\mathbf{r}))d\mathbf{f}_i(\mathbf{r}) = \rho(\mathbf{r})d\mathbf{r}$$

$$\mathbf{f}_1(\mathbf{r}) \equiv \mathbf{r},\ \mathbf{f}_2(\mathbf{r}) \equiv \mathbf{f}(\mathbf{r}),\ \mathbf{f}_3(\mathbf{r}) = \mathbf{f}(\mathbf{f}(\mathbf{r})),\ \mathbf{f}_4(\mathbf{r}) = \mathbf{f}(\mathbf{f}(\mathbf{f}(\mathbf{r}))), \ldots \text{ with } \underbrace{\mathbf{f}(\mathbf{f}(\ldots\mathbf{f}(\mathbf{f}(\mathbf{r}))}_{N \text{ times}} = \mathbf{r}$$

$$V_{ee}^{\mathrm{SCE}}[\rho] = \int d\mathbf{r} \frac{\rho(\mathbf{r})}{N} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{|\mathbf{f}_i(\mathbf{r}) - \mathbf{f}_j(\mathbf{r})|}$$

$$\frac{\delta V_{ee}^{\mathrm{SCE}}[\rho]}{\delta \rho(\mathbf{r})} = v_{\mathrm{SCE}}(\mathbf{r})$$

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$$\frac{\delta V_{ee}^{\mathrm{SCE}}[\rho]}{\delta \rho(\mathbf{r})} = v_{\mathrm{SCE}}(\mathbf{r})$$

$$\nabla v_{\mathrm{SCE}}(\mathbf{r}) = \sum_{i=2}^{N} \frac{\mathbf{r} - \mathbf{f}_i(\mathbf{r})}{|\mathbf{r} - \mathbf{f}_i(\mathbf{r})|^3}$$

shortcut to the functional derivative

F. Malet. et al., PRB ***87*** *115146 (2013)*

The self-consistent KS SCE total energy is a rigorous lower bound to the exact energy

The self-consistent KS SCE total energy is a rigorous lower bound to the exact energy

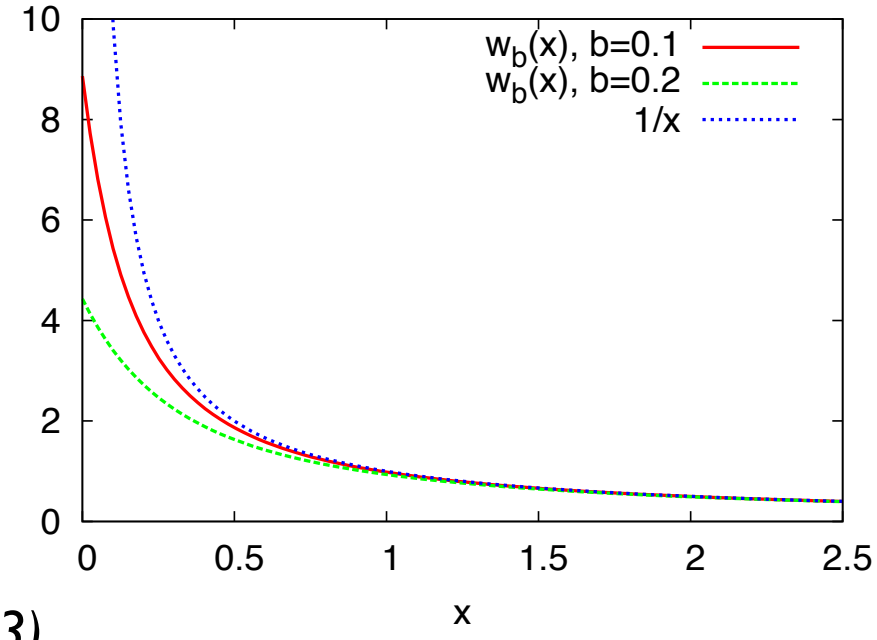
The proof is trivial
(minimum of a sum is always larger than the sum of the minima; self-consistency lowers the energy)

First tests: quasi 1D systems

$$V_\perp(y,z) = \frac{1}{2} m\,\omega_\perp^2 (y^2+z^2) \qquad b^2 = \frac{\hbar}{2m\,\omega_\perp}$$

$$H_{1D} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \sum_{i=1}^{N}\sum_{j>i}^{N} w_b(|x_i - x_j|) + \sum_{i=1}^{N} v_{\rm ext}(x_i)$$

$$w_b(x) = \frac{\sqrt{\pi}}{2}\frac{e_*^2}{b} e^{x^2/4b^2}\,\mathrm{erfc}\left(\frac{x}{2b}\right)$$



Bednarek et al. PRB 68, 045328 (2003)

LDA: Casula, Sorella & Senatore PRB 74, 245427 (2006)

Electrons confined in (quasi)1D

Co-motion functions:

$$f_i(x) = \begin{cases} N_e^{-1}[N_e(x) + i - 1] & x \le a_{N+1-i} \\ N_e^{-1}[N_e(x) + i - 1 - N] & x > a_{N+1-i}, \end{cases}$$

$$N_e(x) = \int_{-\infty}^{x} \rho(x')\, dx' \qquad a_k = N_e^{-1}(k)$$

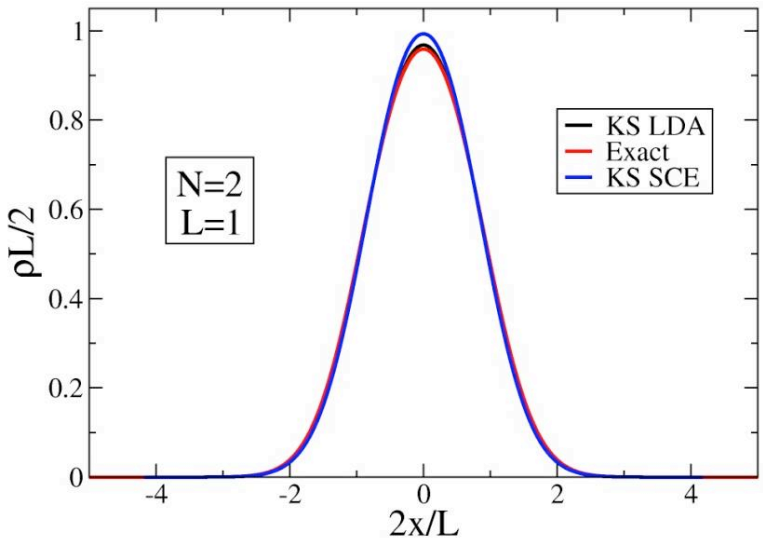
$$v'_{\mathrm{SCE}}[\rho](x) = -\sum_{i=2}^{N} w'_b(|x - f_i(x)|)\mathrm{sgn}(x - f_i(x))$$

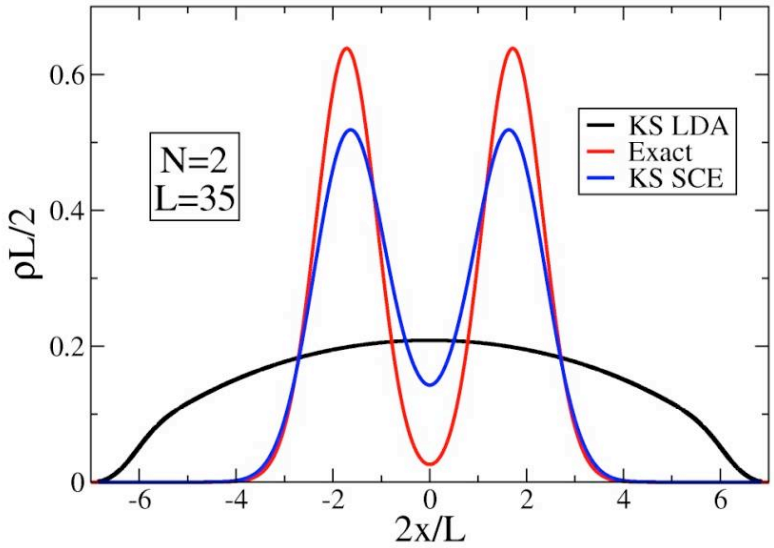
Seidl, *Phys. Rev. A* 60, 4387 (1999)
Buttazzo, De Pascale, & Gori-Giorgi, *Phys. Rev. A* 85, 062502 (2012)
Malet & Gori-Giorgi, *Phys. Rev. Lett.*, 109, 246402 (2012)

Applications to 1D systems

1D harmonic confinement: $v_{\rm ext}(x) = \frac{1}{2}\omega^2 x^2 \qquad \omega = \frac{4}{L^2}$ L: effective length

- **Qualitatively good resuls in both the weak and strong correlation regimes**





*F. Malet and P. Gori-Giorgi, PRL **109** 246402 (2012); F. Malet. et al., PRB **87** 115146 (2013)*

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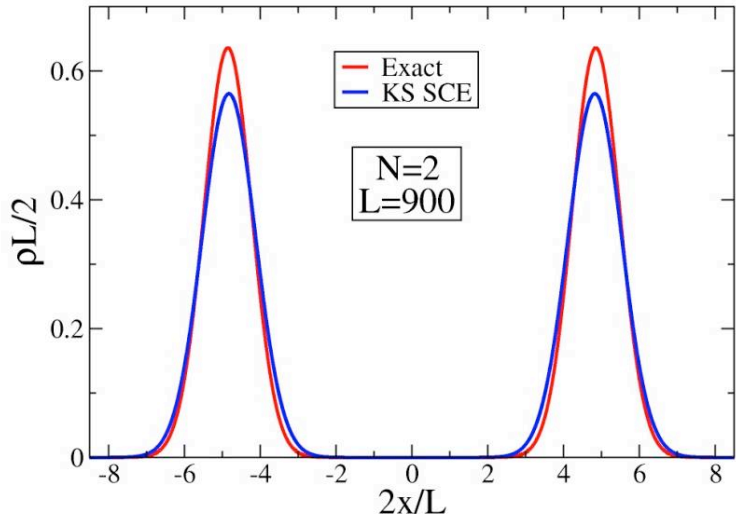
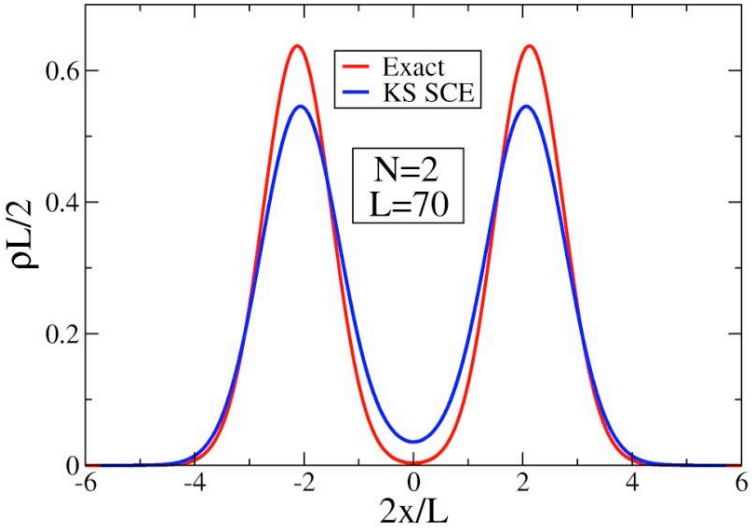
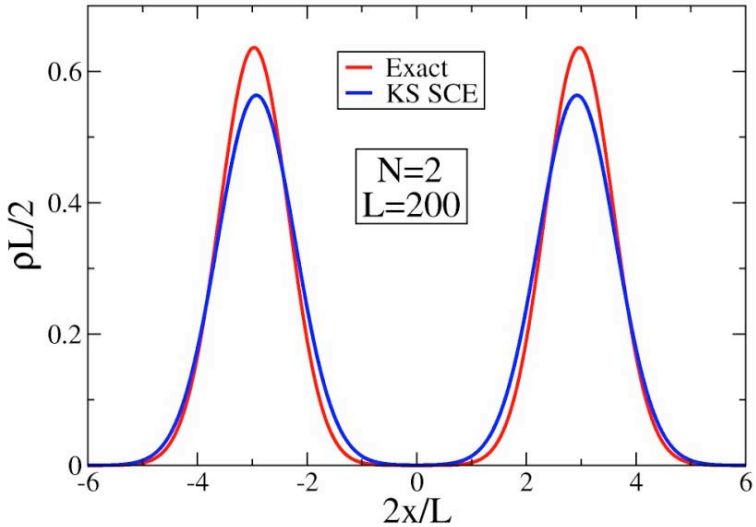
- **Qualitatively good resuls in both the weak and strong correlation regimes**
- **Tends to the exact result in the very strongly-interacting limit**







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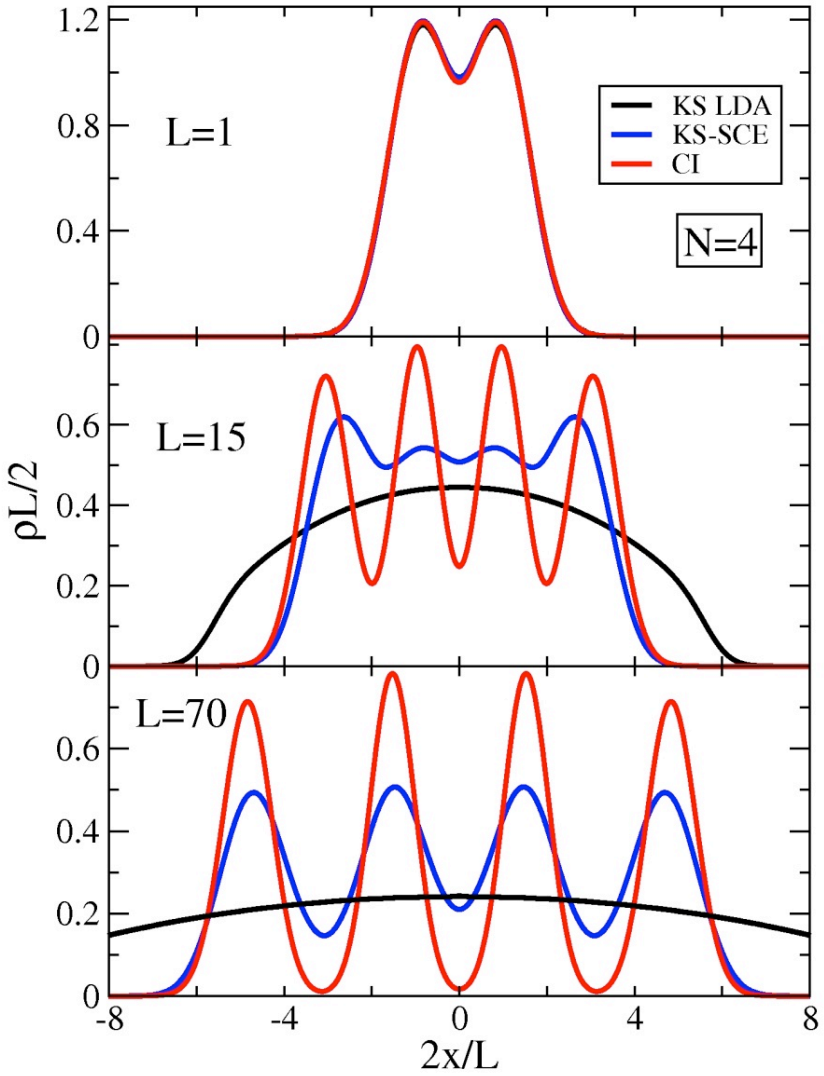

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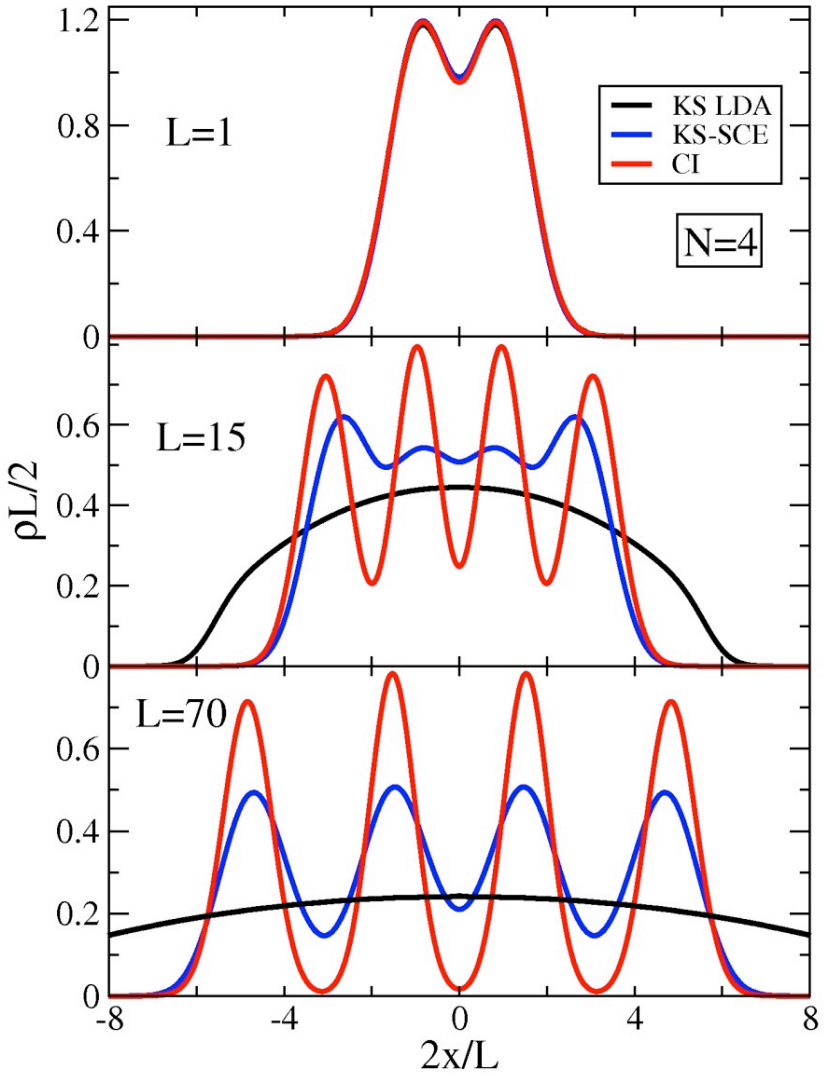

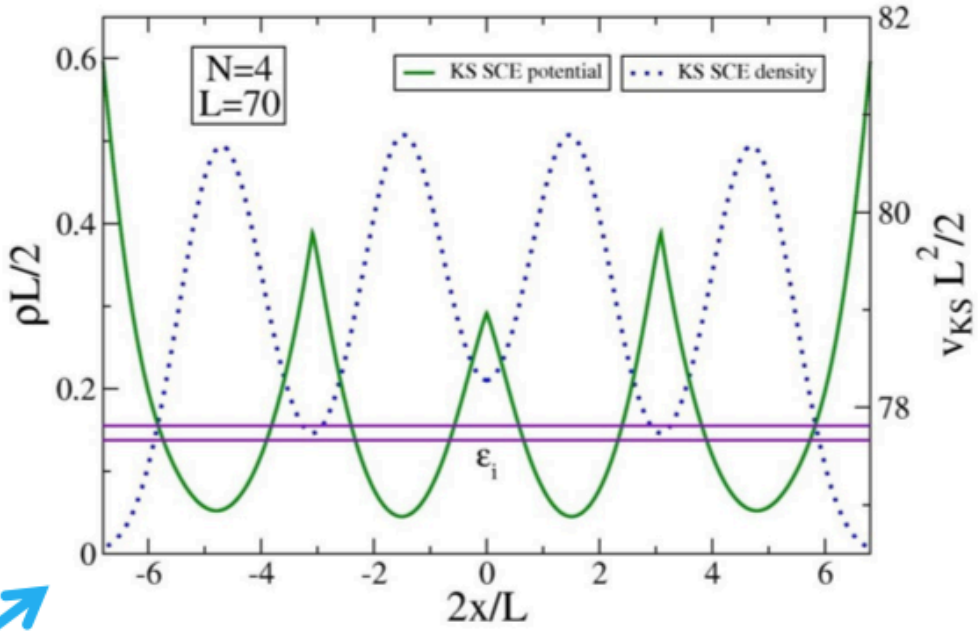

*F. Malet and P. Gori-Giorgi, PRL **109** 246402 (2012); F. Malet. et al., PRB **87** 115146 (2013)*

KS SCE is the first KS DFT approach able to capture the density peak splitting in quasi 1D without introducing magnetic order

Previous attempts include self-interaction corrections (SIC) and GGA:

S. H. Abedinpour, M. Polini, G. Xianlong, and M. P. Tosi, Eur. Phys. J. B 56, 127 (2007)

D. Vieira and K. Capelle, J. Chem. Theory Comput. 6, 3319 (2010)

D. Vieira, Phys. Rev. B 86, 075132 (2012)

Total Energies

N	L	KS SCE	CI	KS LDA
2	2	1.81	2.49	2.59
2	15	0.0942	0.106	0.130
2	70	0.0112	0.0115	0.0182
4	1	25.08	28.42	28.57
4	2	8.46	10.60	10.68
4	15	0.491	0.541	0.580
4	70	0.0602	0.0629	0.0771
5	15	0.787	0.871	0.915
5	70	0.099	0.102	0.121

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CI matrix 10^5 - 10^6

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KS SCE is a rigorous lower bound to the exact ground-state energy

*F. Malet and P. Gori-Giorgi, PRL **109** 246402 (2012); F. Malet. et al., PRB **87** 115146 (2013)*

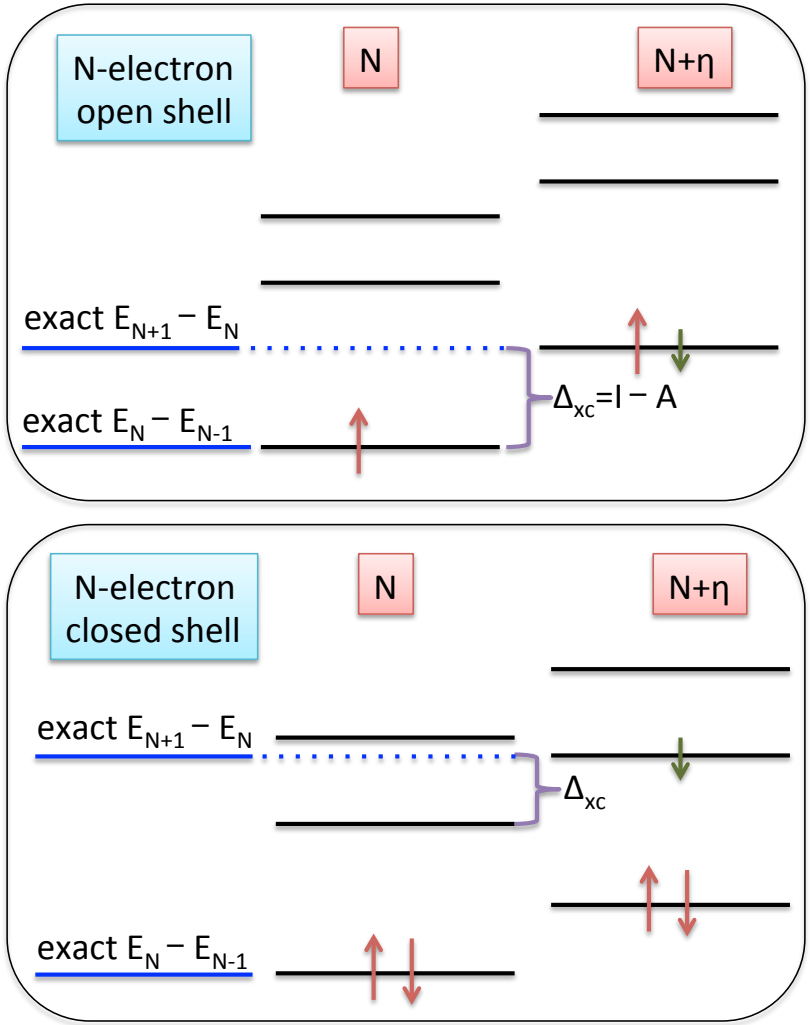
Ionization potentials from minus HOMO

N	L	KS SCE	CI	KS LDA
2	2	1.65	1.99	2.56
2	15	0.104	0.097	0.263
2	70	0.0126	0.0111	0.040 87
4	1	11.26	11.86	12.56
4	2	4.08	4.65	5.02
4	15	0.248	0.256	0.453
4	70	0.0318	0.0304	0.069 09
5	15	0.325	0.330	0.539
5	70	0.0408	0.0391	0.081 72

*F. Malet and P. Gori-Giorgi, PRL **109** 246402 (2012); F. Malet. et al., PRB **87** 115146 (2013)*

Generalization to open systems: The Derivative Discontinuity at integer particle numbers

What exact spin-restricted KS should do



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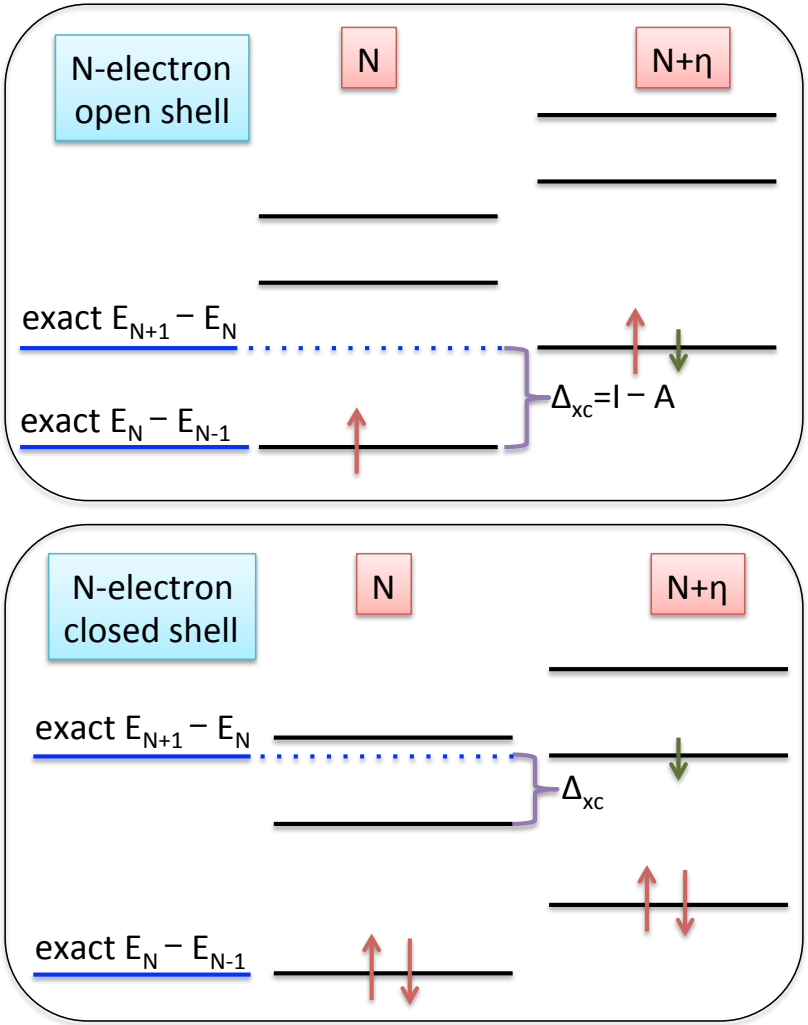
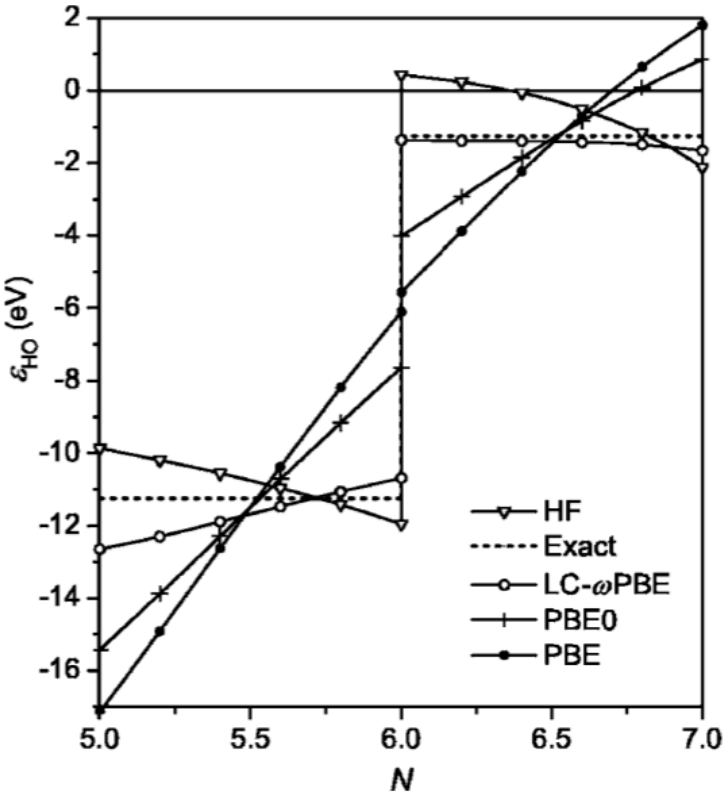
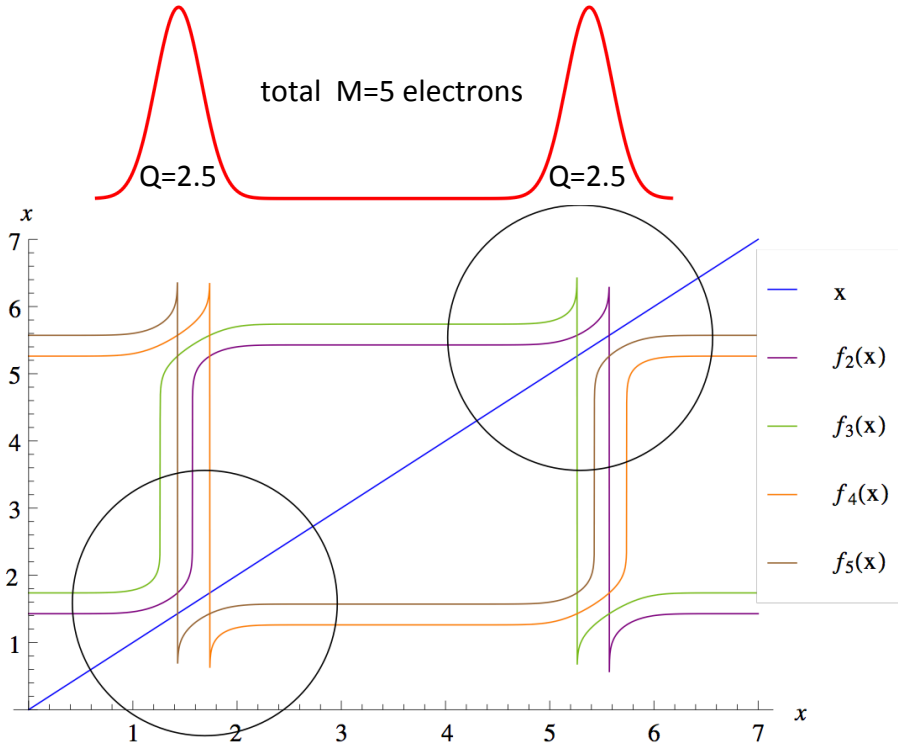


What approximate functionlals do (UKS)



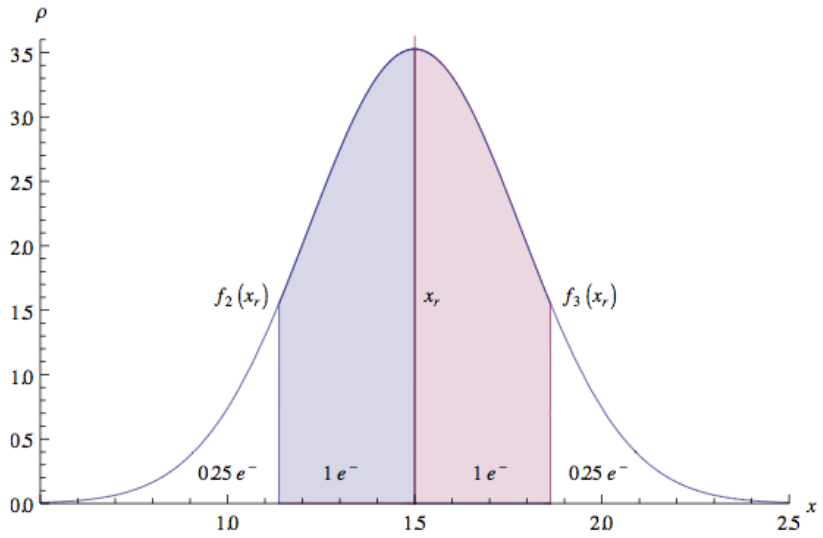
Vydrov, Scuseria & Perdew, JCP 126, 154109 (2007)

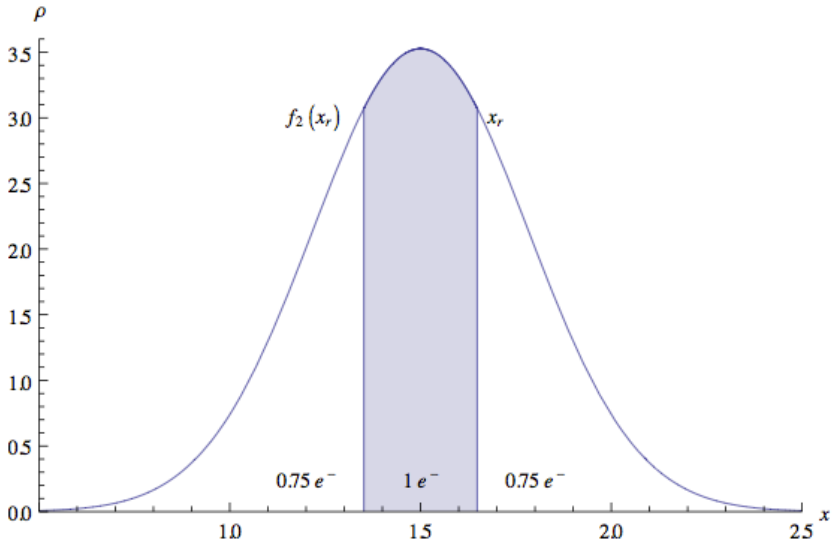
SCE for fractional particle numbers



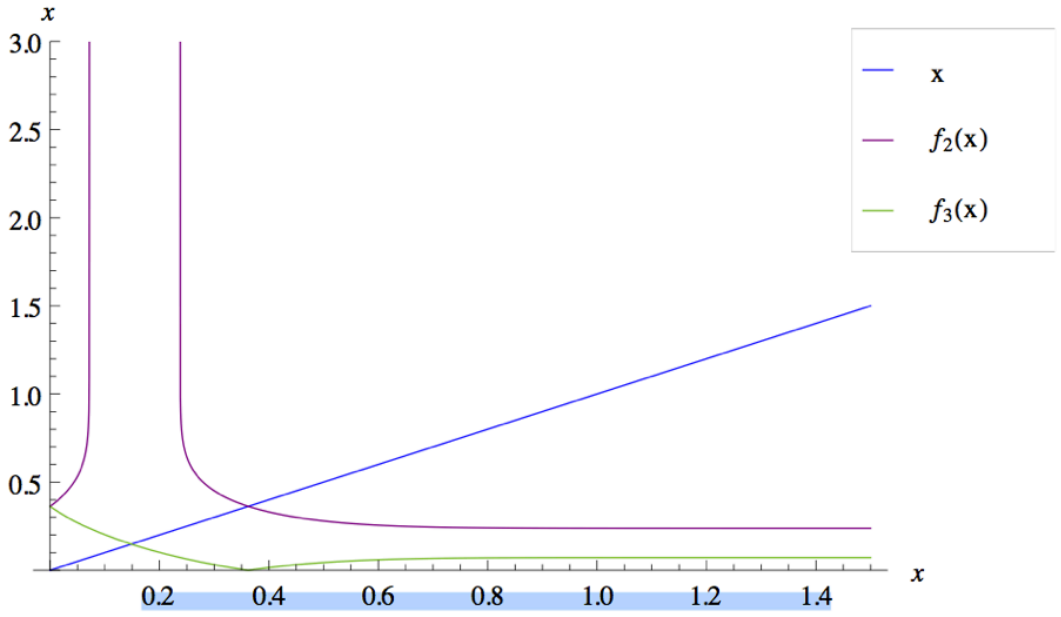
$$\int_{f_i(x)}^{f_{i+1}(x)} \rho(y)dy = 1$$

example: N=2.5





$$\int_{f_i(x)}^{f_{i+1}(x)} \rho(y)dy = 1$$



co-motion functions for $N+\eta$ electrons

$$f_i(x) = \begin{cases} N_e^{-1}[N_e(x) + 2i] & x < a_{N-2i+\eta} \\ N_e^{-1}[|N_e(x) - 2(N+1-i)|] & x > a_{N+2-2i-\eta} \\ \infty & \text{otherwise,} \end{cases}$$

get the SCE potential by integrating

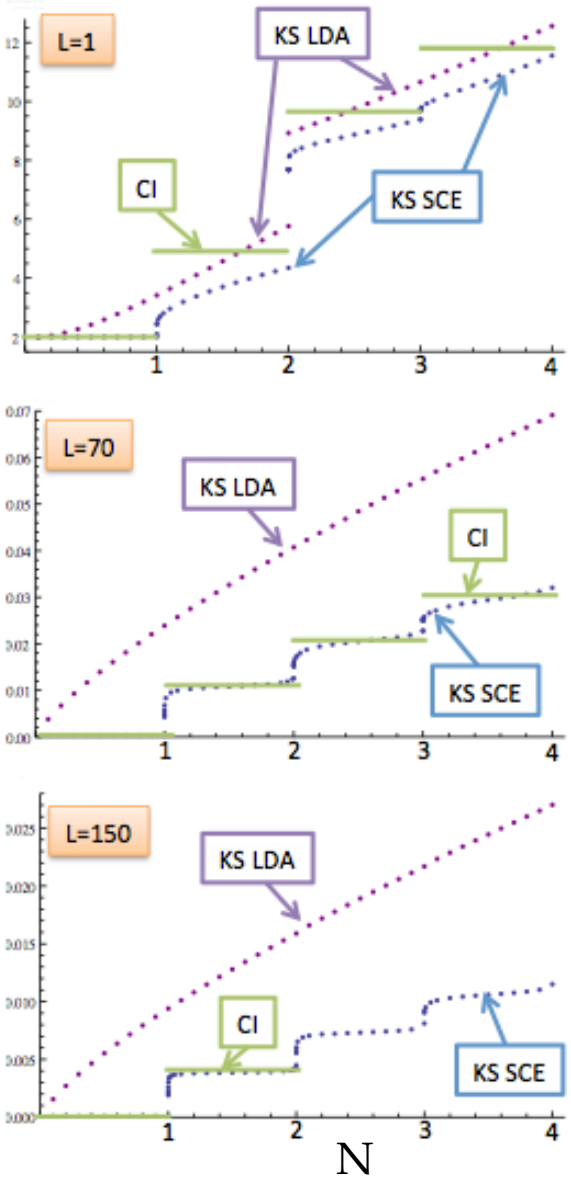
$$v'_{\mathrm{SCE}}[\rho](x) = -\sum_{i=2}^{N} w'_b(|x - f_i(x)|)\mathrm{sgn}(x - f_i(x))$$

with boundary condition

$$v_{\mathrm{SCE}}[\rho](x \to \infty) = 0$$

Self-consistent KS HOMO eigenvalue

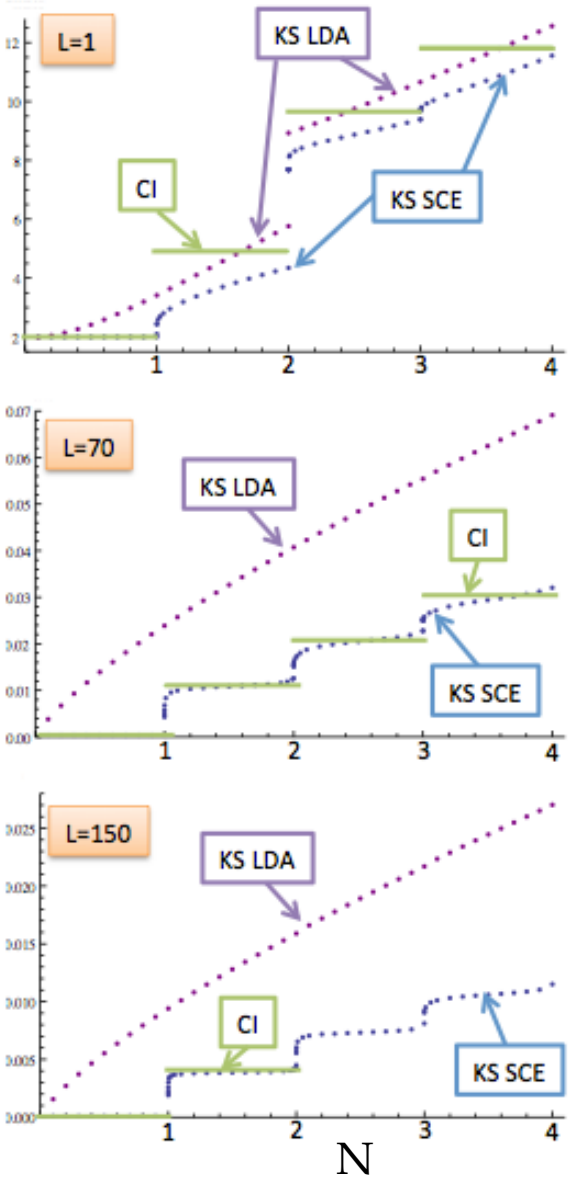
quasi 1D



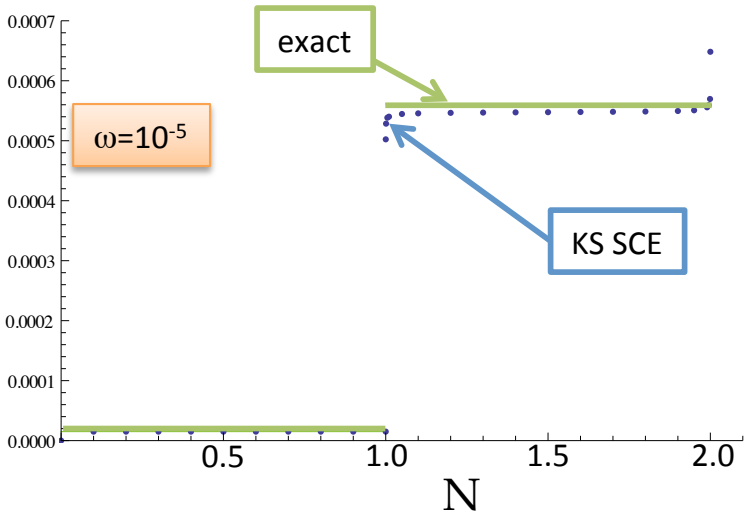
A. Mirtschink, M. Seidl, and P. Gori-Giorgi, arXiv:1305.3982, accepted in PRL

Self-consistent KS HOMO eigenvalue

quasi 1D



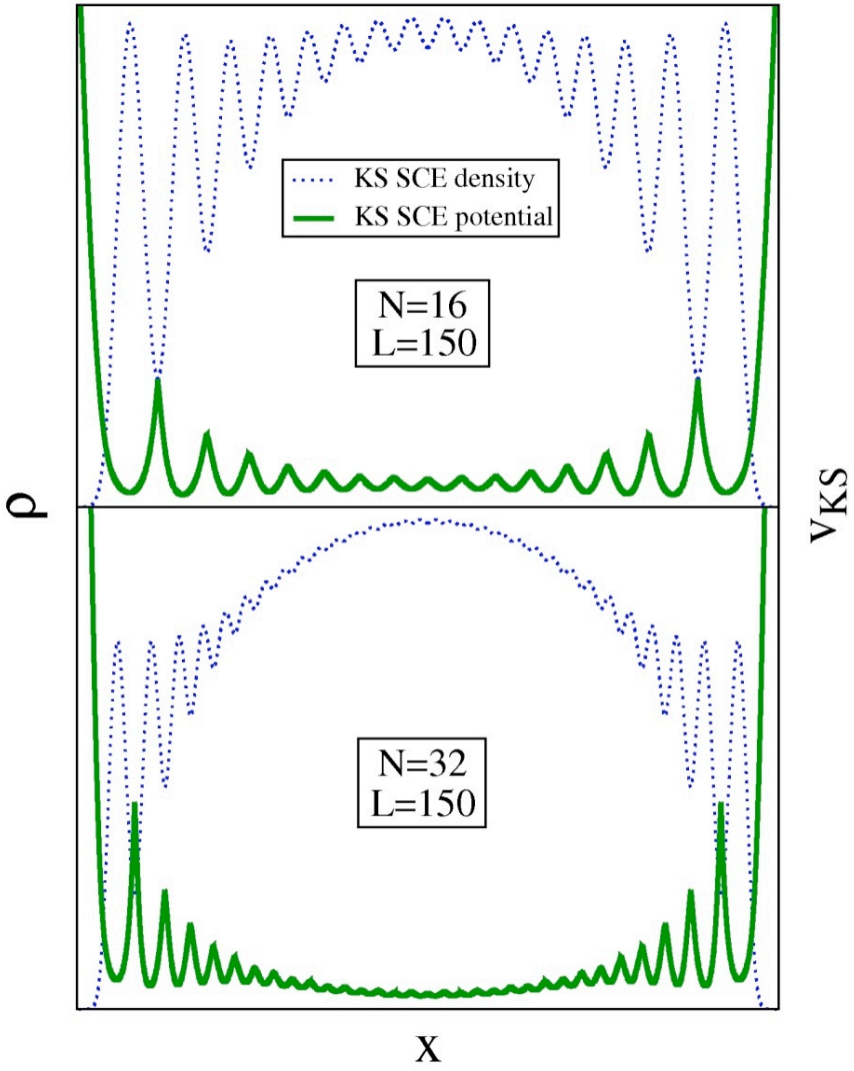
3D (Hooke's atom)



A. Mirtschink, M. Seidl, and P. Gori-Giorgi, arXiv:1305.3982, accepted in PRL

Applications to 1D systems

1D harmonic confinement: $v_{\rm ext}(x) = \frac{1}{2}\omega^2 x^2 \qquad \omega = \frac{4}{L^2}$ L: effective length

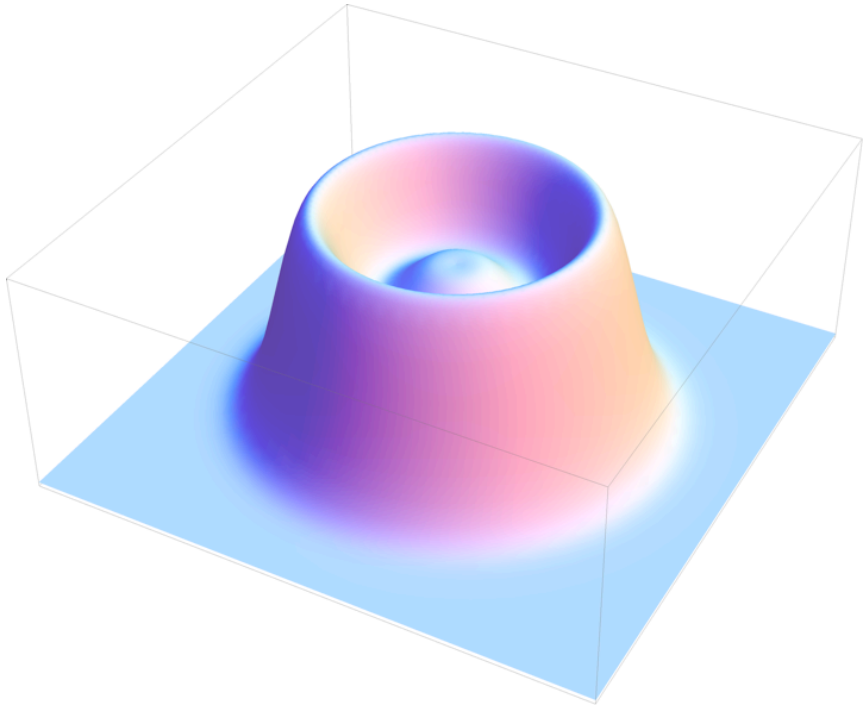


- **KS-SCE allows to treat large strongly-correlated quasi 1D systems (vs CI, limited to 6-8 particles, QMC and DMRG ~ 100 electrons).**
- **Computational time similar to KS LDA calculations**
- **Applications in Physics (model semiconductor quantum wires); nanotransport, quantum computation, ...**

*F. Malet and P. Gori-Giorgi, PRL **109** 246402 (2012); F. Malet. et al., PRB **87** 115146 (2013)*

Electrons confined in two dimensions

$$\hat{H} = -\sum_{i=1}^{N} \frac{\nabla_i^2}{2} + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{\omega^2}{2} \sum_{i=1}^{N} r_i^2$$



$N = 6 \;\; \omega = 0.005$

Self-consistent KS SCE density

C. B. Mendl (Munich Technical University)
F. Malet

What about Chemistry?

1D as a test lab for 3D chemistry

Cite this: *Phys. Chem. Chem. Phys.*, 2012, **14**, 8581–8590

www.rsc.org/pccp **PAPER**

Reference electronic structure calculations in one dimension†

Lucas O. Wagner,*[a] E. M. Stoudenmire,[a] Kieron Burke[ab] and Steven R. White[a]

Received 24th December 2011, Accepted 1st May 2012
DOI: 10.1039/c2cp24118h

THE JOURNAL OF CHEMICAL PHYSICS **131**, 224105 (2009)

Exact Kohn–Sham potential of strongly correlated finite systems

N. Helbig,[1,a] I. V. Tokatly,[1,2] and A. Rubio[1,3]
[1]*Nano-Bio Spectroscopy Group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, Av. Tolosa 72, San Sebastián E-20018, Spain*
[2]*IKERBASQUE, Basque Foundation for Science, Bilbao E-48011, Spain*

PHYSICAL REVIEW A **83**, 032503 (2011)

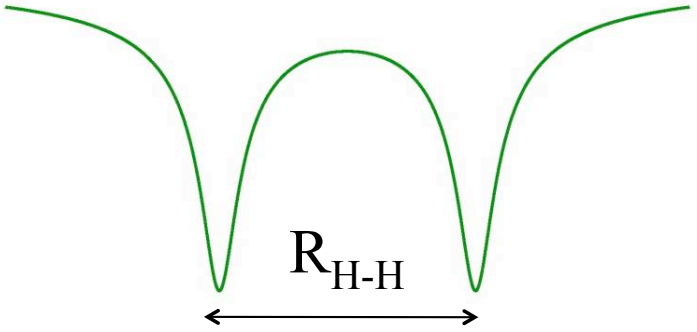
Density functional theory beyond the linear regime: Validating an adiabatic local density approximation

N. Helbig,[1] J. I. Fuks,[1] M. Casula,[2] M. J. Verstraete,[3,4] M. A. L. Marques,[5,4] I. V. Tokatly,[1,6] and A. Rubio[1,7]

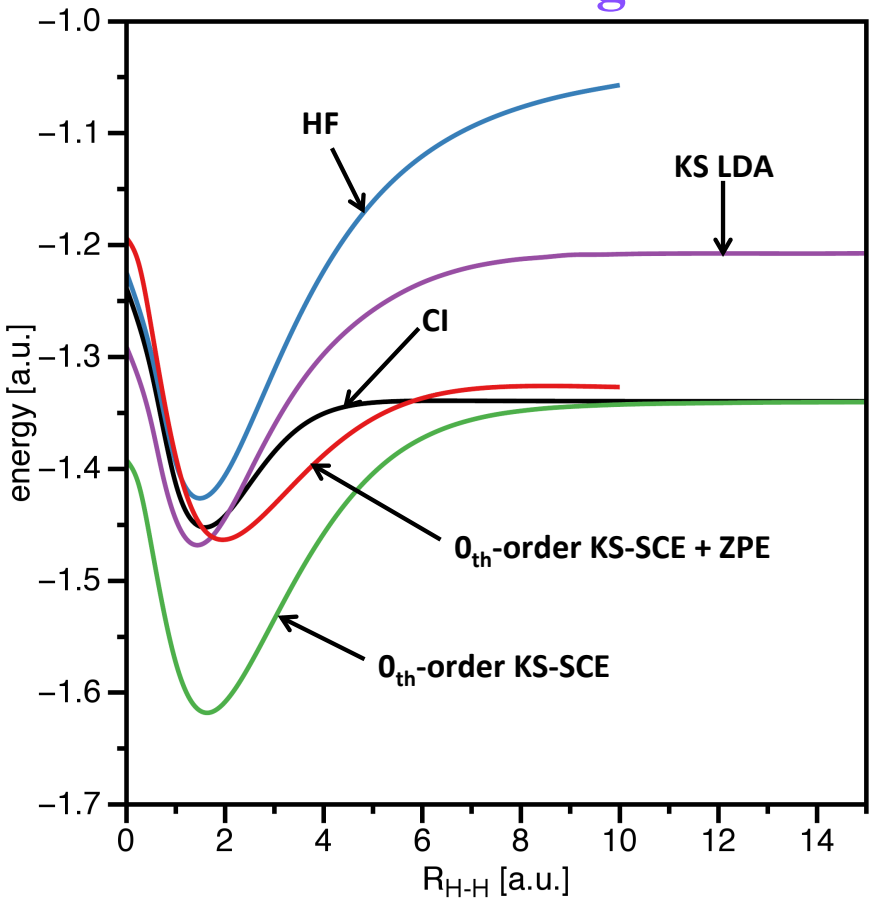
$$w_s(x) = \frac{1}{\sqrt{x^2 + a^2}}$$

Applications to 1D systems

1D model for H_2 :



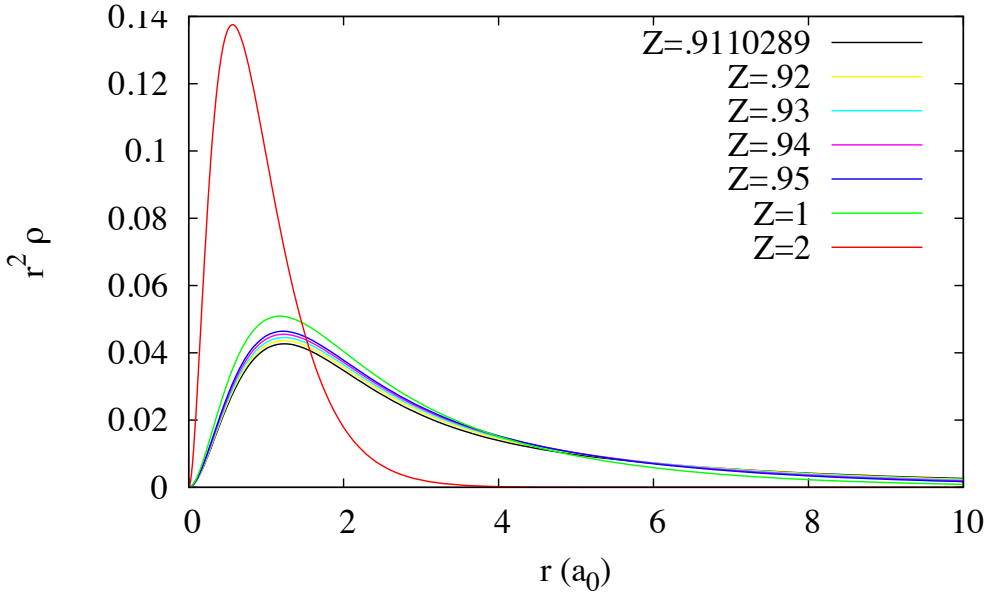
Total energies



Negative ions (3D)

$$N = 2 \qquad v_{\mathrm{ext}}(\mathbf{r}) = -\frac{Z}{r}$$

$$Z \to Z_{\mathrm{crit}} \approx 0.9110289$$ the system looses 1 electron



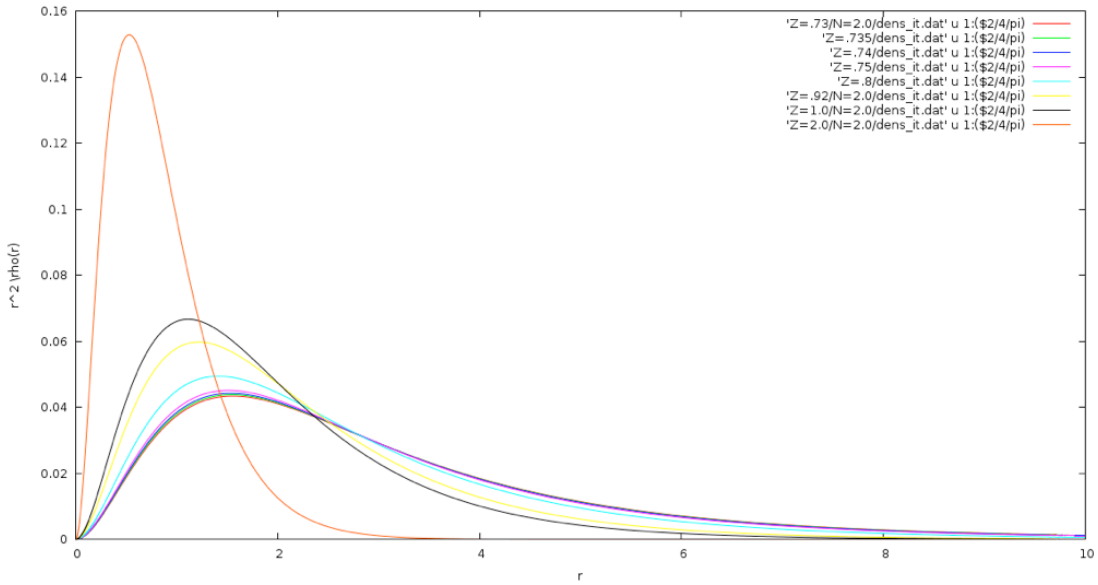
accurate results
(C. Umrigar & J. Morgan)

Negative ions (3D)

$$N = 2 \qquad v_{\text{ext}}(\mathbf{r}) = -\frac{Z}{r}$$

$$Z \to Z_{\text{crit}} \approx 0.9110289$$ the system looses 1 electron

KS SCE self-consistent: $$Z_{\text{crit}} \approx 0.73$$



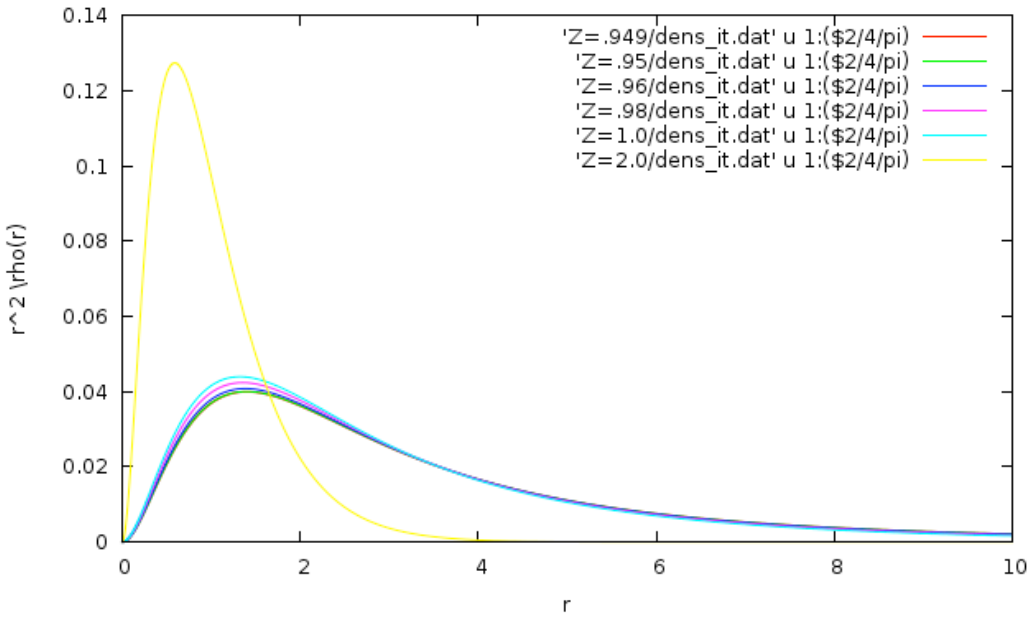
A. Mirtschink

Negative ions (3D)

$$N = 2 \qquad v_{\text{ext}}(\mathbf{r}) = -\frac{Z}{r}$$

$$Z \to Z_{\text{crit}} \approx 0.9110289$$ the system looses 1 electron

KS SCE +local correction (self-consistent): $Z_{\text{crit}} \approx 0.94$



A. Mirtschink

How to treat general 3D systems?

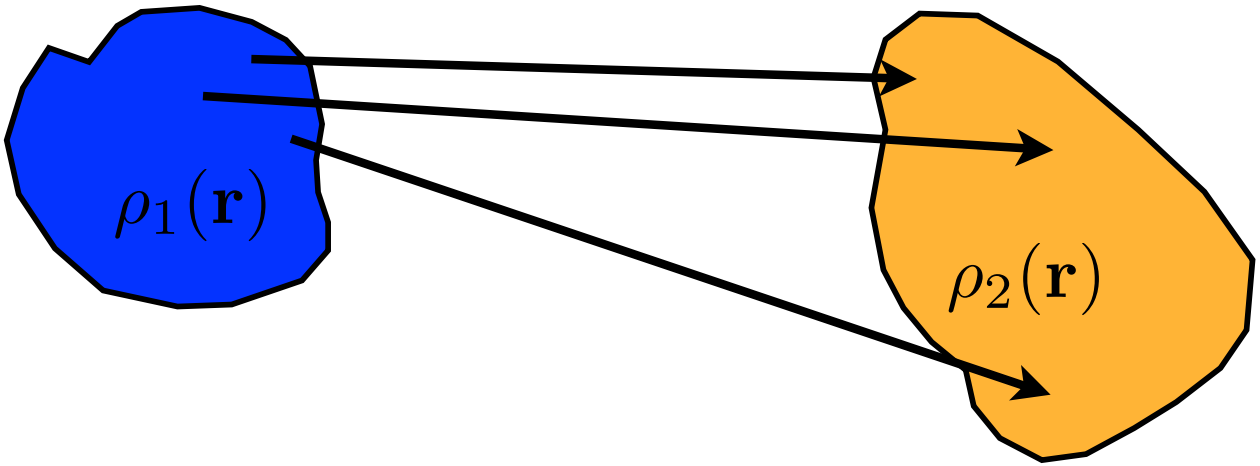
Monge-Kantorovich formulation

Buttazzo, De Pascale, and Gori-Giorgi, *Phys. Rev. A.* **85**, 062502 (2012)
Cotar, Friesecke, and Kluppelberg, *Comm. Pure Appl. Math.* **66**, 548 (2013)

see also talk by Gero Friesecke!

Optimal transport formulation

(Monge-Kantorovich)



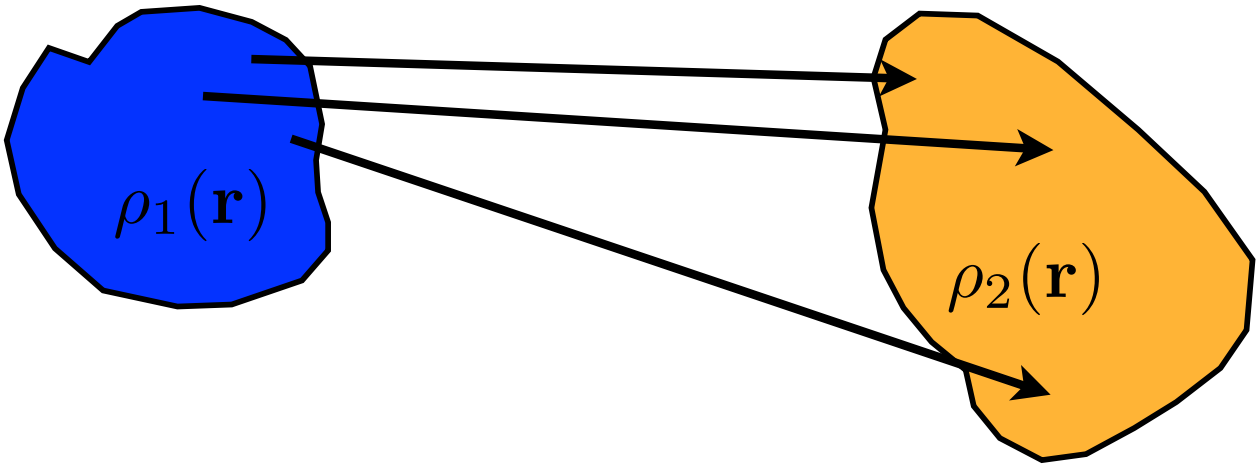
$$\int \rho_1(\mathbf{r})d\mathbf{r} = \int \rho_2(\mathbf{r})d\mathbf{r}$$

cost function (work necessary to move a unit mass)

$$c(\mathbf{r}_1, \mathbf{r}_2) = |\mathbf{r}_2 - \mathbf{r}_1|$$

Optimal transport formulation

(Monge-Kantorovich)



$$\int \rho_1(\mathbf{r})d\mathbf{r} = \int \rho_2(\mathbf{r})d\mathbf{r}$$

cost function (work necessary to move a unit mass)

$$c(\mathbf{r}_1, \mathbf{r}_2) = |\mathbf{r}_2 - \mathbf{r}_1|$$

optimal map

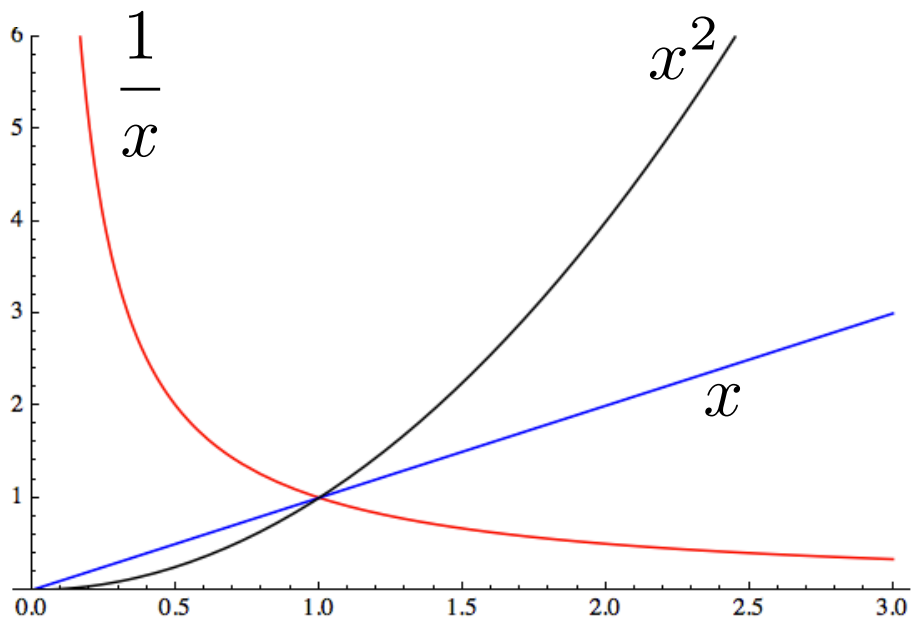
$$\text{minimize total cost} \Rightarrow \min_{\mathbf{f}} \int c(\mathbf{r}, \mathbf{f}(\mathbf{r}))\rho_1(\mathbf{r})d\mathbf{r}$$

$$\min_P \left\{ \int c(x_1, ..., x_N) P(dx_1, ...dx_N) : \pi_j^{\#} P = \frac{\rho}{N} \text{ for } j = 1, ..., N \right\}$$

$$c(x_1, ..., x_N) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{|x_i - x_j|}$$

$$\min_P \left\{ \int c(x_1, ..., x_N) P(dx_1, ...dx_N) : \pi_j^{\#} P = \frac{\rho}{N} \text{ for } j = 1, ..., N \right\}$$

$$c(x_1, ..., x_N) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{1}{|x_i - x_j|}$$



here: the further, the better!

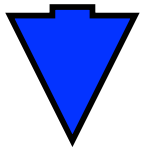
Things you can prove from Optimal Transport

- Existence of $P(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) (= |\Psi_{\rm SCE}(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N)|^2)$
- $v_{\rm SCE}(\mathbf{r})$ exists and it is bounded (Kantorovich potential)
- Not possible (so far) to prove general existence of $\mathbf{f}_i(\mathbf{r})$
- Dual Kantorovich problem

Buttazzo, De Pascale, and Gori-Giorgi, *Phys. Rev. A.* **85**, 062502 (2012)

Dual Kantorovich problem

$$V_{\rm SCE}[\rho] = \min_{\Psi\to\rho} \langle \Psi | \hat{V}_{ee} | \Psi \rangle$$



$$V_{\rm SCE}[\rho] = \max_{u} \left\{ \int \rho(\mathbf{r}) u(\mathbf{r}) d\mathbf{r} \quad : \quad \sum_{i=1}^{N} u(\mathbf{r}_i) \leq \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \right\}$$

$$v_{\rm SCE}(\mathbf{r}) = u(\mathbf{r}) + C$$

Kantorovich potential

Buttazzo, De Pascale, and Gori-Giorgi, *Phys. Rev. A.* **85**, 062502 (2012)

Kantorovich formulation: key to treat the 3D case?

PHYSICAL REVIEW B **87**, 125106 (2013)

Kantorovich dual solution for strictly correlated electrons in atoms and molecules

Christian B. Mendl[1] and Lin Lin[2]

[1]*Mathematics Department, Technische Universität München, Boltzmannstraße 3, 85748 Garching bei München, Germany*

[2]*Computational Research Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

(Received 26 October 2012; published 6 March 2013)

The many-body Coulomb repulsive energy of strictly correlated electrons provides direct information on the exact Hohenberg-Kohn exchange-correlation functional in the strong interaction limit. Until now the treatment of strictly correlated electrons has been based on the calculation of comotion functions with the help of semianalytic formulations. This procedure is system-specific and has been limited to spherically symmetric atoms and strictly one-dimensional systems. We develop a nested optimization method which solves the Kantorovich dual problem directly, and thus facilitates a general treatment of strictly correlated electrons for systems including atoms and small molecules.

Conclusions and outlook

- **Strongly-interacting limit of DFT: approximations for the xc functional able to describe strong correlation within the restricted KS scheme (no artificial symmetry breaking)**

- **One can treat strongly-correlated quasi 1D systems with large electron numbers**

Perspectives:

- **Improve the algorithms for 2D and 3D systems**
- **Corrections to the KS SCE functional:**

$$F[\rho] = T_s[\rho] + V_{ee}^{\mathrm{SCE}}[\rho] + T_c[\rho] + V_{ee}^{d}[\rho]$$

- **Inclusion of spin states**
- **Approximate SCE forms for new non-local functionals**
- **Nanotransport**

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Andreas Savin (CNRS, University Paris VI)
Giuseppe Buttazzo (University of Pisa)
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Thank you for your attention!