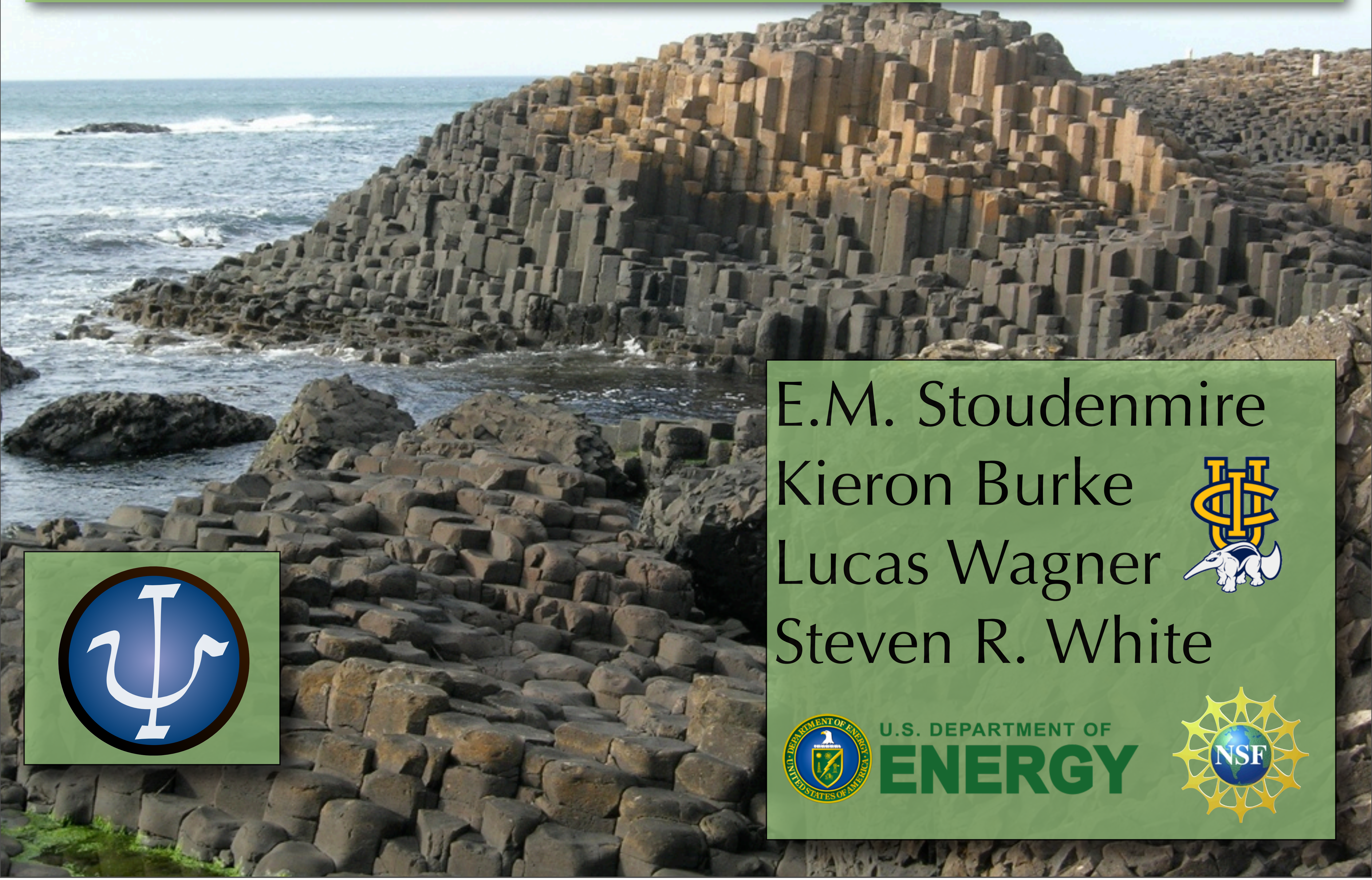
Exact DFT with DMRG



E.M. Stoudenmire
Kieron Burke
Lucas Wagner
Steven R. White

Summary:

Using an exact numerical solver for 1d systems (known as DMRG), we can learn more about density functional theory (DFT) and find ways to make it better

Density functional theory (DFT) is an efficient method that works extremely well for molecules and materials....

...except when it doesn't

Strong Correlation

Transport

Derivative Discontinuity

Predicting Gaps

Ideas for correcting these issues, but how to test them?

S-DFA

HSE

DMFT+DFT

GGA+U

To check if they work, and for the right reasons, must give something up:

- Continuum
- Long-range interactions
- ~~Three Dimensions~~

Keeping the continuum and long-range interactions, we find 1d chemistry to be a good mimic of real 3d world

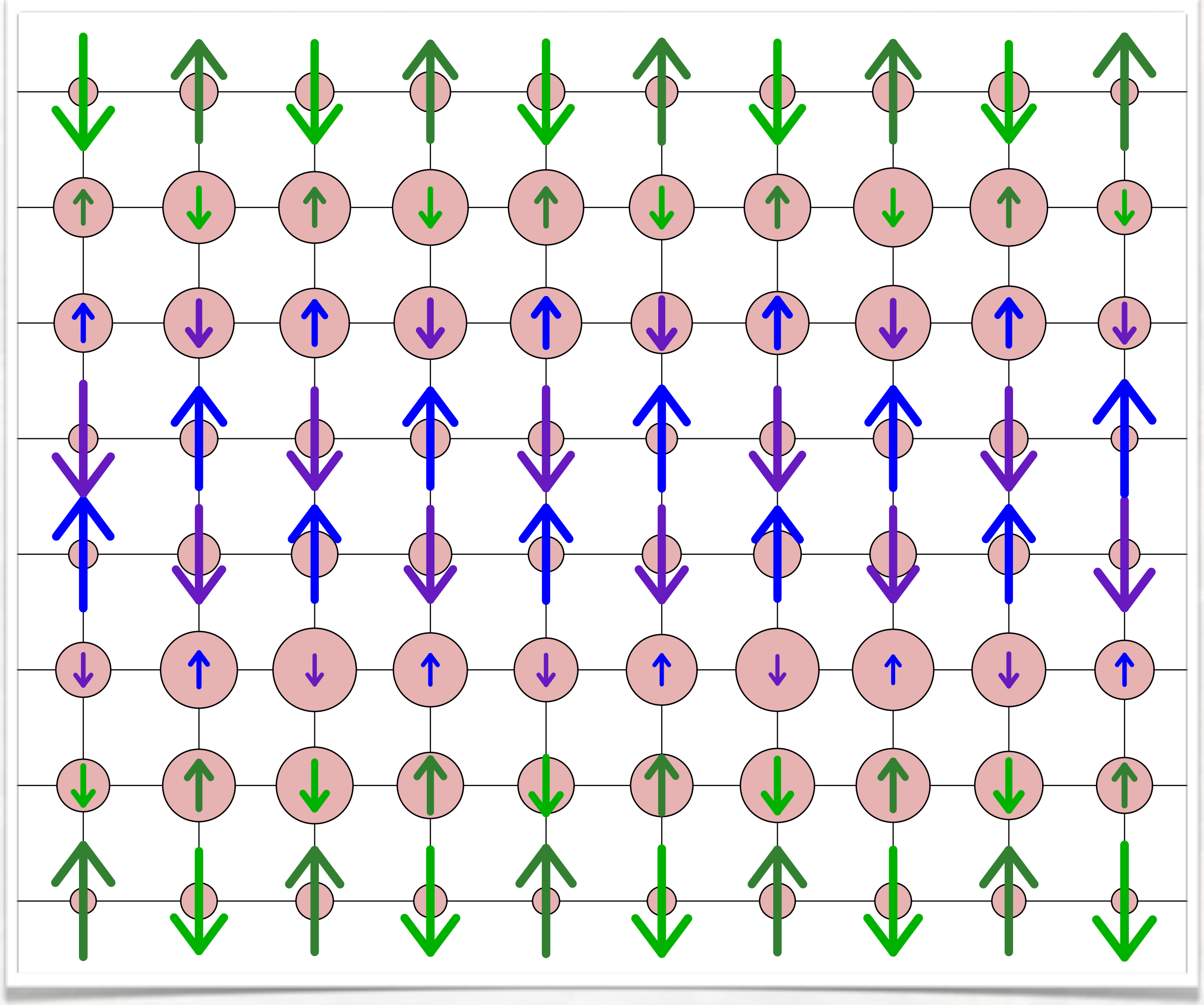
→ *(see next talk by Lucas Wagner)*

Working in 1d lets us use the powerful density matrix renormalization group (DMRG) method...

DMRG - a powerful numerical method:

- 👍 Essentially exact solutions
- 👍 Linear scaling in 1d
- 👍 Access entire wavefunction
- 👍 Time dependence, finite T
- 👎 1d and narrow 2d systems

DMRG usually applied to lattice models (such as t-J or Hubbard)

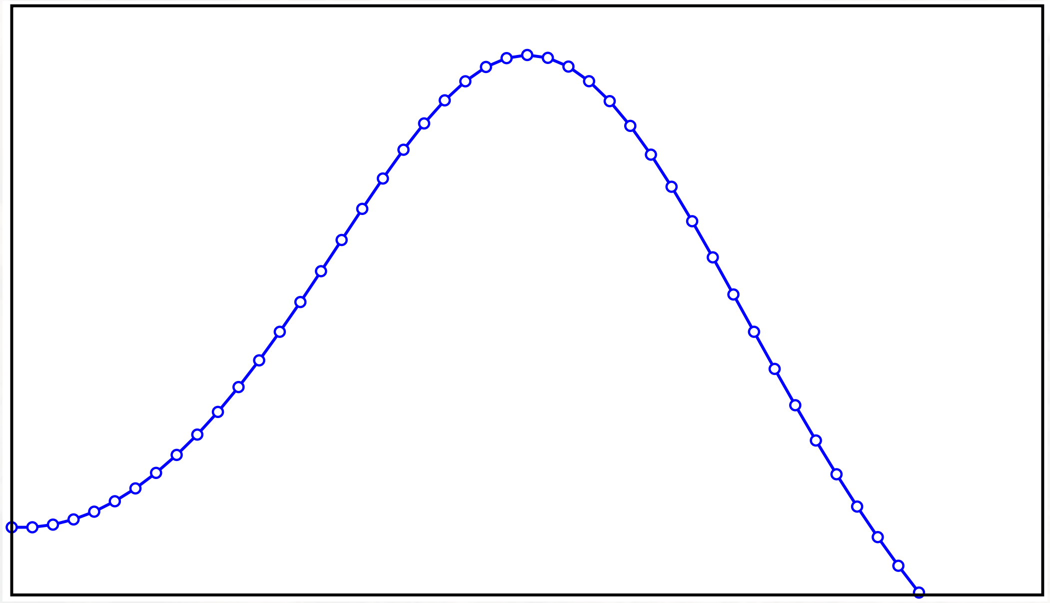


White and
Scalapino (2008)

Lattice sites ⟷ Discretized atoms

But can also describe the continuum:

$$T = -\frac{1}{2}\int_x c^\dagger(x)\,\frac{\partial^2}{\partial x^2}c(x)$$



$$\simeq -\frac{1}{2a^2}\sum_j (c_j^\dagger c_{j+1} + 2n_j + c_{j+1}^\dagger c_j)$$

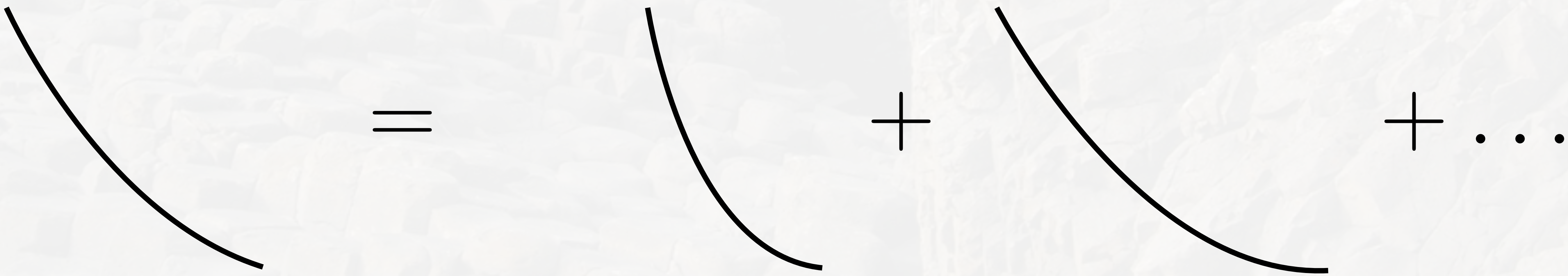
Grid sites ⟷ Discretized space

Long Range Interactions?

Obstacle: Including all pairwise interactions on the grid makes scaling N^3

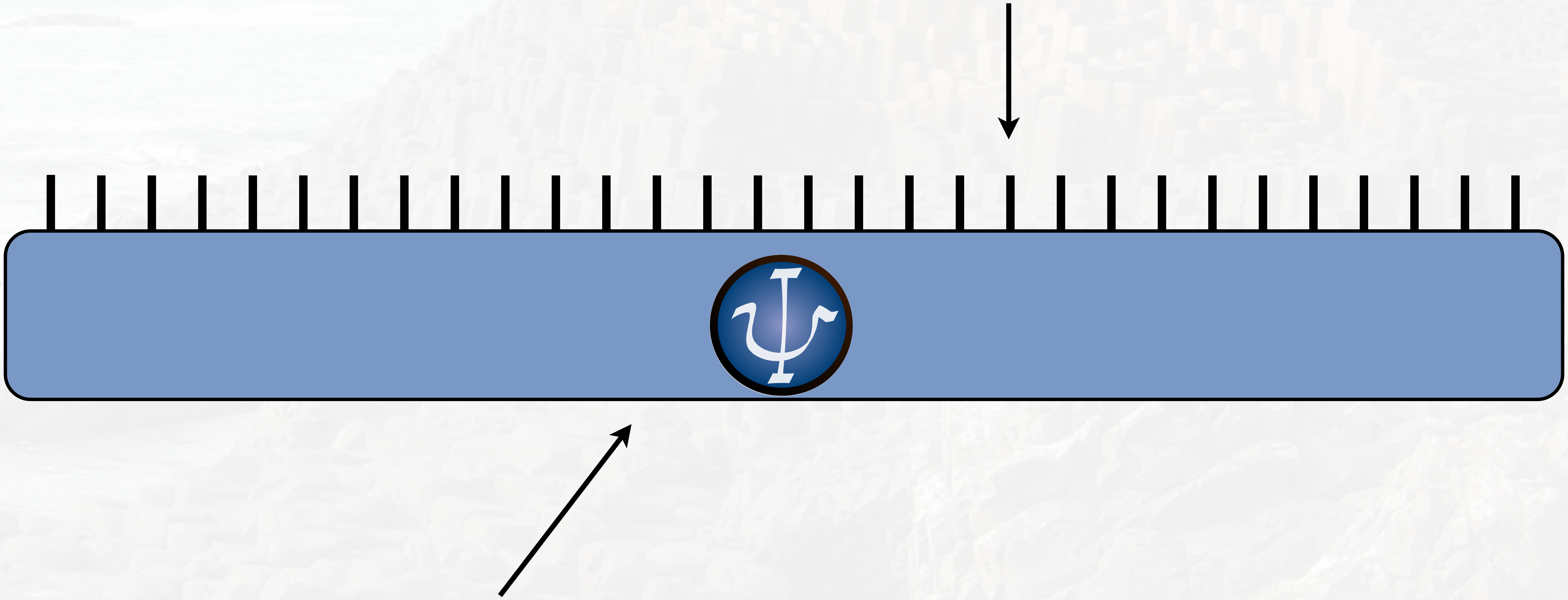
Solution:

1. No extra cost in DMRG for exponential long-range interactions
2. Fit Coulomb law to sum of exponentials



Pirvu, Murg, Cirac and Verstraete, NJP **12** 025012, (2010)

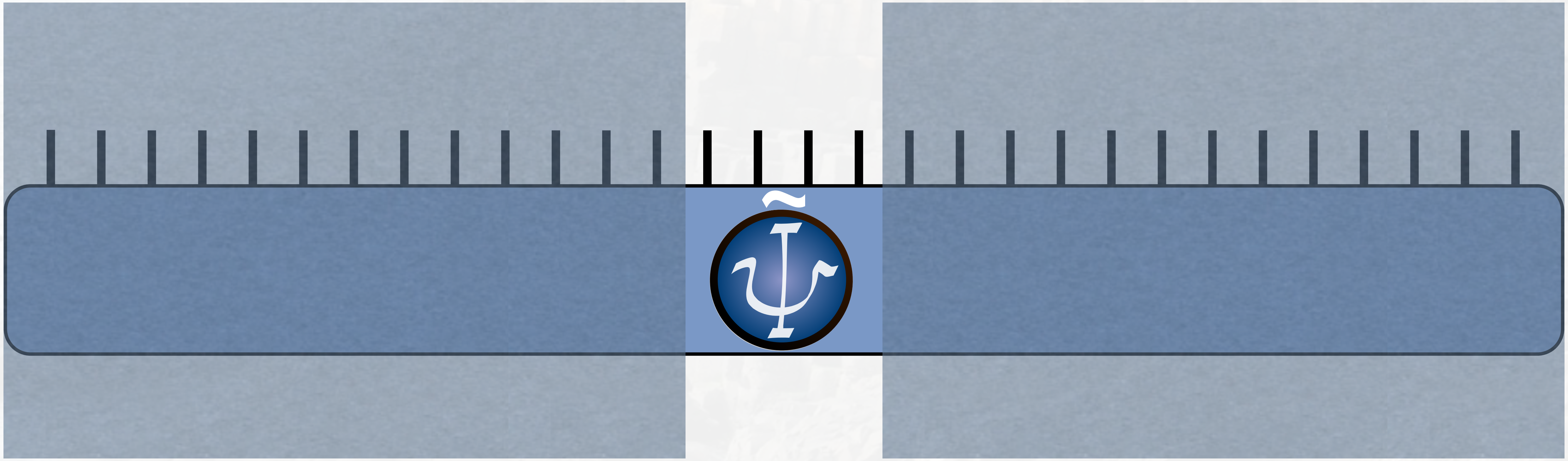
How does DMRG work?



Grid sites

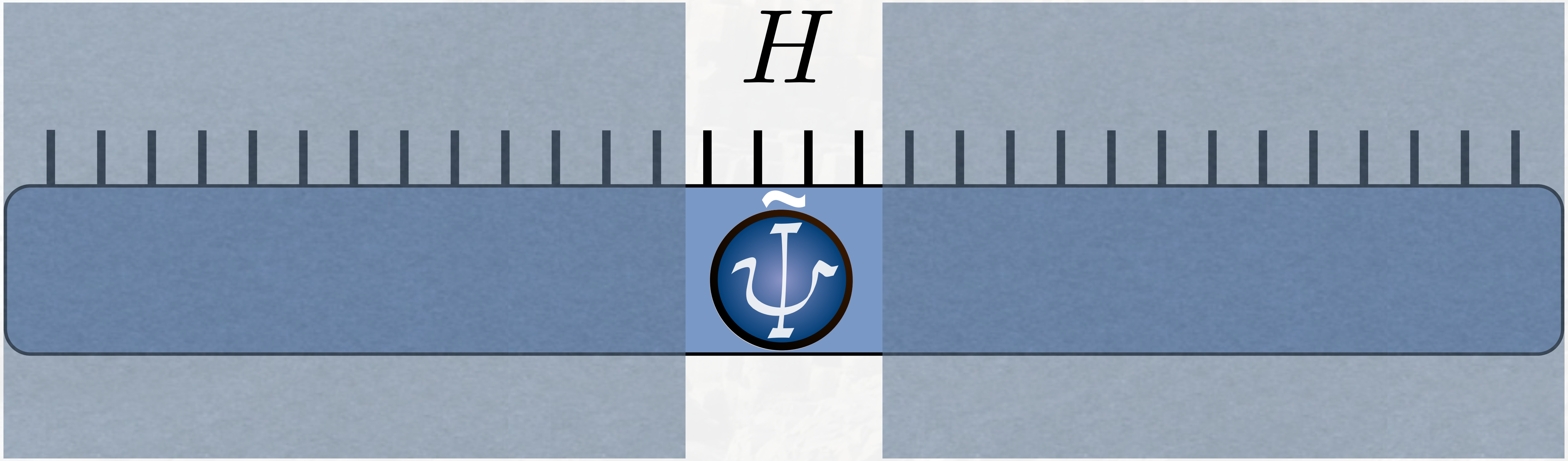
Many-body wavefunction

How does DMRG work?



Freeze out all but a small
piece of wavefunction

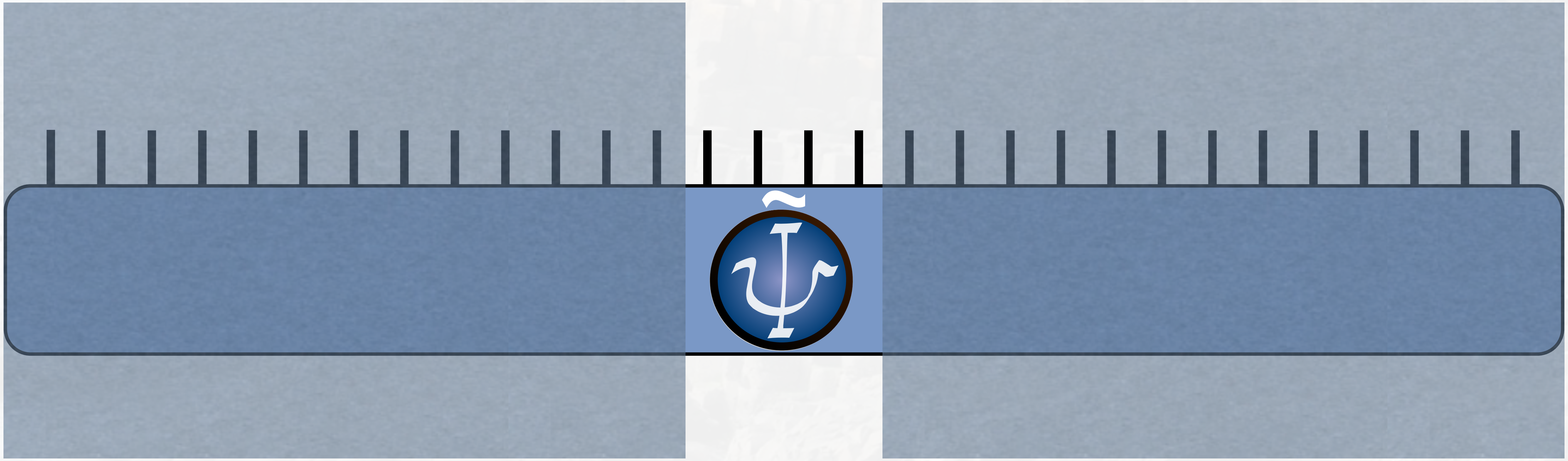
How does DMRG work?



Solve Schrodinger equation exactly for remaining piece

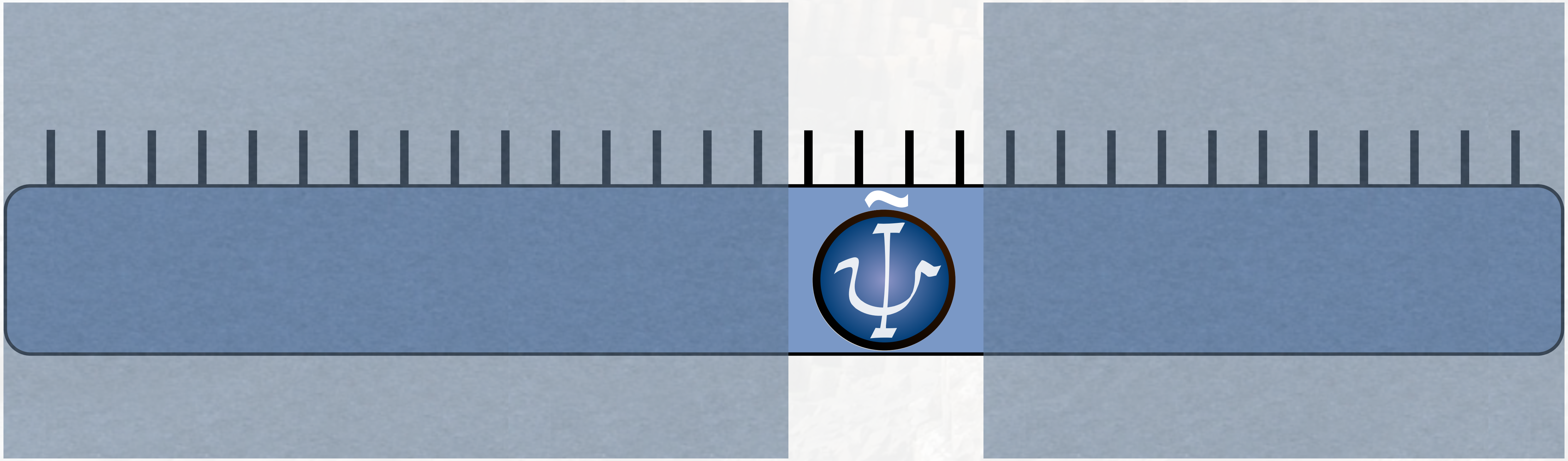
$$\tilde{H}|\tilde{\Psi}\rangle = \tilde{E}|\tilde{\Psi}\rangle$$

How does DMRG work?



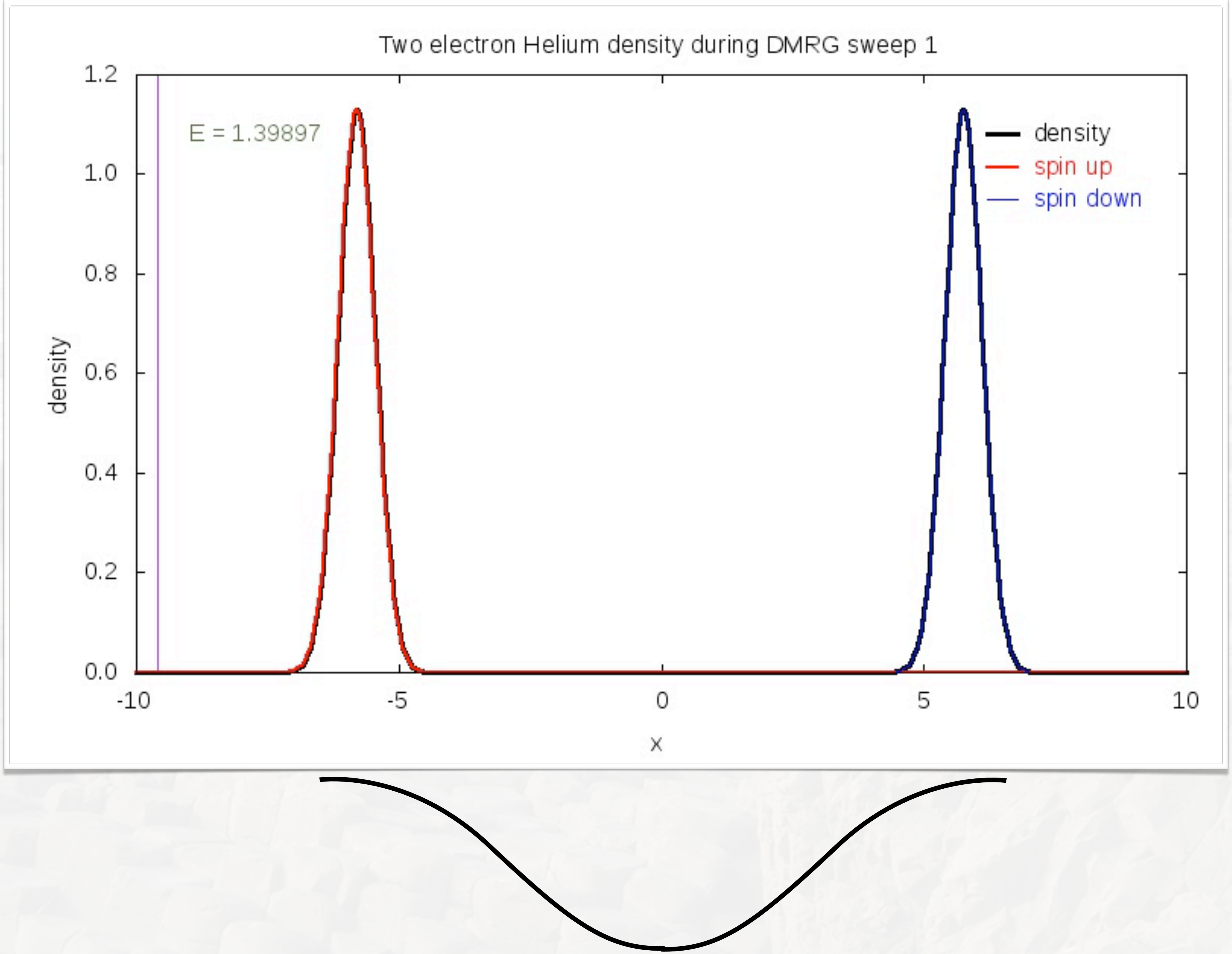
Shift exposed region, keeping only
the most important states in the basis

How does DMRG work?



Shift exposed region, keeping only
the most important states in the basis

DMRG Demo - 1d “Helium” Atom



Three levels of application to DFT:

Level I: compare exact results to DFT approximations

● Easier

Level II: study the exact Kohn-Sham system

■ More Difficult

Level III: self-consistent KS calculation with the exact functional

◆◆ Most Difficult: Use Extra Caution

Level I: compare exact results to DFT approximations

● Easier

Model system: 1d matter

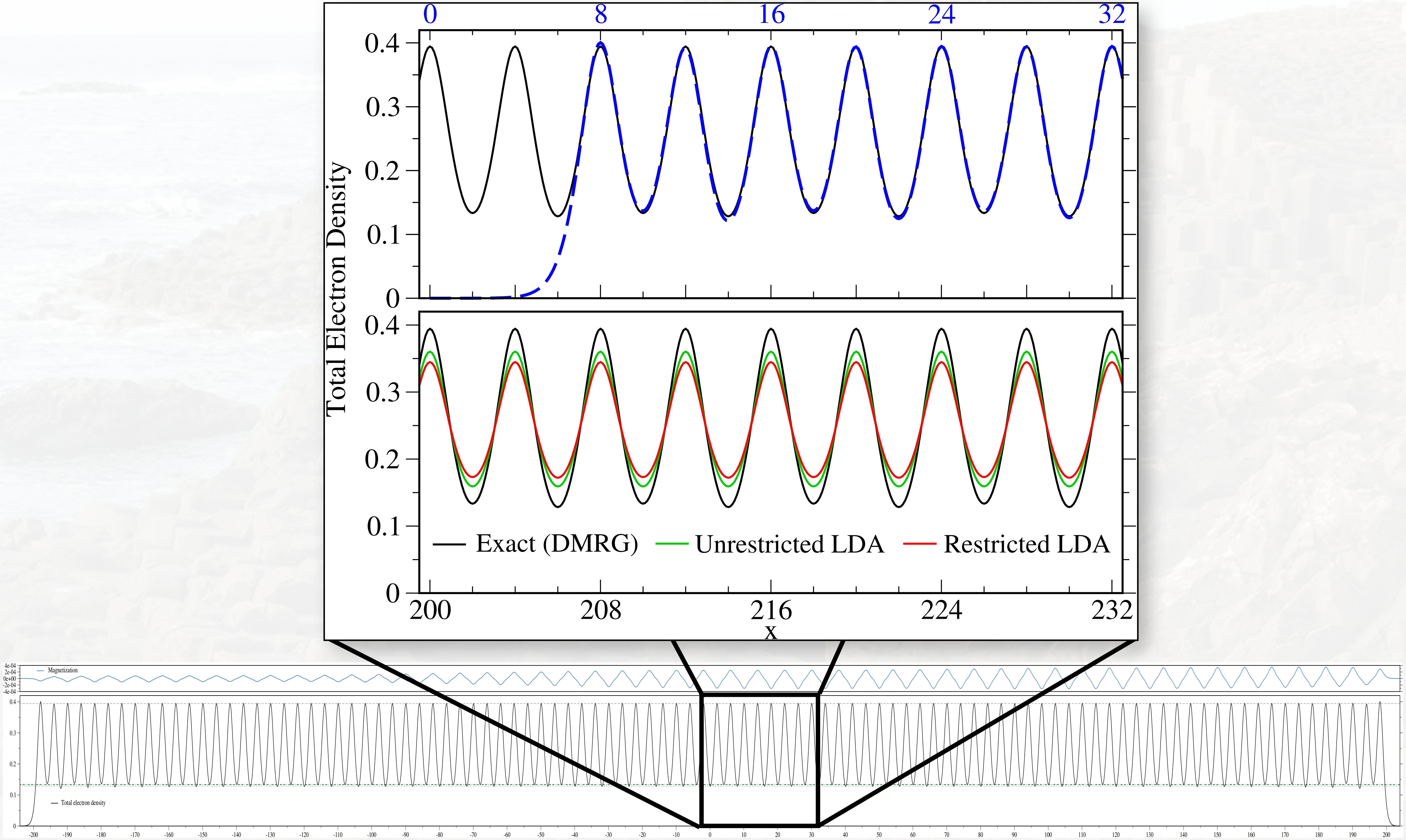
$$v_{\text{ee}}(x) = \frac{1}{\sqrt{x^2+1}}$$

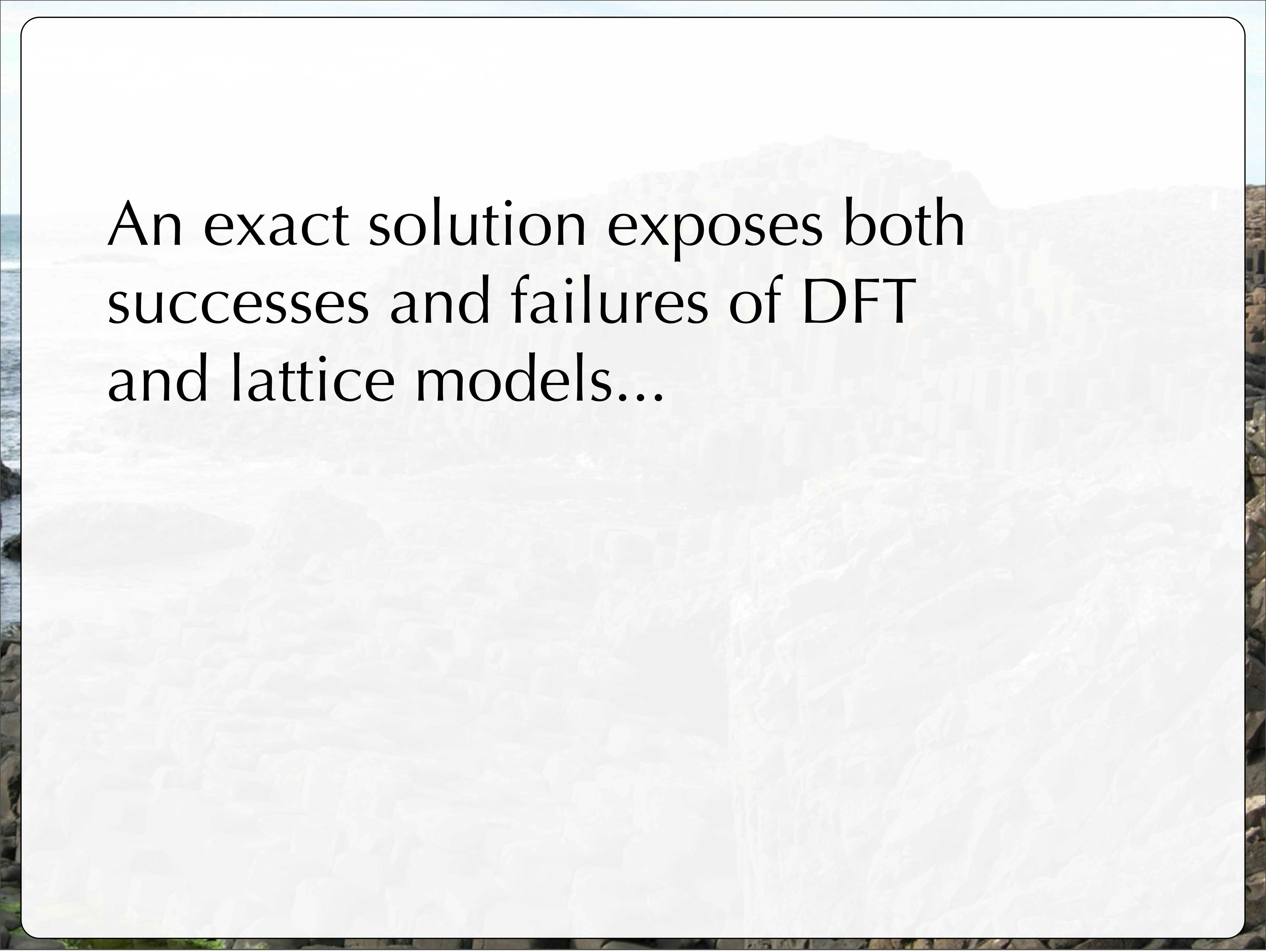
$$v_{\text{atom}}(x) = -Z v_{\text{ee}}(x)$$

$$\hat{V}_{\text{int}} = \frac{1}{2}\int_{x,x'} v_{\text{ee}}(|x-x'|)\hat{n}(x)\hat{n}(x')$$

"soft Coulomb" interaction

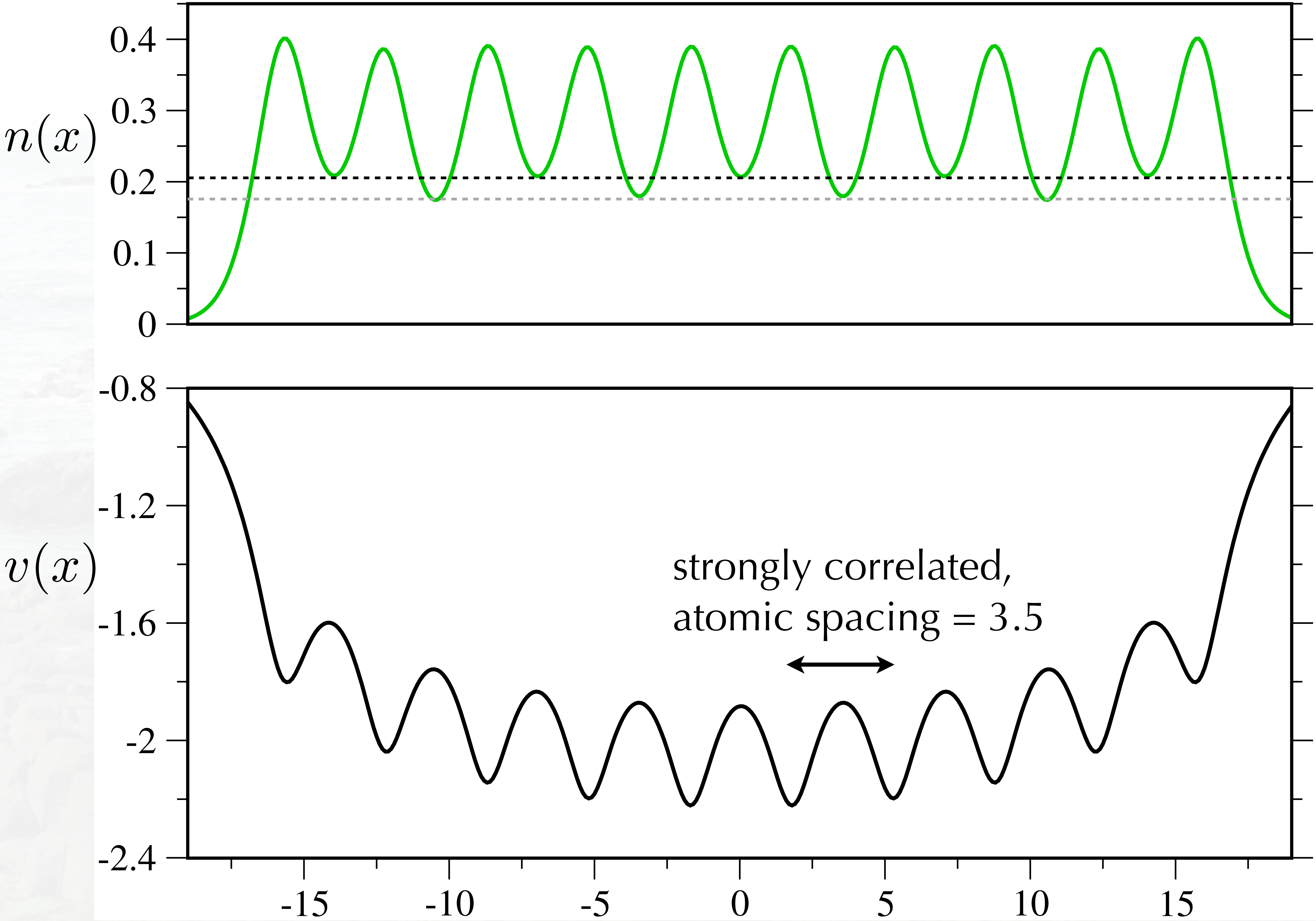
DMRG powerful enough to solve a chain of 100 stretched soft Hydrogen atoms





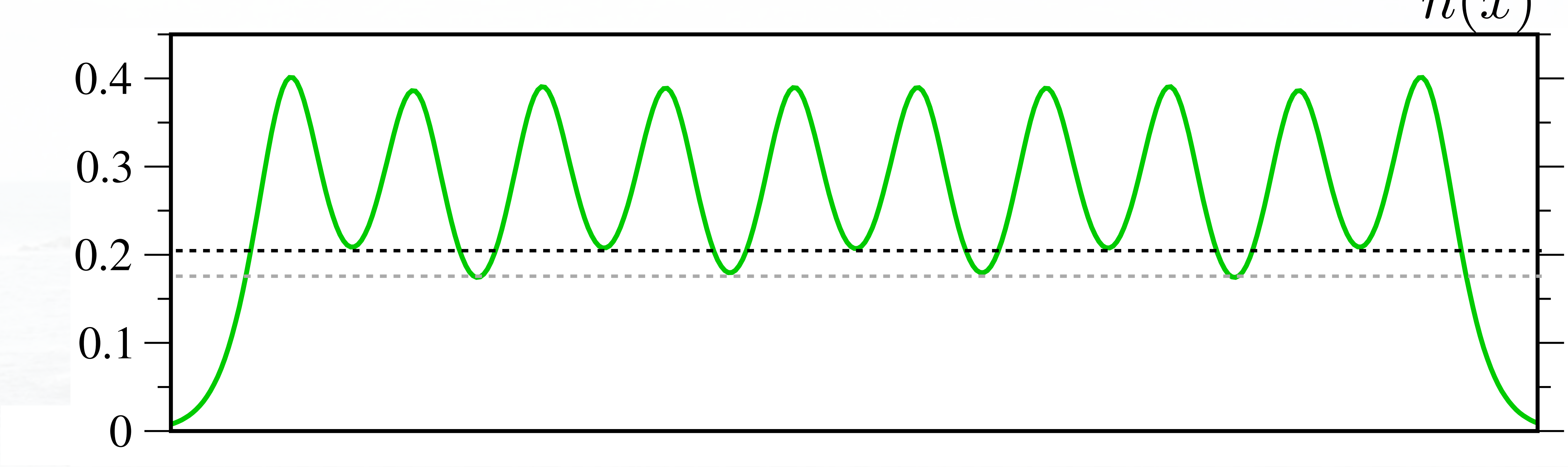
An exact solution exposes both successes and failures of DFT and lattice models...

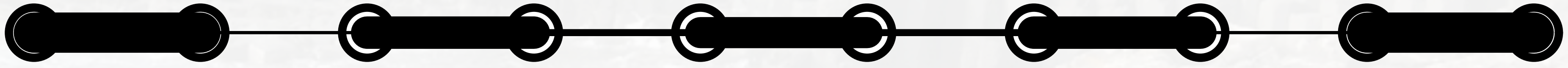
Stretched chain of 10 soft Hydrogen atoms



strongly correlated,
atomic spacing = 3.5

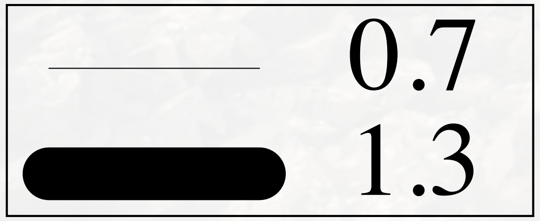
Continuum Model





Hubbard Model (U/t = 4)

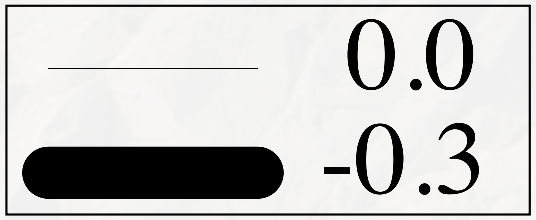
$$H = \sum_j -t(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) + U\,n_j(n_j - 1)$$



$\langle c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \rangle$

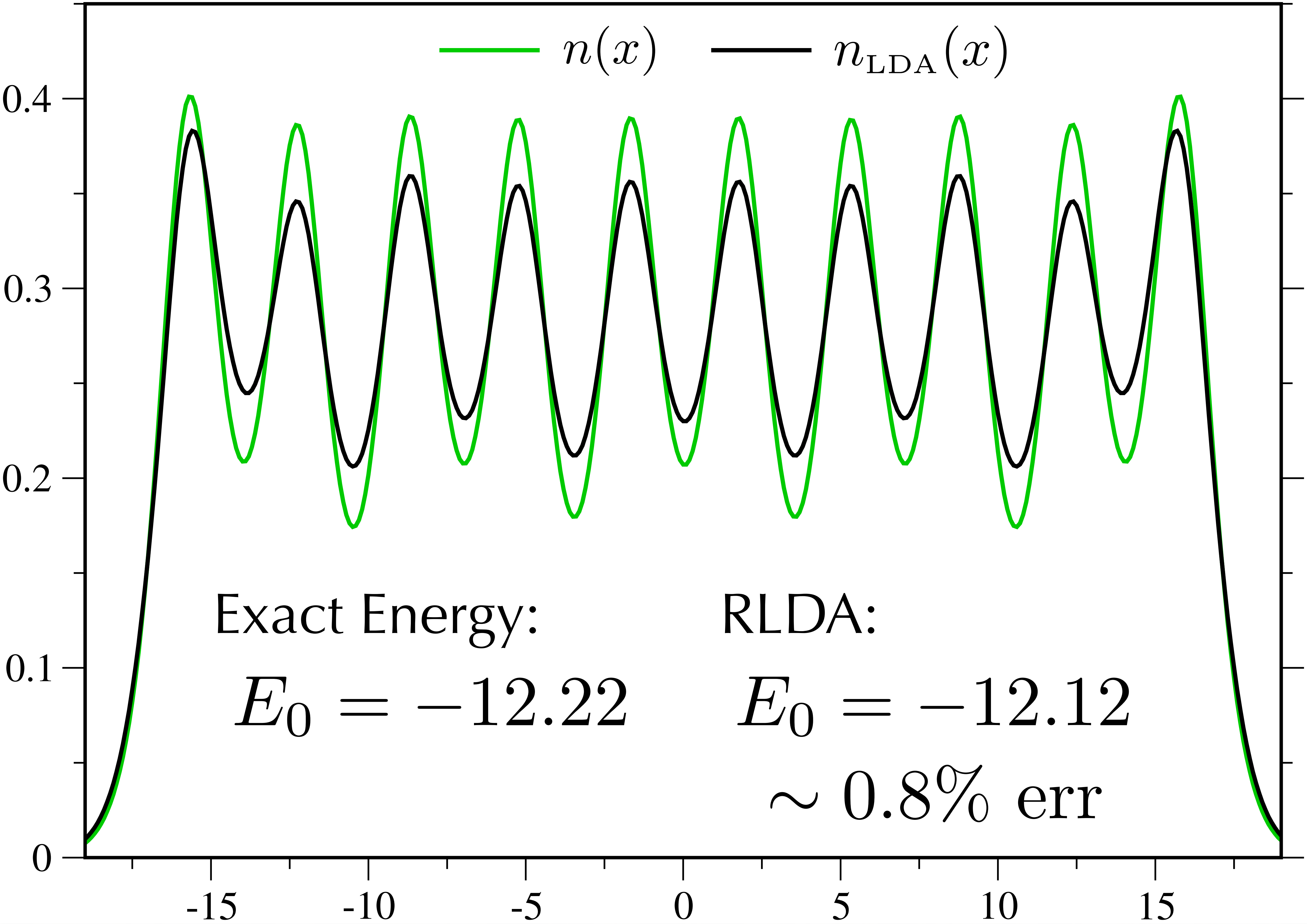
Heisenberg Model (J = 1)

$$H = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$



$\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle$

Comparison to LDA* Results (restricted)



Exact Energy:

$$E_0 = -12.22$$

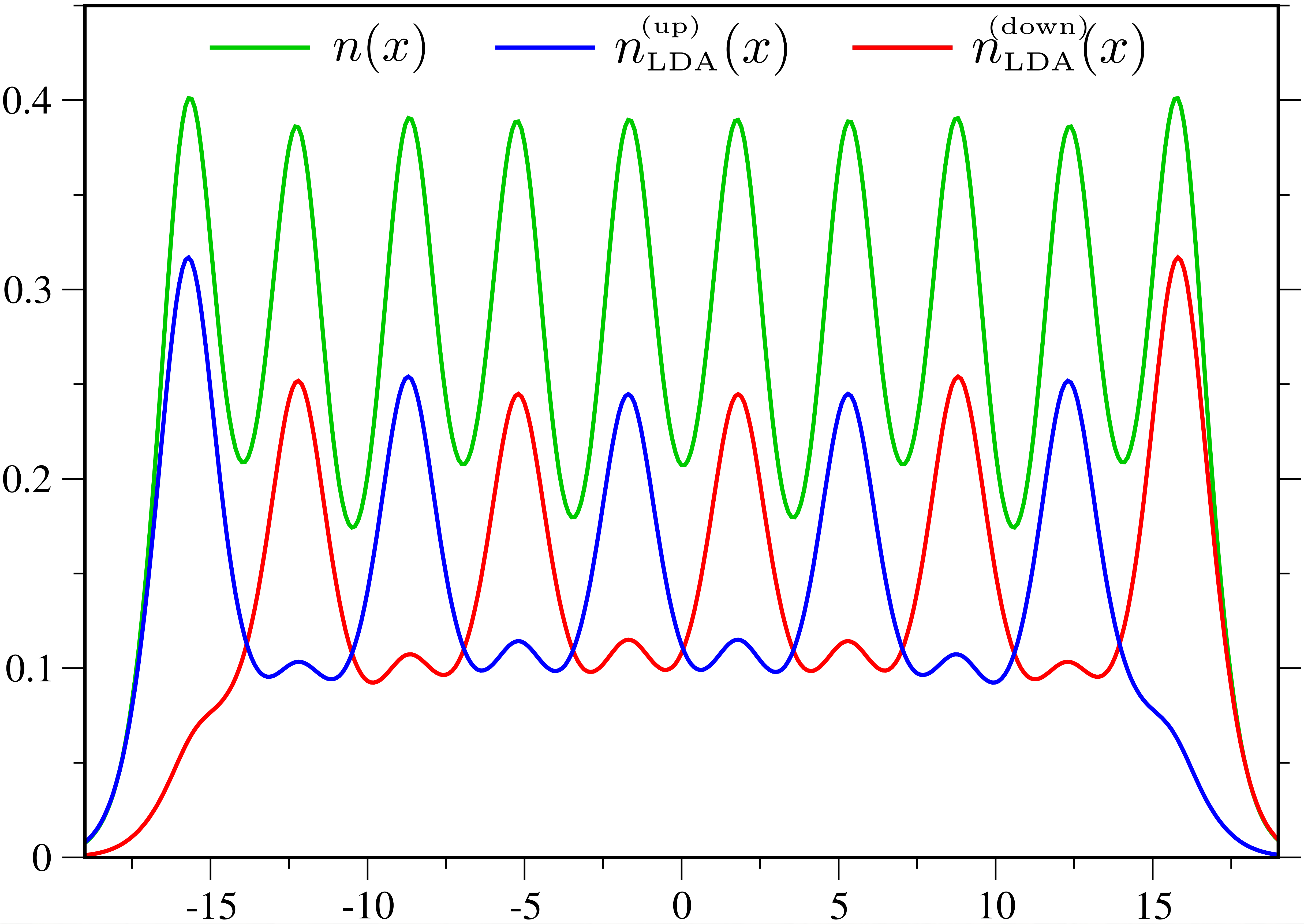
RLDA:

$$E_0 = -12.12$$

$$\sim 0.8\% \text{ err}$$

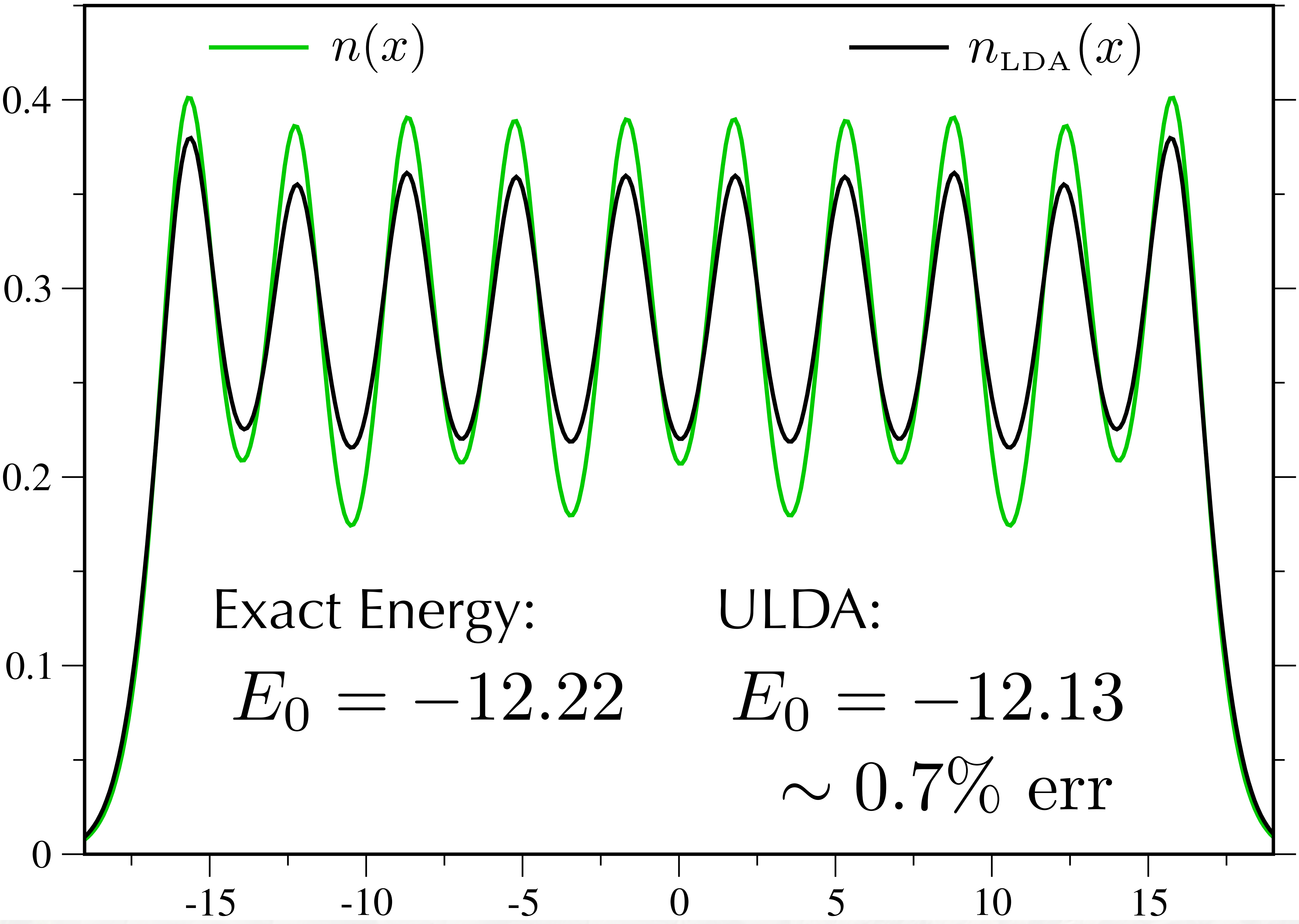
*Helbig et al. Phys. Rev. A **83**, 032503 (2011).

Comparison to LDA* Results (unrestricted)



*Helbig et al. Phys. Rev. A **83**, 032503 (2011).

Comparison to LDA* Results (unrestricted)



Exact Energy:

$$E_0 = -12.22$$

ULDA:

$$E_0 = -12.13$$

$$\sim 0.7\% \text{ err}$$

*Helbig et al. Phys. Rev. A **83**, 032503 (2011).

Nearly all essential physics relevant to e.g. strong correlation is present in 1d

Plan to benchmark many more DFT approximations

Level II: study the exact Kohn-Sham system

More Difficult

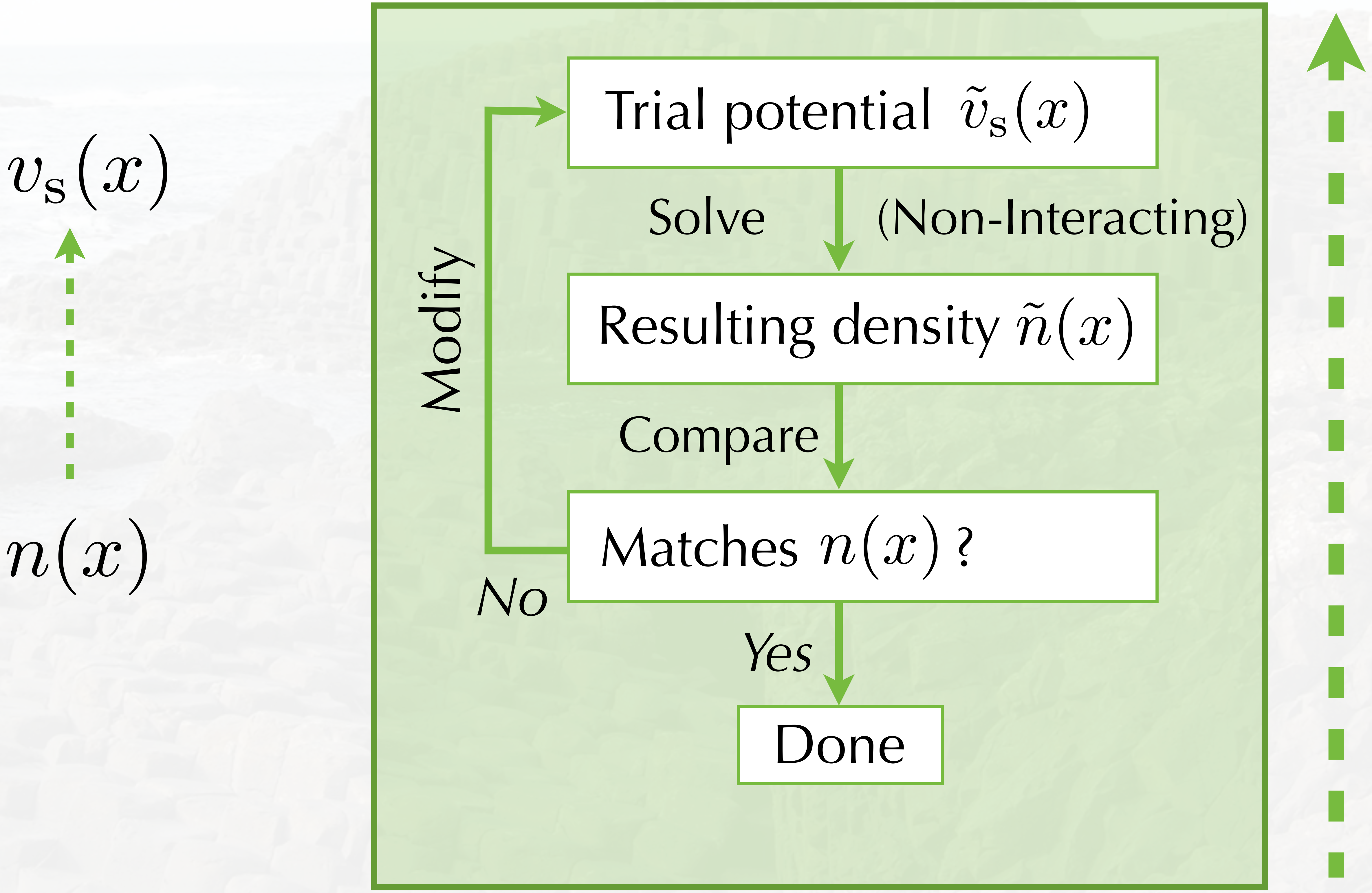
Having the exact ground state density means we can "invert" it to find the exact KS potential.

Hohenberg-Kohn theorem:
KS potential is unique if it exists

$$\begin{tikzcd}
v_{\mathrm{s}}(x) \arrow[d, shift right, "\text{Solve}"'] \\
n(x) \arrow[u, shift right, dashed, "\text{Invert}"']
\end{tikzcd}$$

Inversion means finding this unique KS potential for the density $n(x)$

How to perform an inversion?



$v_{\mathrm{s}}(x)$

$n(x)$

Trial potential $\tilde{v}_{\mathrm{s}}(x)$

Solve (Non-Interacting)

Resulting density $\tilde{n}(x)$

Compare

Matches $n(x)$?

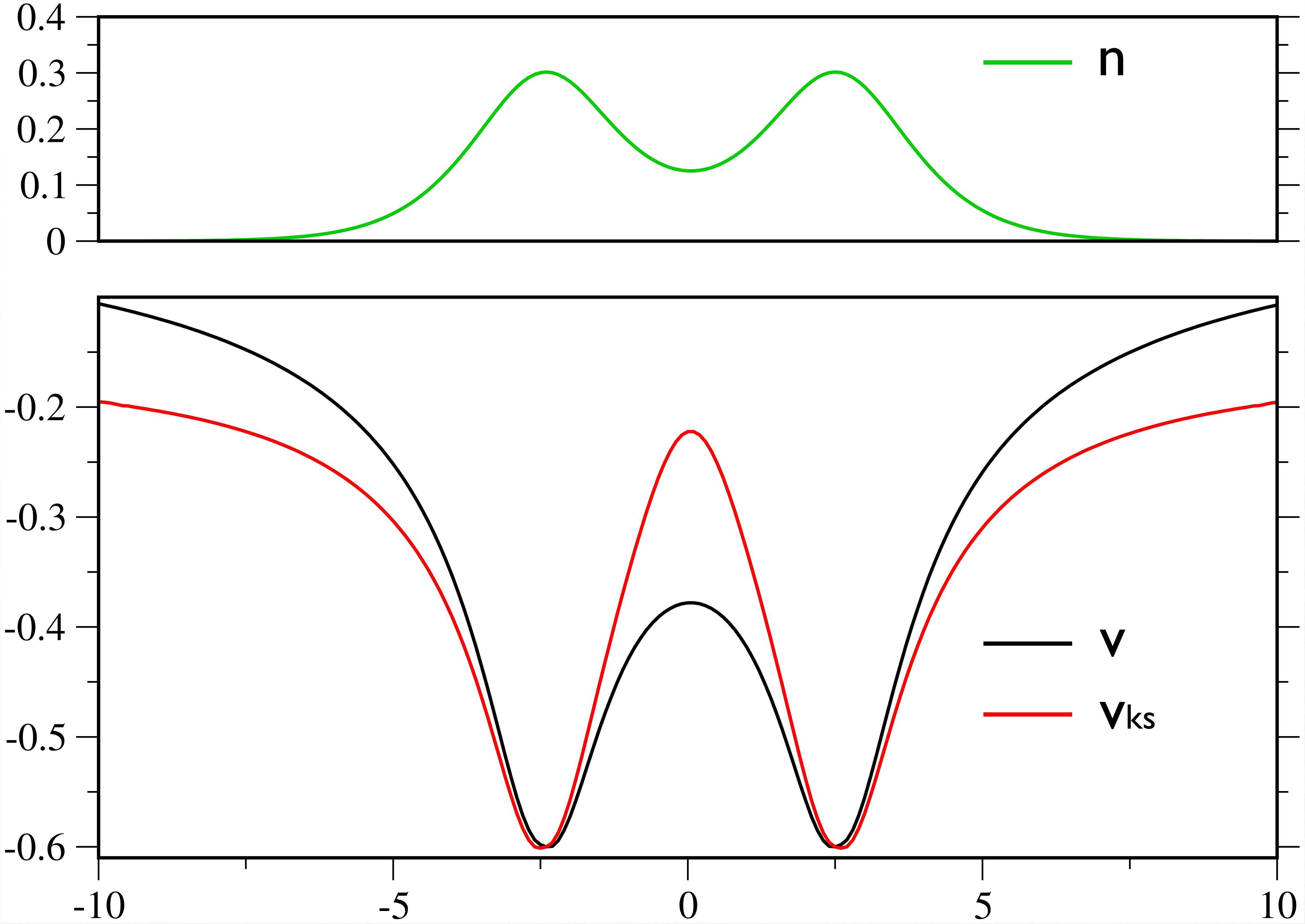
No

Modify

Yes

Done

Example: stretched H_2



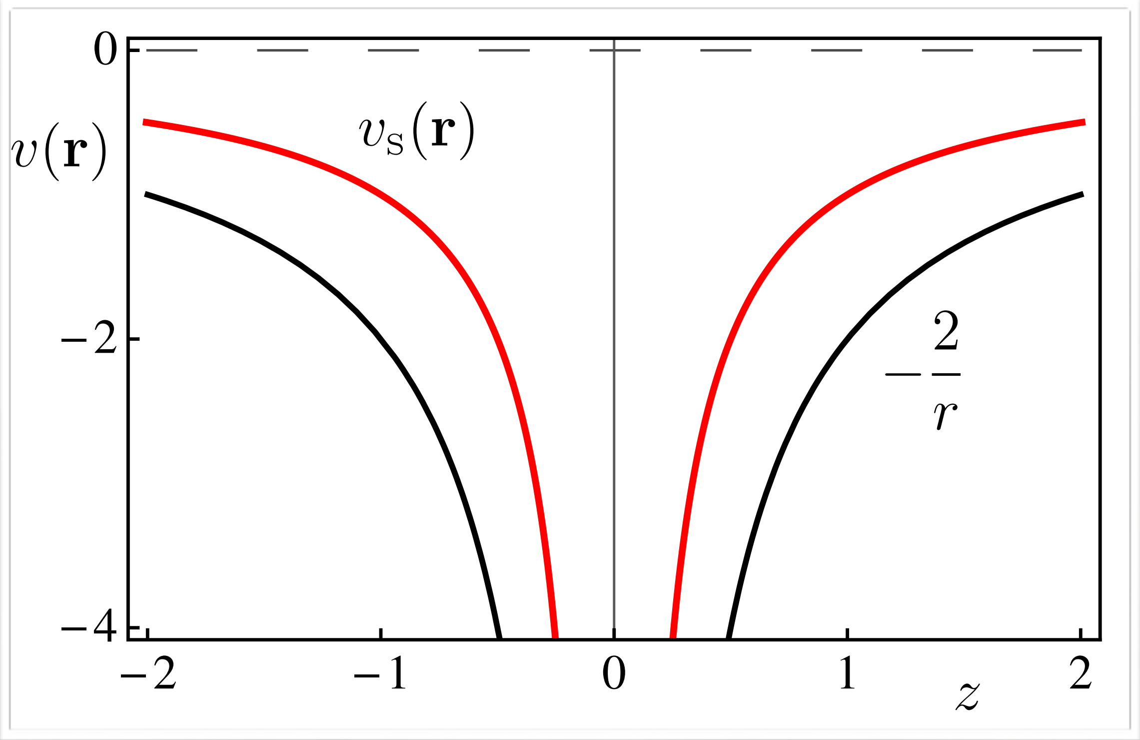
It's important to understand the KS wavefunction.

In a transport calculation, is it ever ok to replace $G(k,\omega) \rightarrow G^{\mathrm{KS}}(k,\omega)$?

(See talk by Zhenfei Liu, today 3pm in 107B)

Also: arxiv:1201.1310, Liu et al.

Exact KS potential
of He atom:



Umrigar and Gonze, PRA **50**, 3827 (1994)
(figure adapted by Burke and Wagner)

In contrast to previous calculations, we can approach the thermodynamic limit and study matter

$\longrightarrow$ Kohn-Sham gap

Level III: self-consistent KS calculation with the exact functional

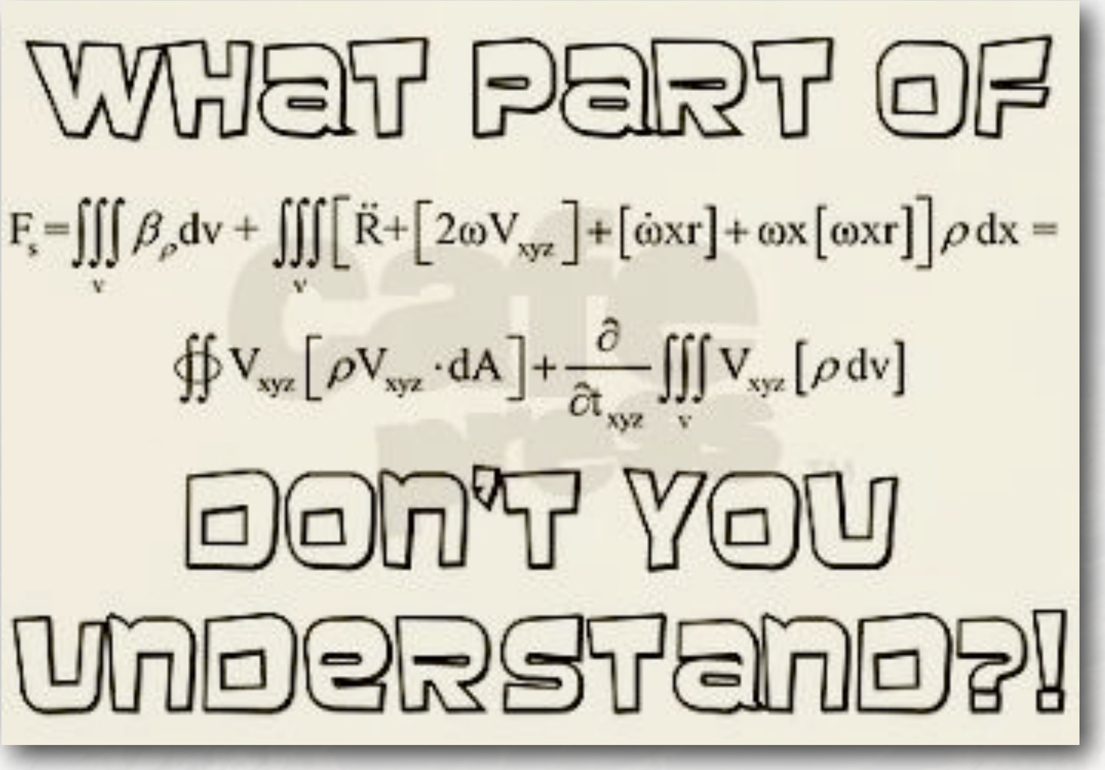
What *is* the functional?

Given a density $n(x)$, computes the ground state energy for a given type of interactions

$$E_0 = E[n]$$

the functional

Often spoken about as if it's some closed-form, analytic expression...



$$F_s = \iiint_v \beta_\rho \, dv + \iiint_v \left[\ddot{R} + \left[2\omega V_{xyz} \right] + \left[\dot{\omega} x r \right] + \omega x \left[\omega x r \right] \right] \rho \, dx =$$

$$\oiint V_{xyz} \left[\rho V_{xyz} \cdot dA \right] + \frac{\partial}{\partial t_{xyz}} \iiint_v V_{xyz} \left[\rho \, dv \right]$$

...but this can't be right - writing down the exact functional is QMA hard.*

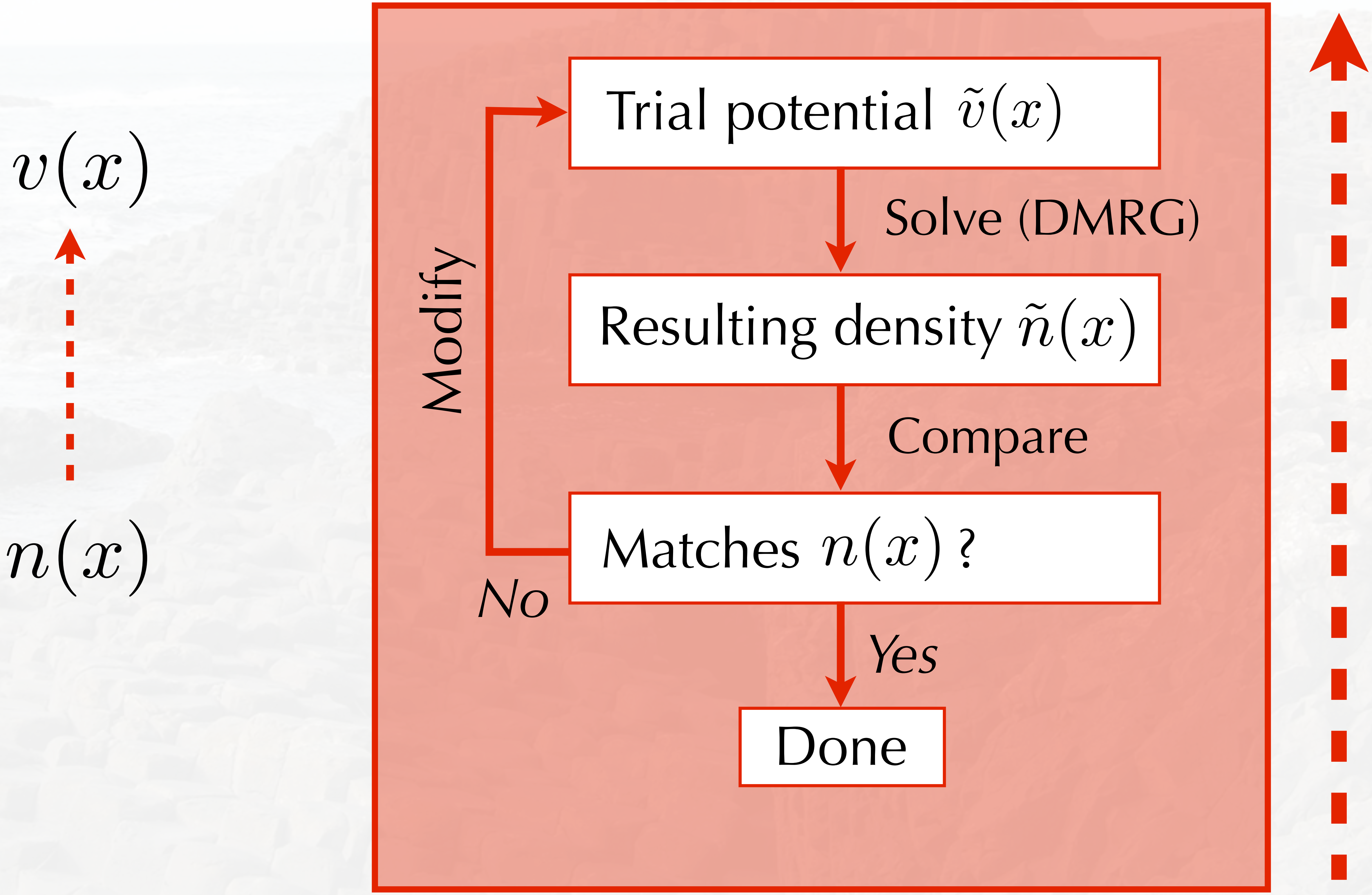
*N. Schuch and F. Verstraete, Nature Phys. **5**, 732 (2009).

In reality, the functional is not an expression but an algorithm.

Key ingredient: interacting inversion

$$\begin{tikzcd}
v(x) \arrow[d, shift right=2, "\text{Solve}"'] \\
n(x) \arrow[u, dashed, shift right=2, "\text{Invert}"']
\end{tikzcd}$$

Similar to non-interacting inversion:



$v(x)$

$n(x)$

Trial potential $\tilde{v}(x)$

Solve (DMRG)

Resulting density $\tilde{n}(x)$

Compare

Matches $n(x)$?

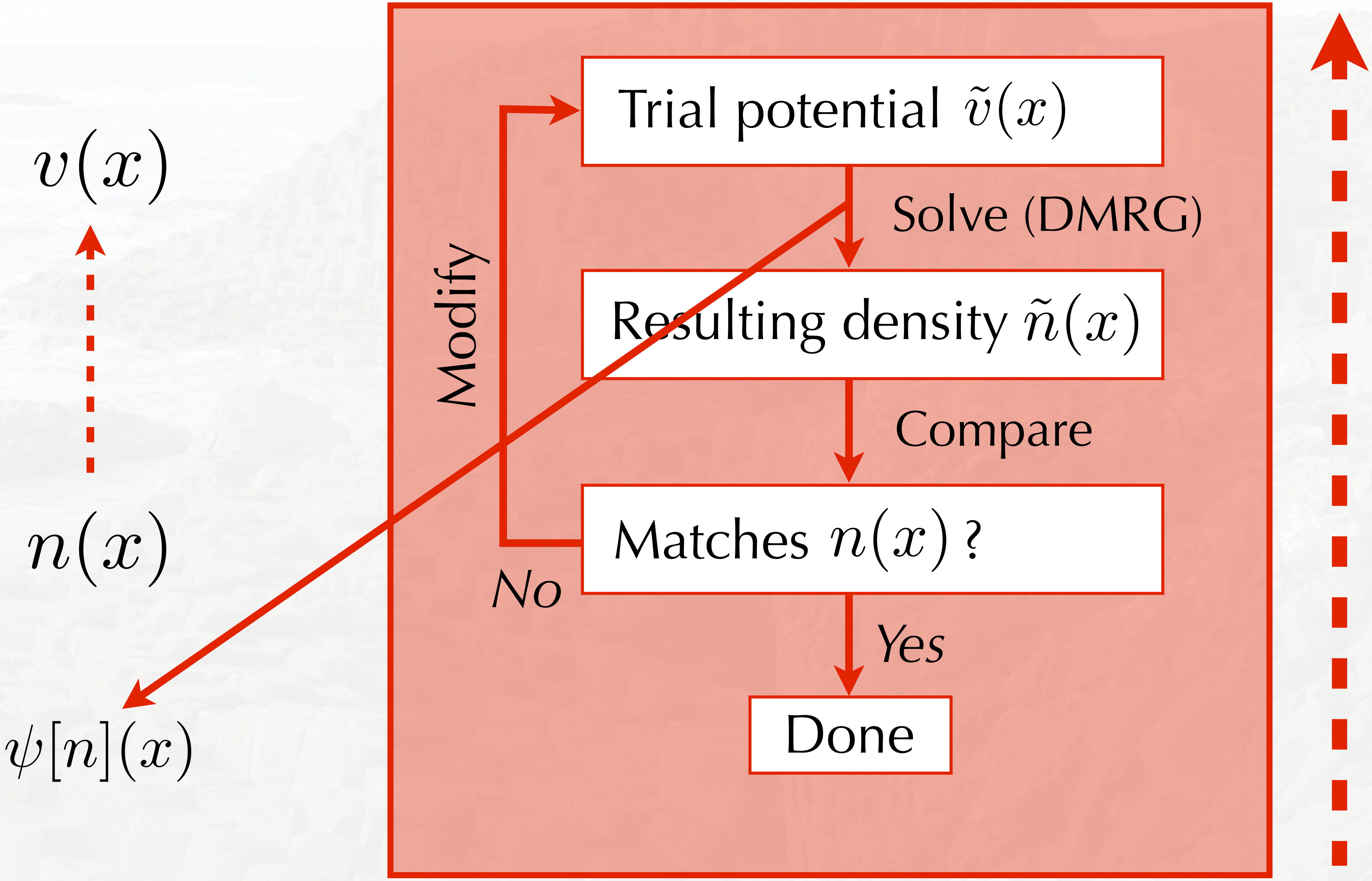
Modify

No

Yes

Done

Last step gives the wavefunction $\psi[n](x)$



$v(x)$

$n(x)$

$\psi[n](x)$

Trial potential $\tilde{v}(x)$

Solve (DMRG)

Resulting density $\tilde{n}(x)$

Compare

Matches $n(x)$?

Modify

No

Yes

Done

Finally, with

✓ $v[n](x)$

✓ $\psi[n](x)$

$$E[n] =$$

$$= \langle\psi[n]|\ \hat{H}_{v[n]}\ |\psi[n]\rangle$$

$$= \langle\psi[n]|\ \hat{T} + \hat{V}_{\rm ee} + \int_x v[n](x)\hat{n}(x)\ |\psi[n]\rangle$$

Can also do self-consistent Kohn-Sham with exact functional.

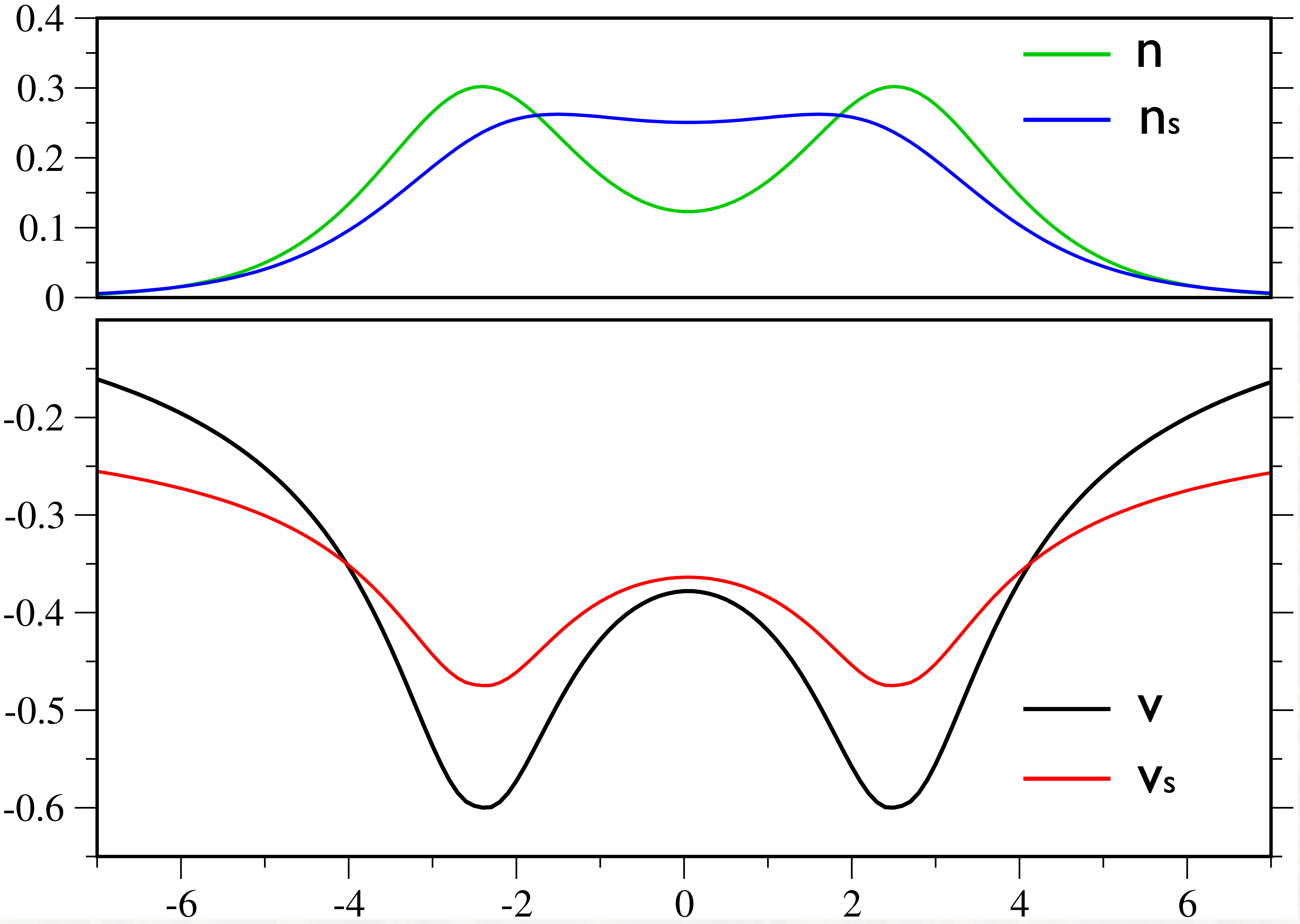
Given any $n(x)$:

1. Invert (no interactions) $\dashrightarrow v_s[n](x)$
2. Invert (with interactions) $\dashrightarrow v[n](x)$
3. Compute

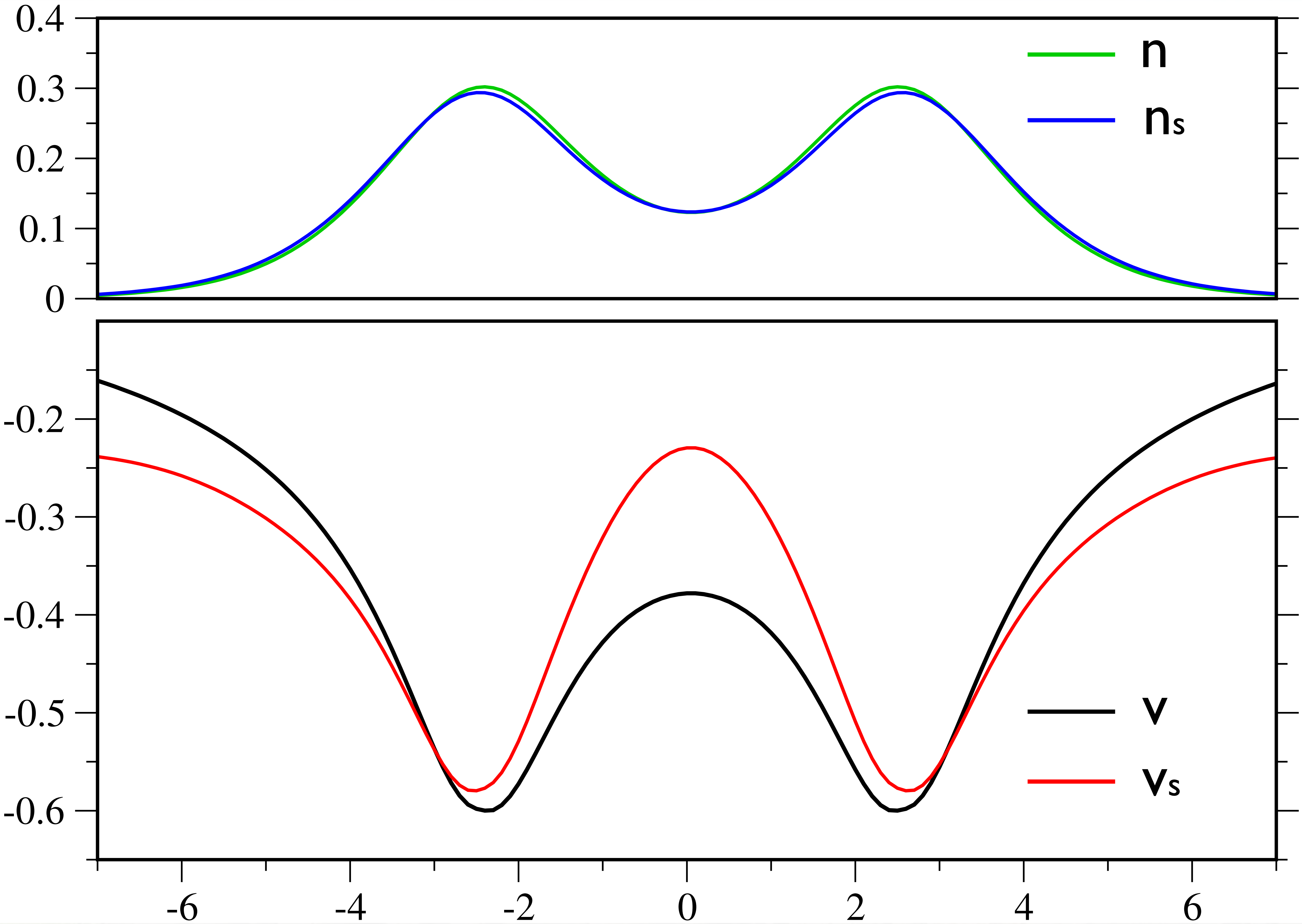
$$v_{\mathrm{HXC}}[n](x) = v_s(x) - v(x)$$

Example Kohn-Sham Calculations

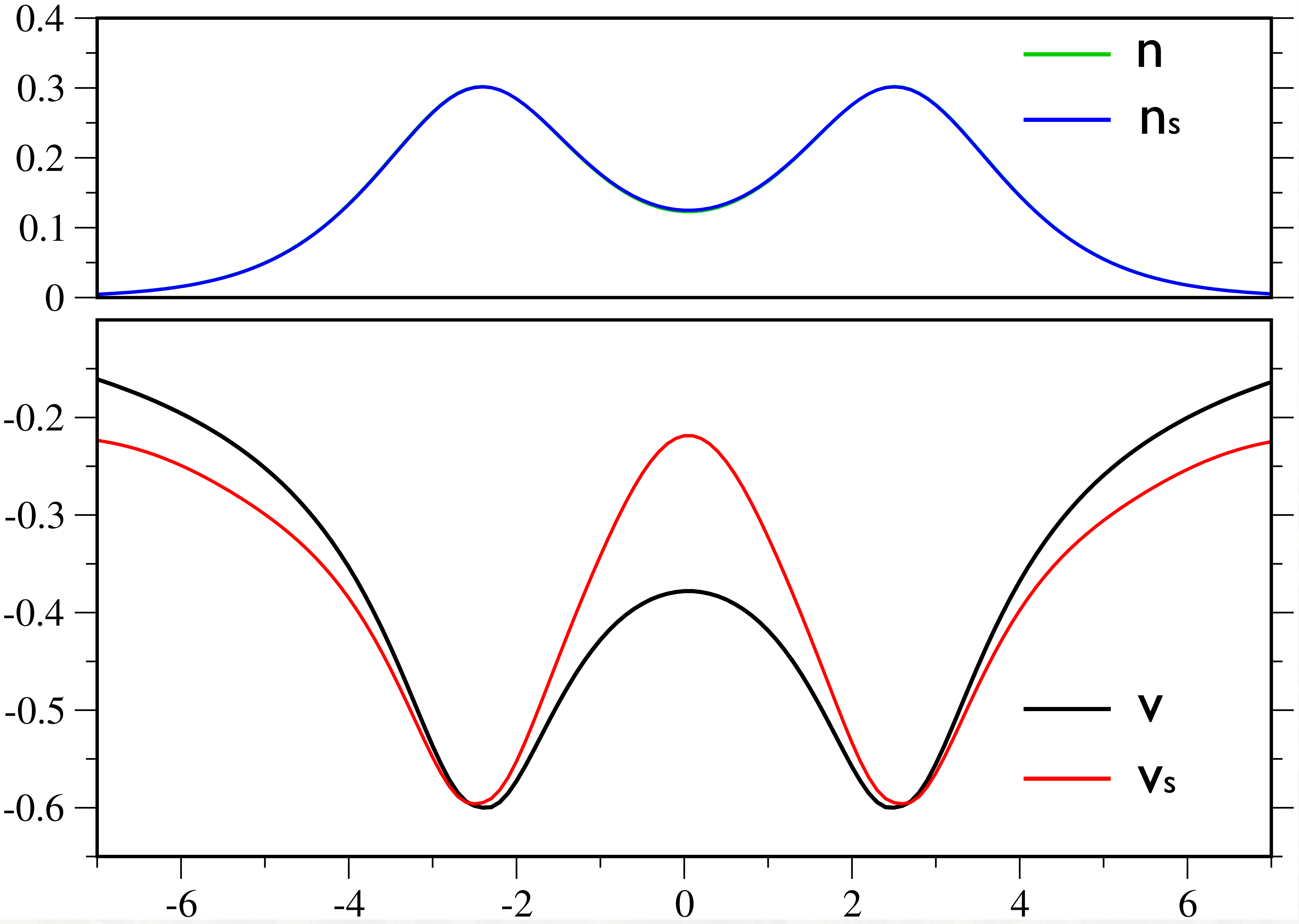
2 electrons, atomic spacing b=4



2 electrons, atomic spacing b=4



2 electrons, atomic spacing b=4



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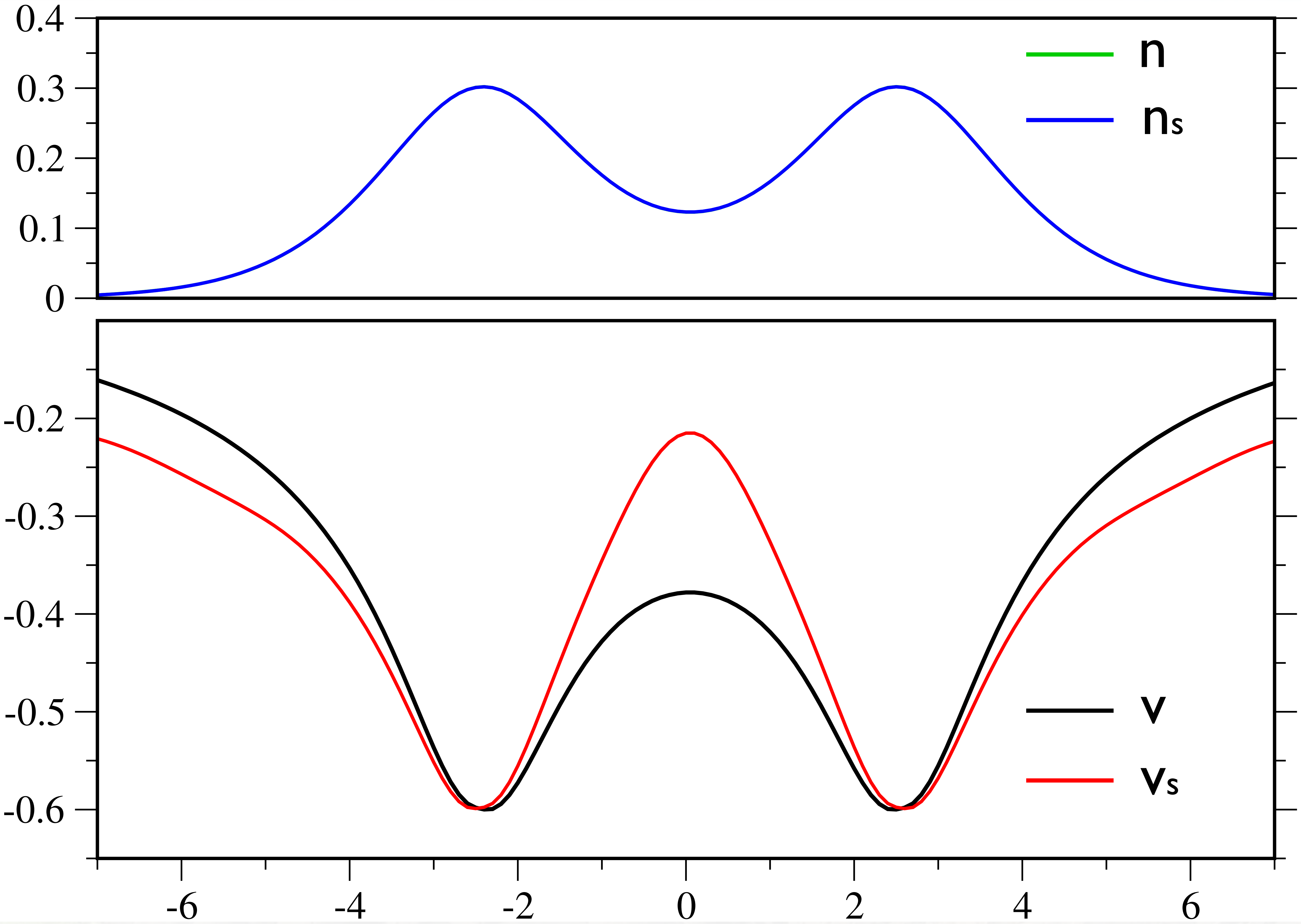
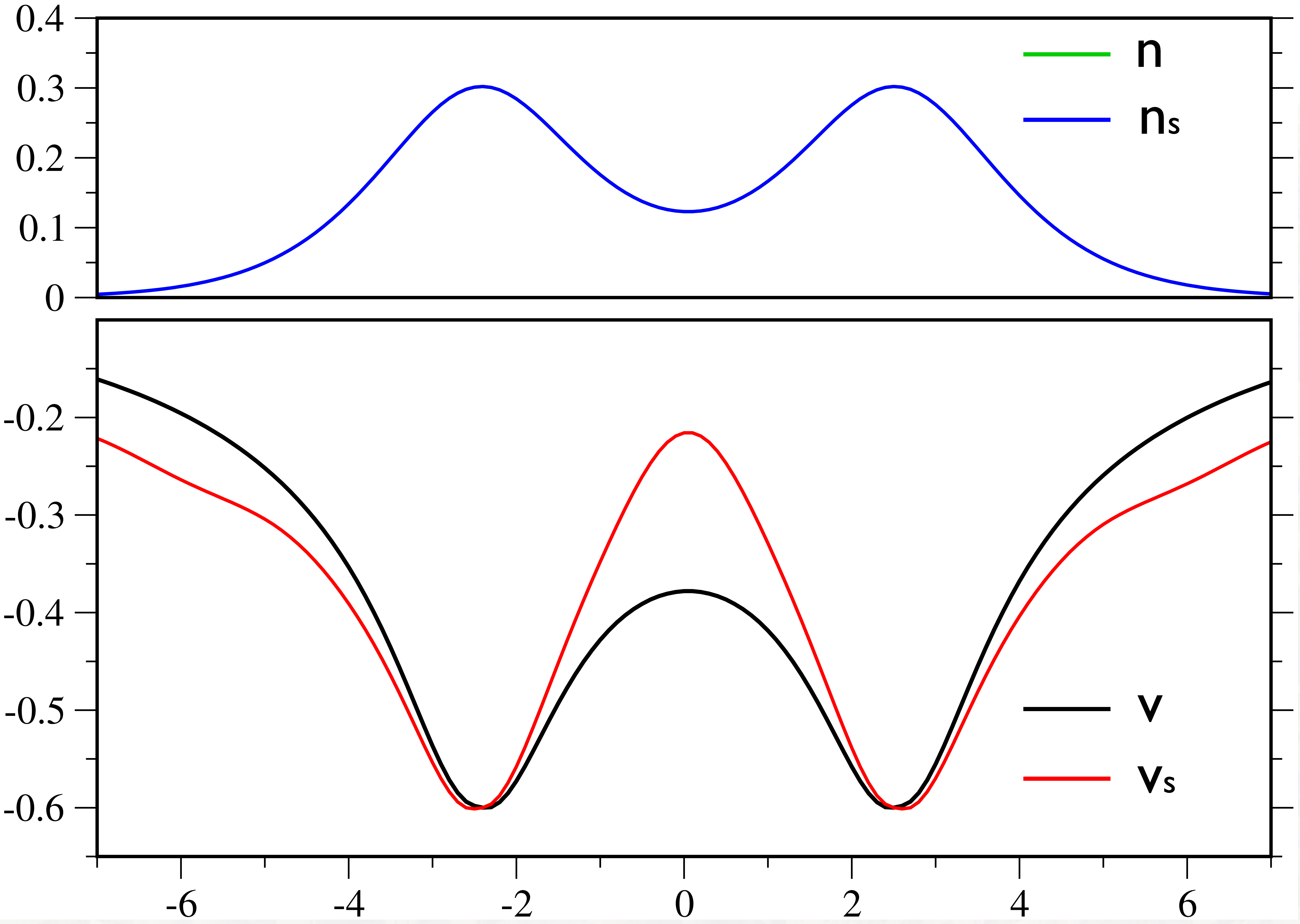
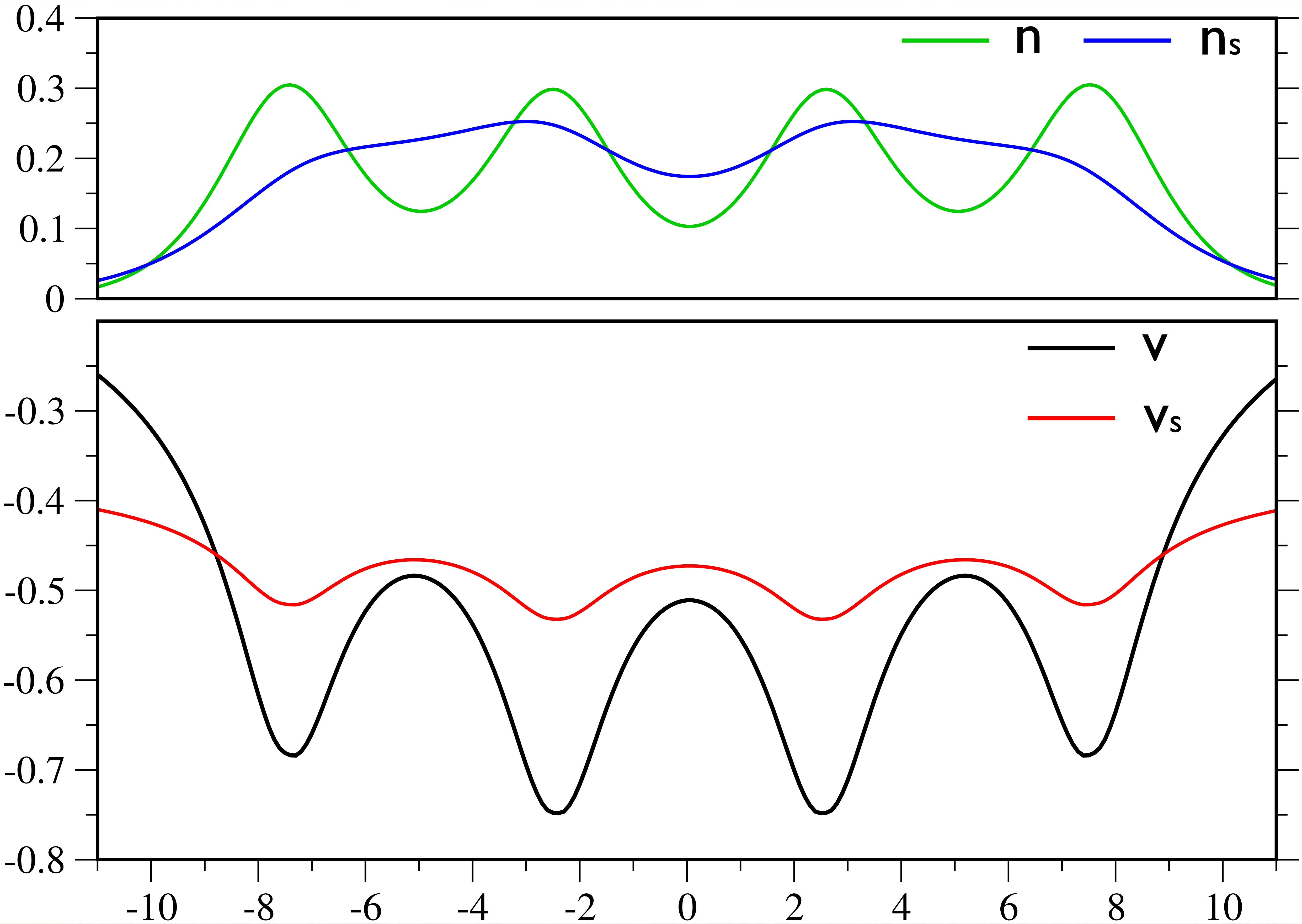


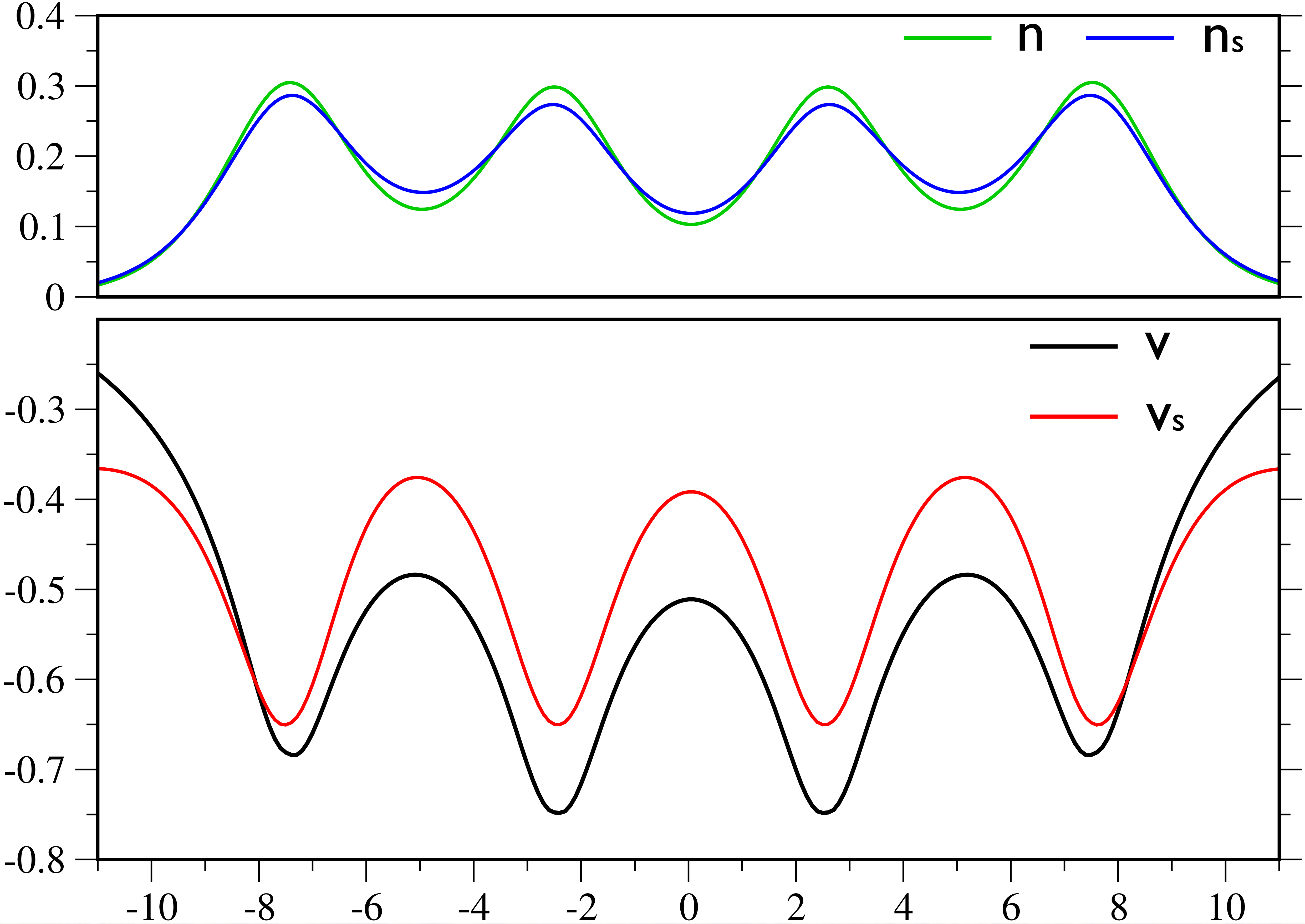
2 electrons, atomic spacing b=4



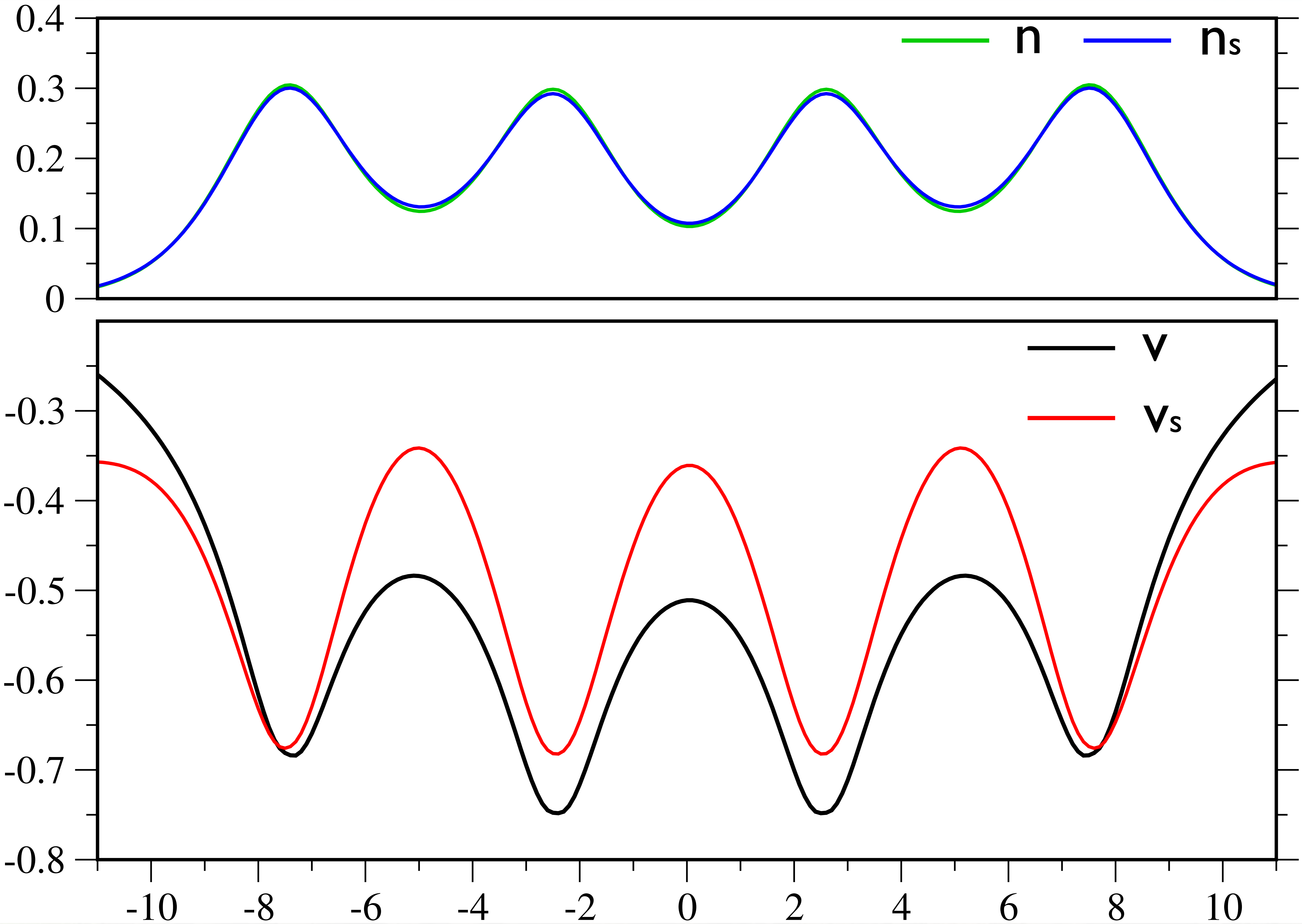
4 electrons, atomic spacing b=5



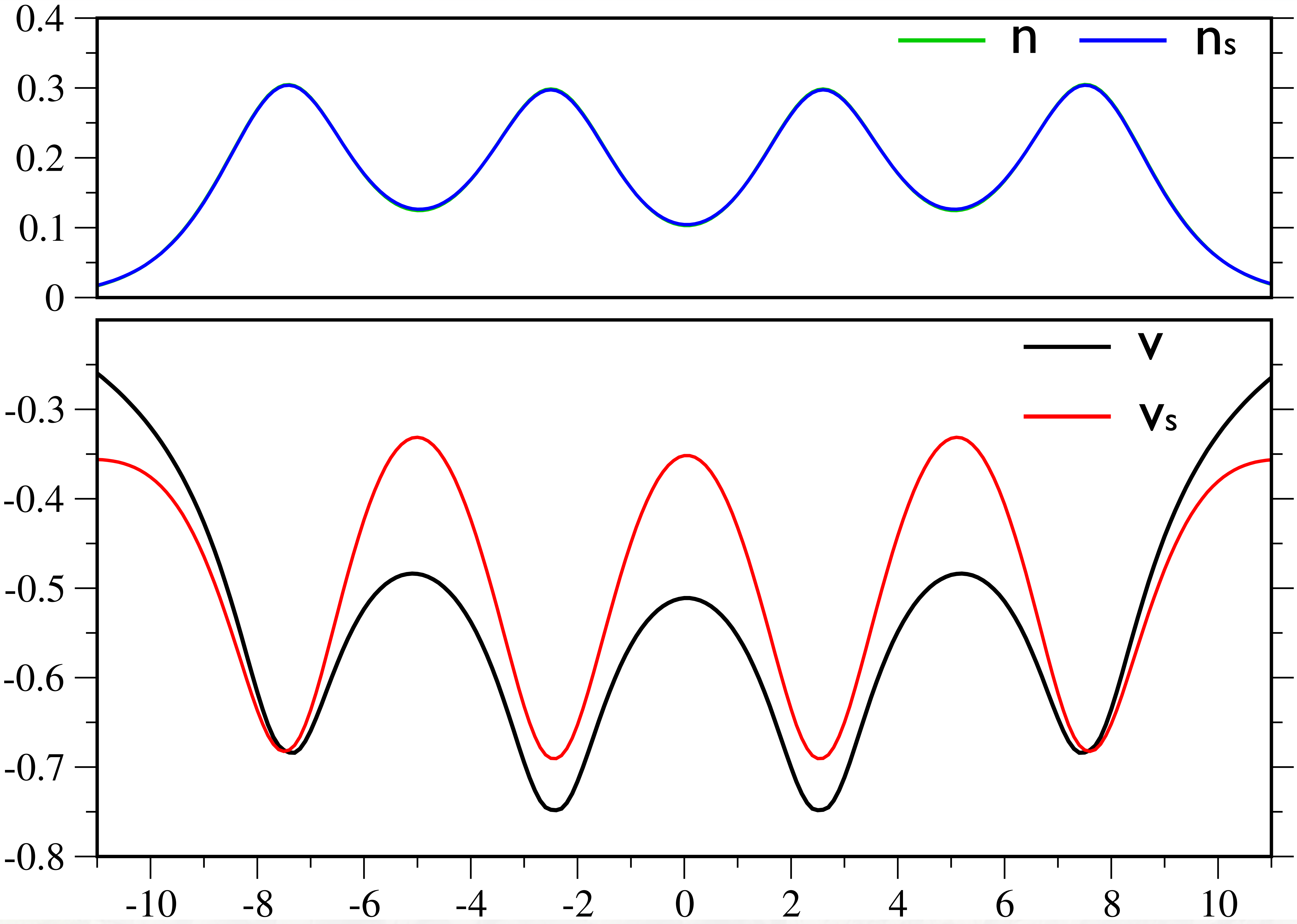
4 electrons, atomic spacing b=5



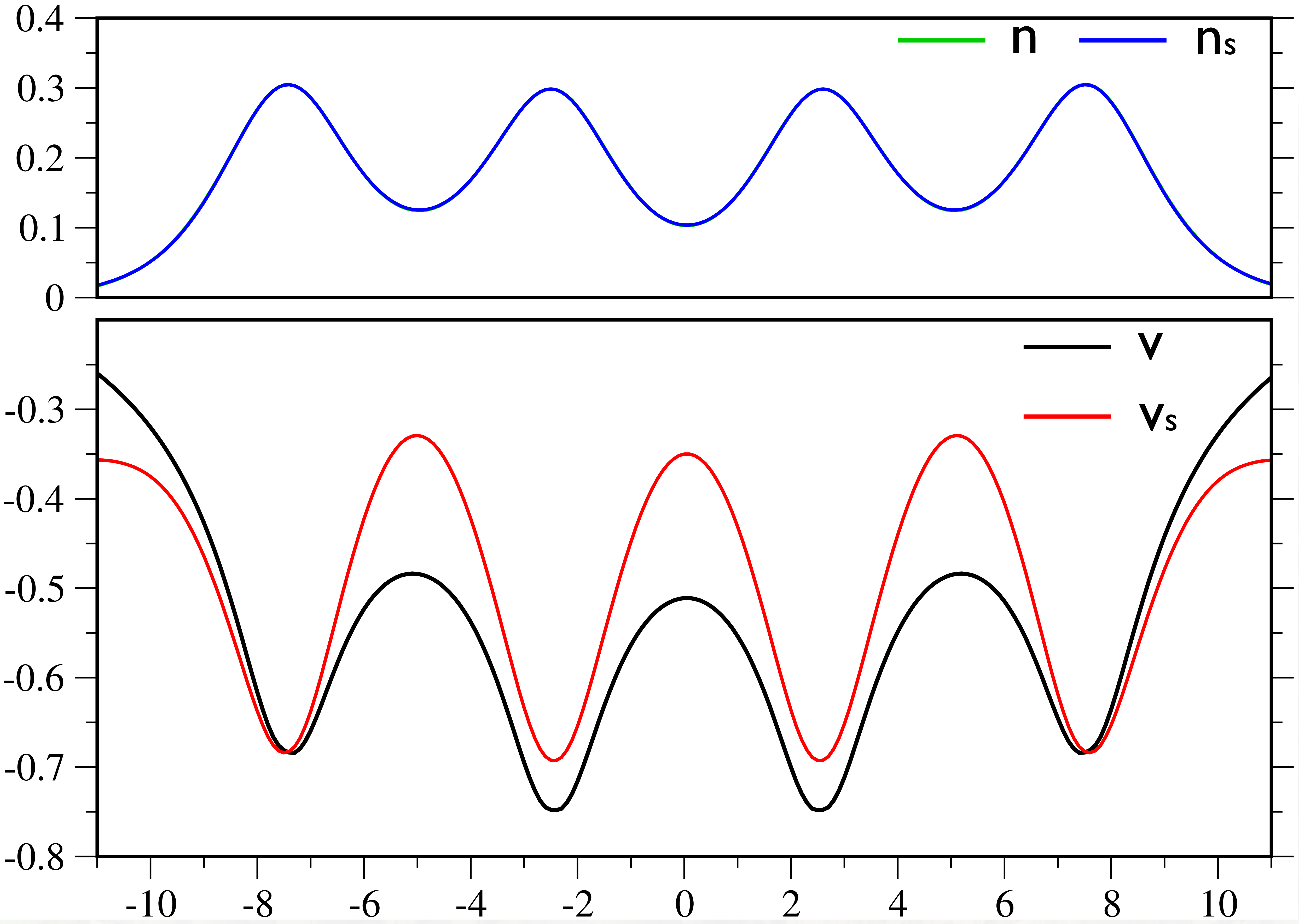
4 electrons, atomic spacing b=5



4 electrons, atomic spacing b=5



4 electrons, atomic spacing b=5



- Exact Kohn-Sham can be embedded within approximate DFT calculation (partition DFT)

- Also explore fundamental DFT questions:
  V-representability
  Local minima of exact functional

Future plans:

- Apply 1d lessons to 3d approximate functionals
- Continuum DMRG for 1d cold atom experiments
- Answer questions about effective models (such as Hubbard) e.g. physics of screening

For more information, please see the following preprints:

arxiv:1107.2394
arxiv:1202.4788