Title: Exact Calculations in the 1D Continuum for DFT and Beyond

Date: Nov 27, 2012 02:00 PM

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Abstract: Most applications of the density matrix renormalization group (DMRG) have been to lattice models with short range interactions. But recent developments in DMRG technology open the door to studying continuum systems with long-range interactions in one dimension (1d). One key motivation is simulating cold atom experiments, where it is possible to engineer Hamiltonians of precisely this type.

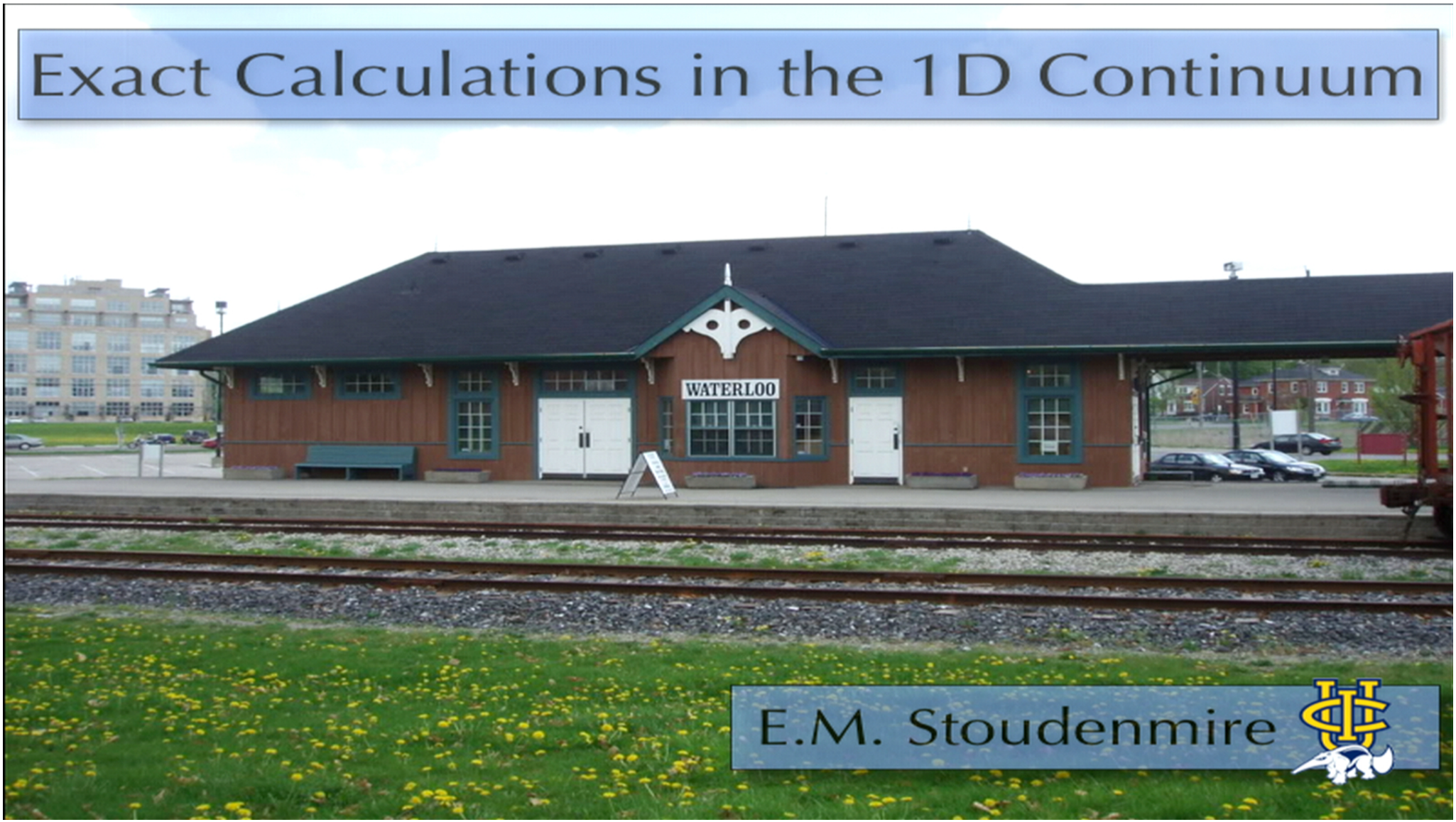
We have been applying DMRG in the 1d continuum with another

motivation: to investigate and improve density functional theory (DFT). DFT has exact mathematical foundations, but in practice one must use approximations. These approximations work incredibly well for weakly correlated systems yet fail when correlations are strong.

Improving DFT directly for realistic 3d systems is hard because few systems can be solved exactly. By working in the 1d continuum instead, we can use the power of DMRG to study DFT. We can implement both the exact DFT formalism and standard DFT approximations.

After showing how to overcome the challenges in performing these calculations, I will discuss some of the key questions we are investigating, for example, the ability of DFT to predict gaps of insulating systems.

Exact Calculations in the 1D Continuum



E.M. Stoudenmire

Collaborators

Steven R. White

Kieron Burke

Lucas O. Wagner

Summary:

Density matrix renormalization group (DMRG) a powerful method for 1d quantum systems

With recent improvements/extensions can study 1d continuum with long-range interactions

Why study 1d continuum?

- Can realize in cold atom/molecule experiment

  Liang, Kitagawa, Alicea et al. PRL **106**, 220402 (2011)
  Kinoshita, Wenger, Weiss Science **305**, 1125 (2004)

- Understand continuum-lattice mappings

- Laboratory for studying density functional theory (DFT) [*today*]

  Knorr and Godby PRL **68**, 639 (1992); PRB **50**, 1779 (1994)
  Wagner, Stoudenmire, Burke, White PCCP **14**, 7559 (2012)
  Stoudenmire, Wagner, White, Burke PRL **109**, 056402 (2012)

Outline:

I. Background: DMRG

II. DMRG tools for 1d continuum

III. Exact charge gaps of atomic chains

IV. Exact DFT band gaps

DMRG: almost ideal numerical method

 Essentially exact results

 Linear scaling in 1d

 Access wavefunction

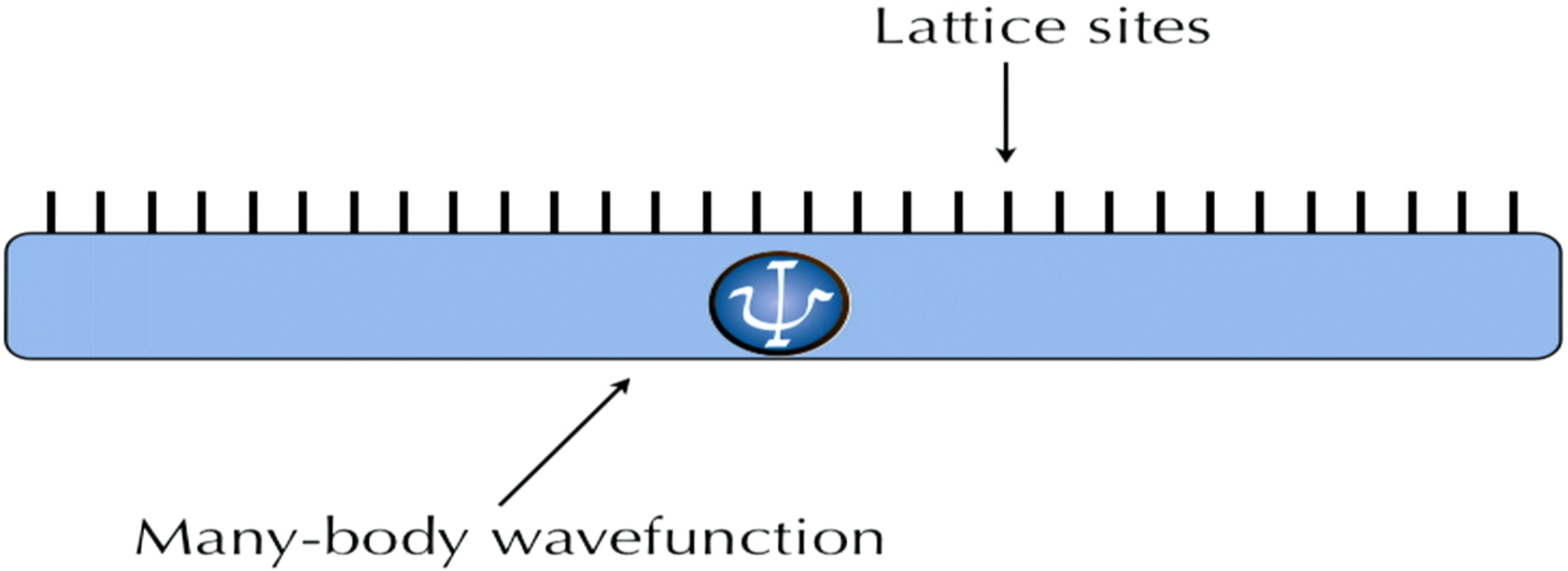
 Dynamics, finite T

 Parallelizable*

 1d and narrow 2d systems

*Stoudenmire and White [in preparation]

How does DMRG work?



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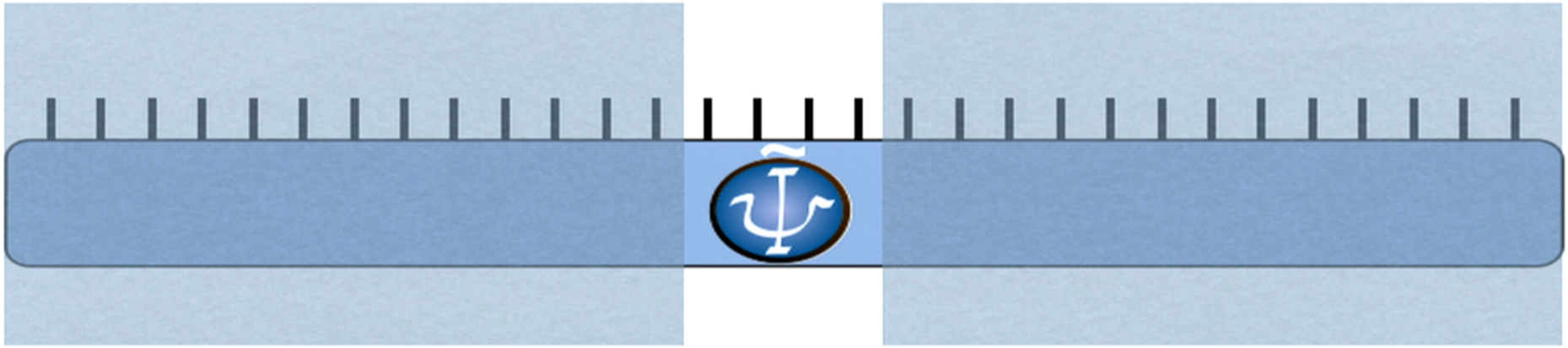
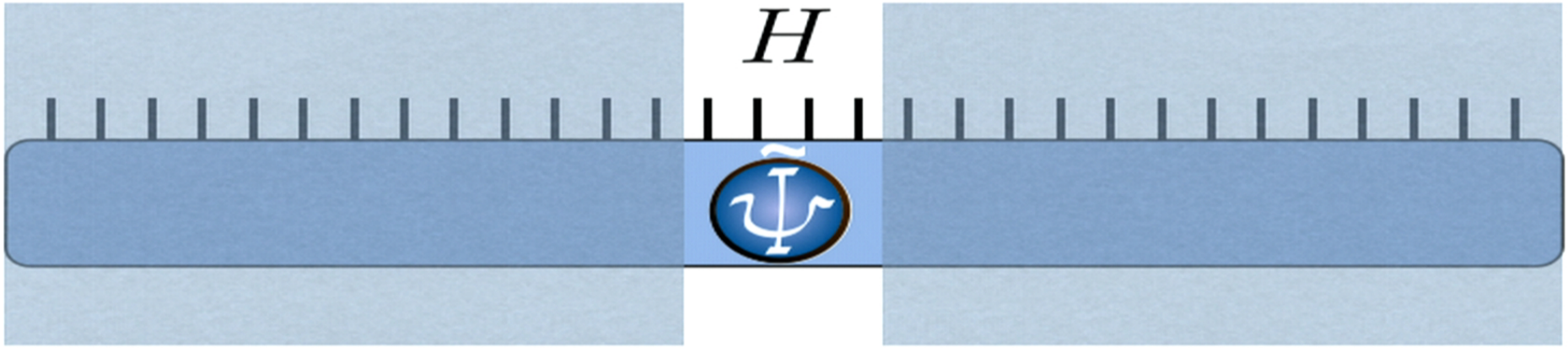


Freeze out all but a small piece of wavefunction

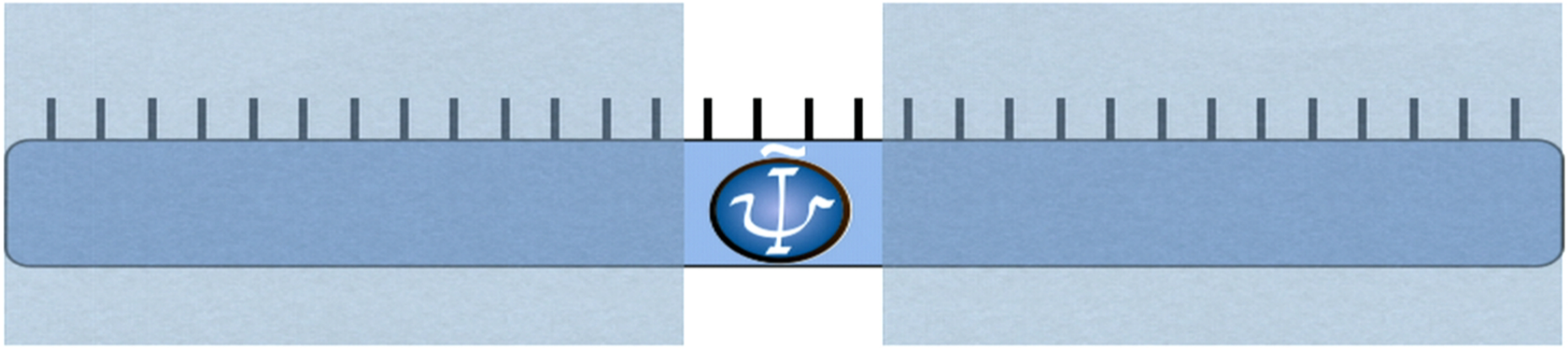
How does DMRG work?



Solve Schrodinger equation exactly for remaining piece

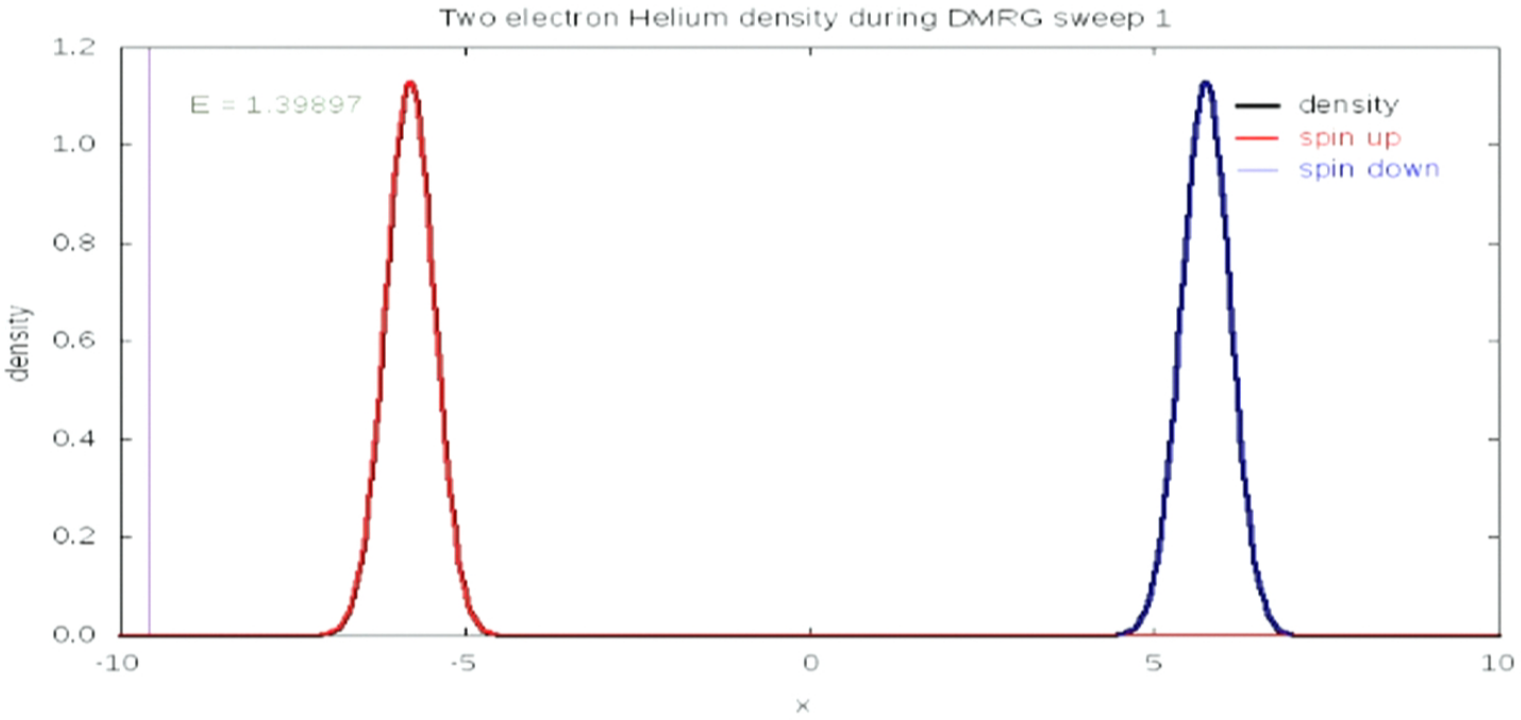
$$\tilde{H}|\tilde{\Psi}\rangle = \tilde{E}|\tilde{\Psi}\rangle$$

How does DMRG work?



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

DMRG Demo - 1d "Helium" Atom



$v(x)$

Applying DMRG to the continuum

Two approaches...

Method 1:

Continuous matrix product states (cMPS)

Continuum limit of DMRG wavefunctions.

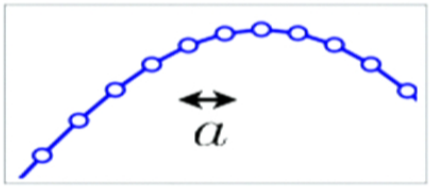
Verstraete and Cirac PRL **104**, 190405 (2010)

Haegeman et al. PRL **105**, 251601 (2010)

Method 2: (*this talk*)

Discretize real space

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



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

"Grid sites" instead of lattice sites

Dolfi, Bauer, et al., PRL **109** 020604 (2012)

Stoudenmire, Wagner, White, Burke, PRL **109** 056402 (2012)

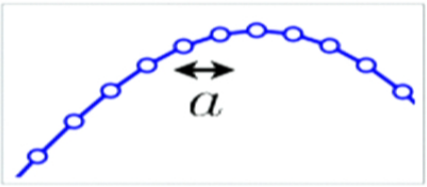
Continuum Hamiltonian:

$$\hat{H} = -\frac{1}{2}\sum_{\sigma}\int_{x}\psi^{\dagger}_{\sigma}(x)\frac{\partial^2}{\partial x^2}\psi_{\sigma}(x)$$

$$+\frac{1}{2}\int_{x,x'} v_{\mathrm{ee}}(x-x')\,\hat{n}(x)\,\hat{n}(x')$$

$$+\int_{x} v(x)\,\hat{n}(x)$$

Grid Hamiltonian:



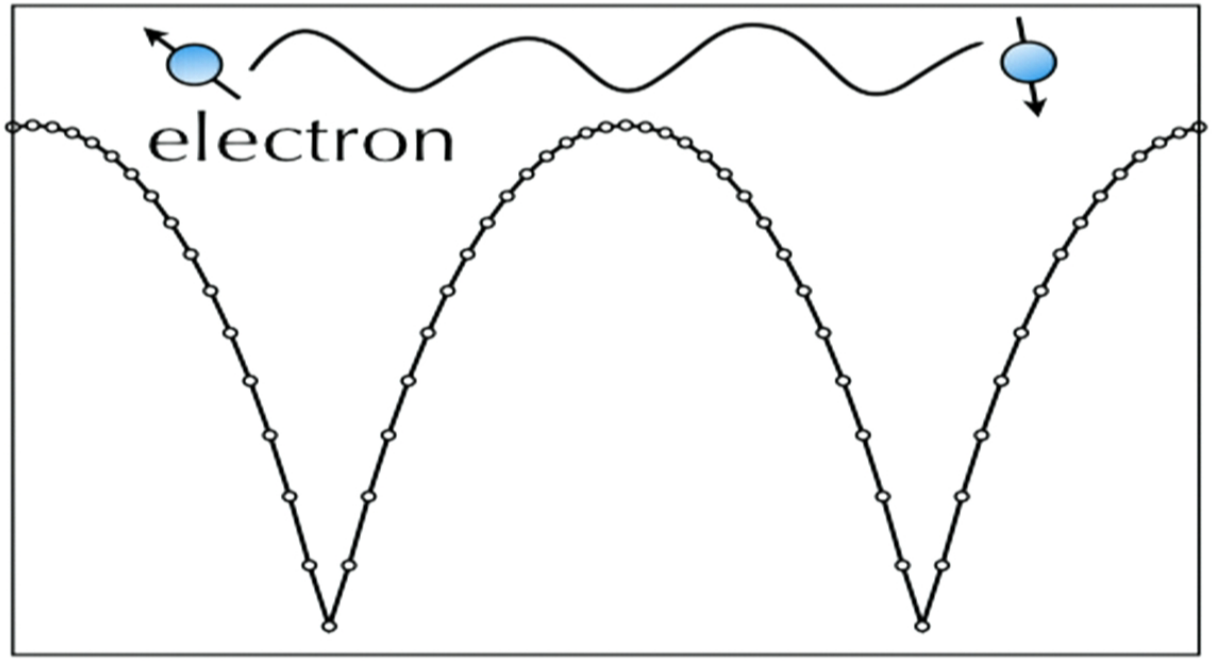
$$\hat{H} = -\frac{1}{2a^2}\sum_{\sigma,j}(c^{\dagger}_{\sigma j}c_{\sigma j+1} - 2n_{\sigma j} + c^{\dagger}_{\sigma j+1}c_{\sigma j})$$

$$+\frac{1}{2}\sum_{i,j} v^{ij}_{\mathrm{ee}}\, n_i\,(n_j - \delta_{ij})$$

$$+\sum_{j} v^{j}\, n_j$$

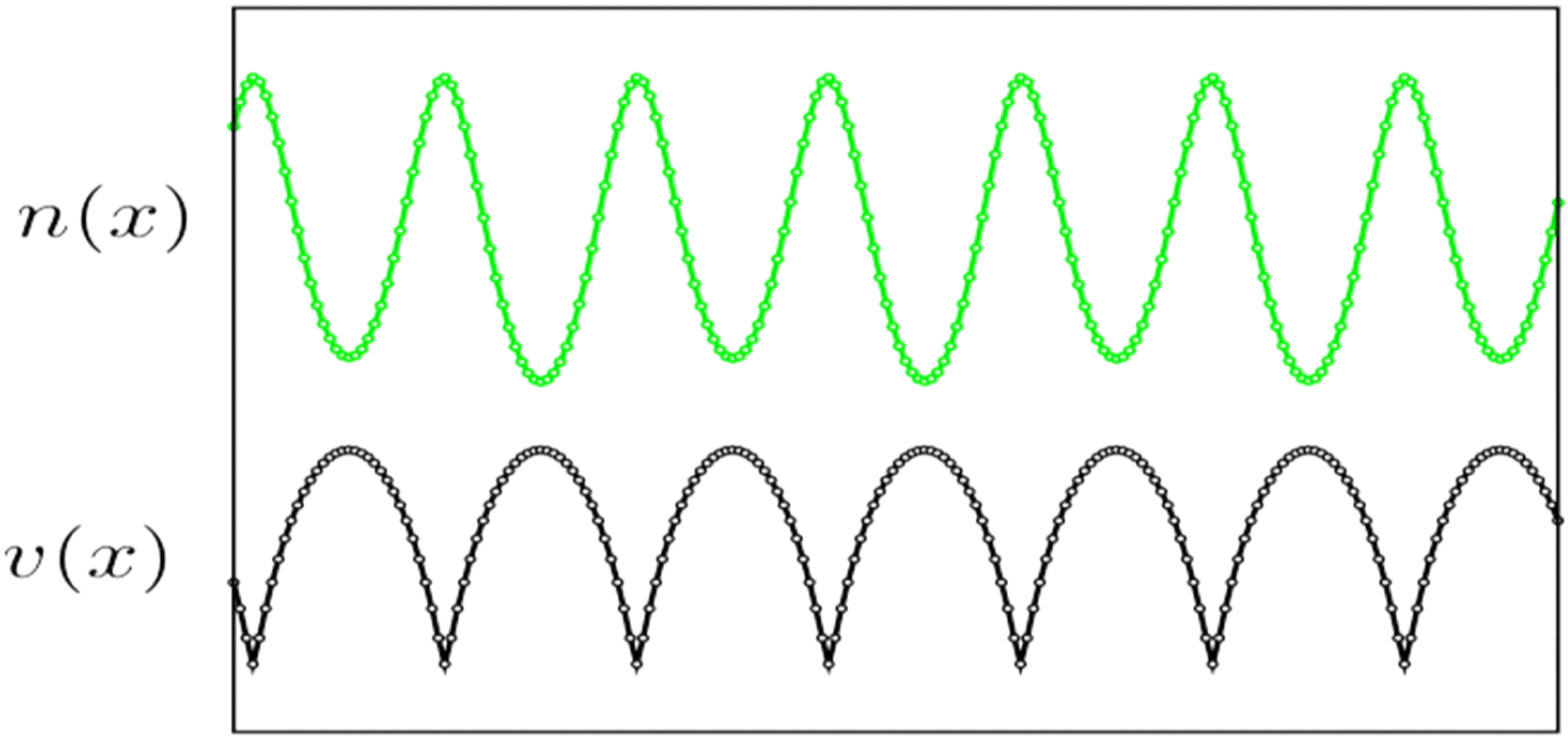
$\longrightarrow$ Extrapolate results to small a limit

Model systems: 1d chains of atoms



$$v_{\rm ee}(x-x') = e^{-|x-x'|} \; ; \; v_{\rm atom}(x) = -Z v_{\rm ee}(x)$$

When plotting, leave off grid points



Why hasn't DMRG been applied to these systems before?

Long-range interactions

Conventional approach: include pairwise interactions separately

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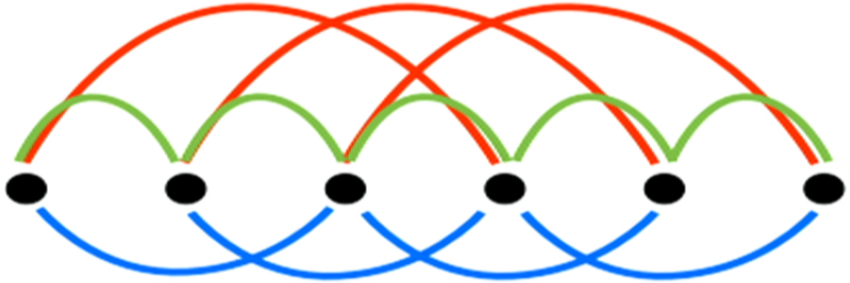

Long-range interactions

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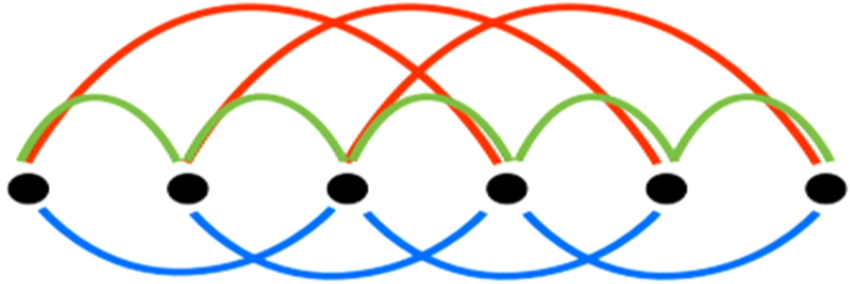

Normally DMRG scales $\propto N$,

with this approach $\propto N^2 \times N = N^3$

Disaster for the continuum! $(N \sim 1000)$

We now have better understanding of DMRG wavefunctions

product of transfer matrices carrying quantum entanglement (matrix product states)

Useful for representing Hamiltonians?

Östlund and Rommer, PRL **75**, 3537 (1995)

Yes, can "bundle" finite number of operators to obtain infinite-range exponential interactions:

$$H = \cdots \begin{bmatrix} \hat{I} & & \\ \hat{\sigma}^z & \lambda\hat{I} & \\ 0 & \hat{\sigma}^z & \hat{I} \end{bmatrix} \cdots \begin{bmatrix} \hat{I} & & \\ \hat{\sigma}^z & \lambda\hat{I} & \\ 0 & \hat{\sigma}^z & \hat{I} \end{bmatrix} \cdots$$

$$\hat{\sigma}^z \quad \lambda\hat{I} \quad \lambda\hat{I} \quad \lambda\hat{I} \quad \lambda\hat{I} \quad \lambda\hat{I} \quad \lambda\hat{I} \quad \lambda\hat{I} \quad \hat{\sigma}^z$$

McCulloch, arxiv: 0804.2509 (2008)
Crosswhite, Doherty, Vidal, PRB **78**, 035116 (2008)

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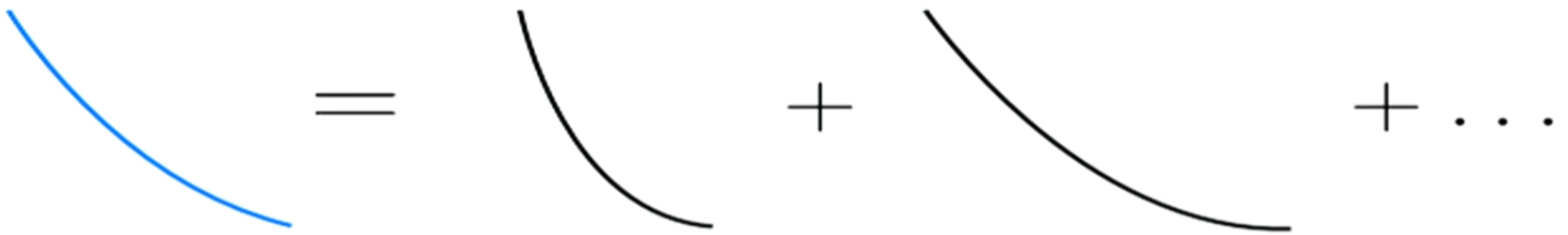
McCulloch, arxiv: 0804.2509 (2008)
Crosswhite, Doherty, Vidal, PRB **78**, 035116 (2008)

Can approximate power-law interactions as sums of exponentials:

$$\frac{1}{|i-j|^{\alpha}} \simeq \sum_{p} \chi_p \ \lambda_p^{i-j}$$



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

Convergence Issues

At least 3 widely separated energy scales:

Grid kinetic energy $(1/a^2)$

$\ggg$

Density fluctuations (U)

$\gg$

Spin fluctuations (t^2/U)

Convergence Issues

Leads to unique situation for DMRG:

Typical limitation is states kept "m".
Convergence in 5-10 sweeps.

Here m~500 required (no problem),
but may need 1000's of sweeps!

Solution is that–from grid point of view–systems are highly dilute:

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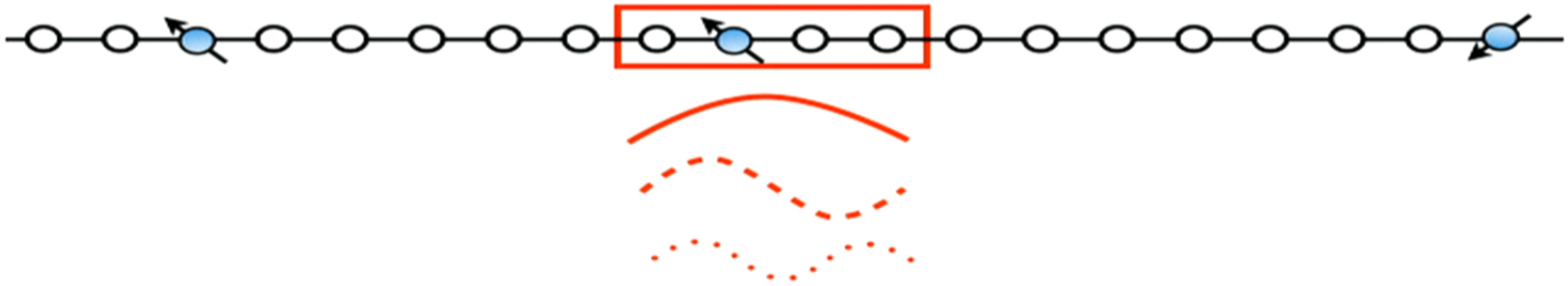
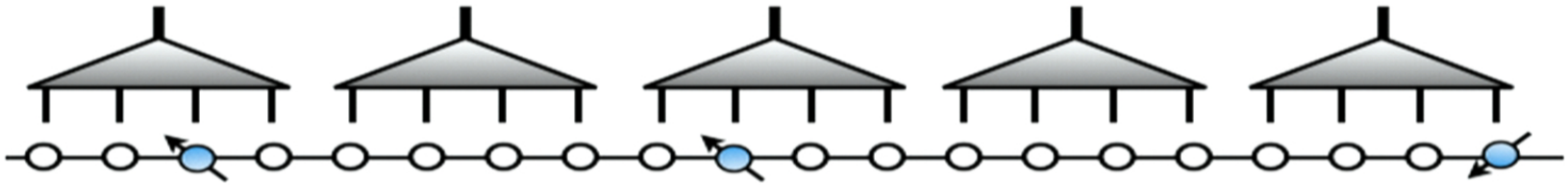


For small region, only first few reduced-density-matrix eigenstates significant

Apply isometries (truncated unitaries) to keep highest weight states



Actually, best to use 2 to 1 map:

Dolfi, Bauer, et al., PRL **109** 020604 (2012)

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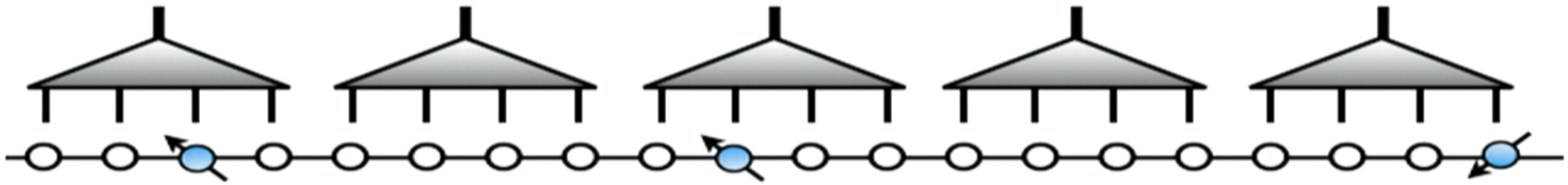

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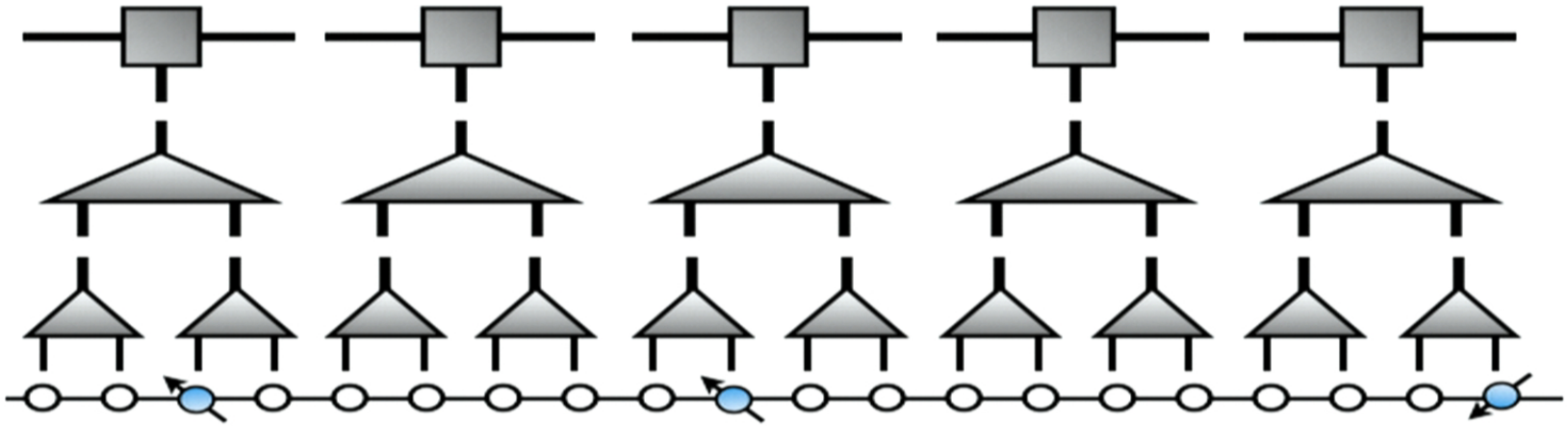
Leads to interesting tensor-network state: a tree-tensor-network / MPS hybrid



Dolfi, Bauer, et al., PRL **109** 020604 (2012)

Can determine optimal isometries from converged wavefunction.

Verstraete, Cirac, Latorre, Rico & Wolf, PRL **94** 140601 (2005)

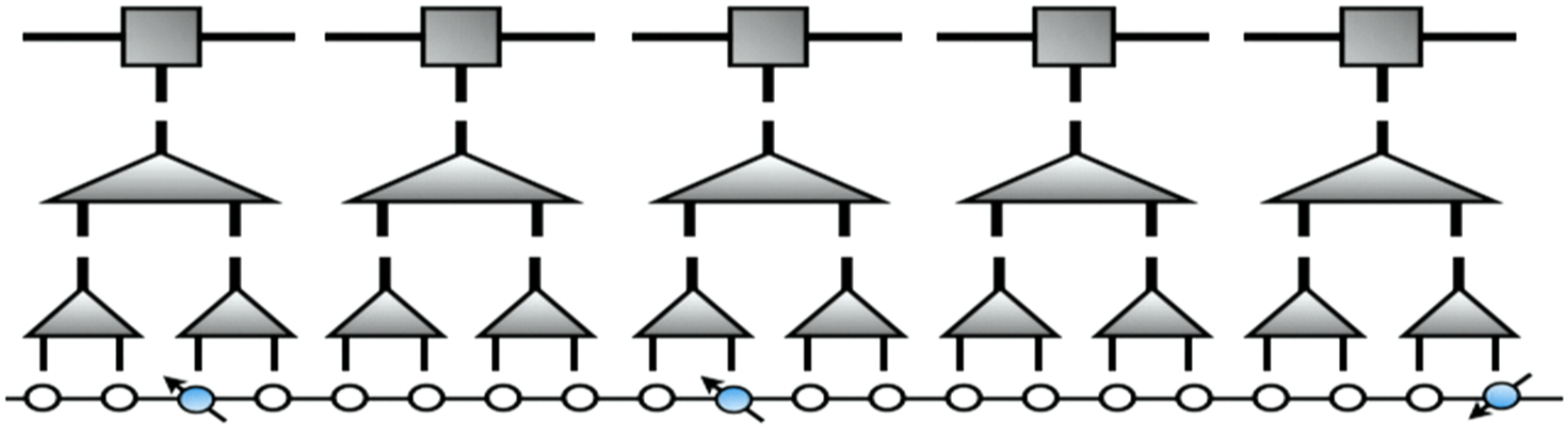
In practice, initial wavefunction poor so use "flat" isometries, let DMRG correct

Dolfi, Bauer, et al., PRL **109** 020604 (2012)

Optimal: 

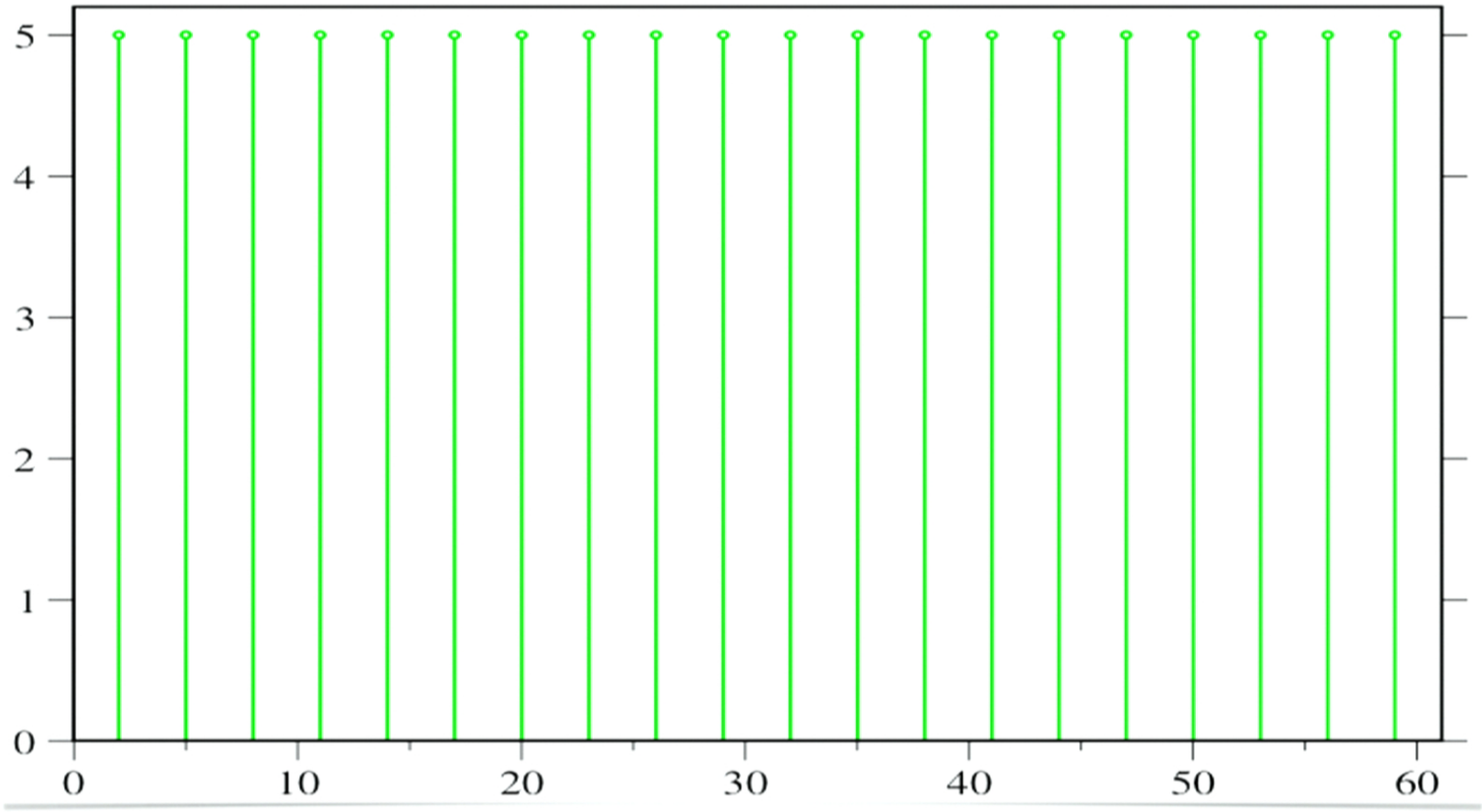
Flat: 

Leads to interesting tensor-network state: a tree-tensor-network / MPS hybrid



Dolfi, Bauer, et al., PRL **109** 020604 (2012)

Demonstration: 40 Grid Points



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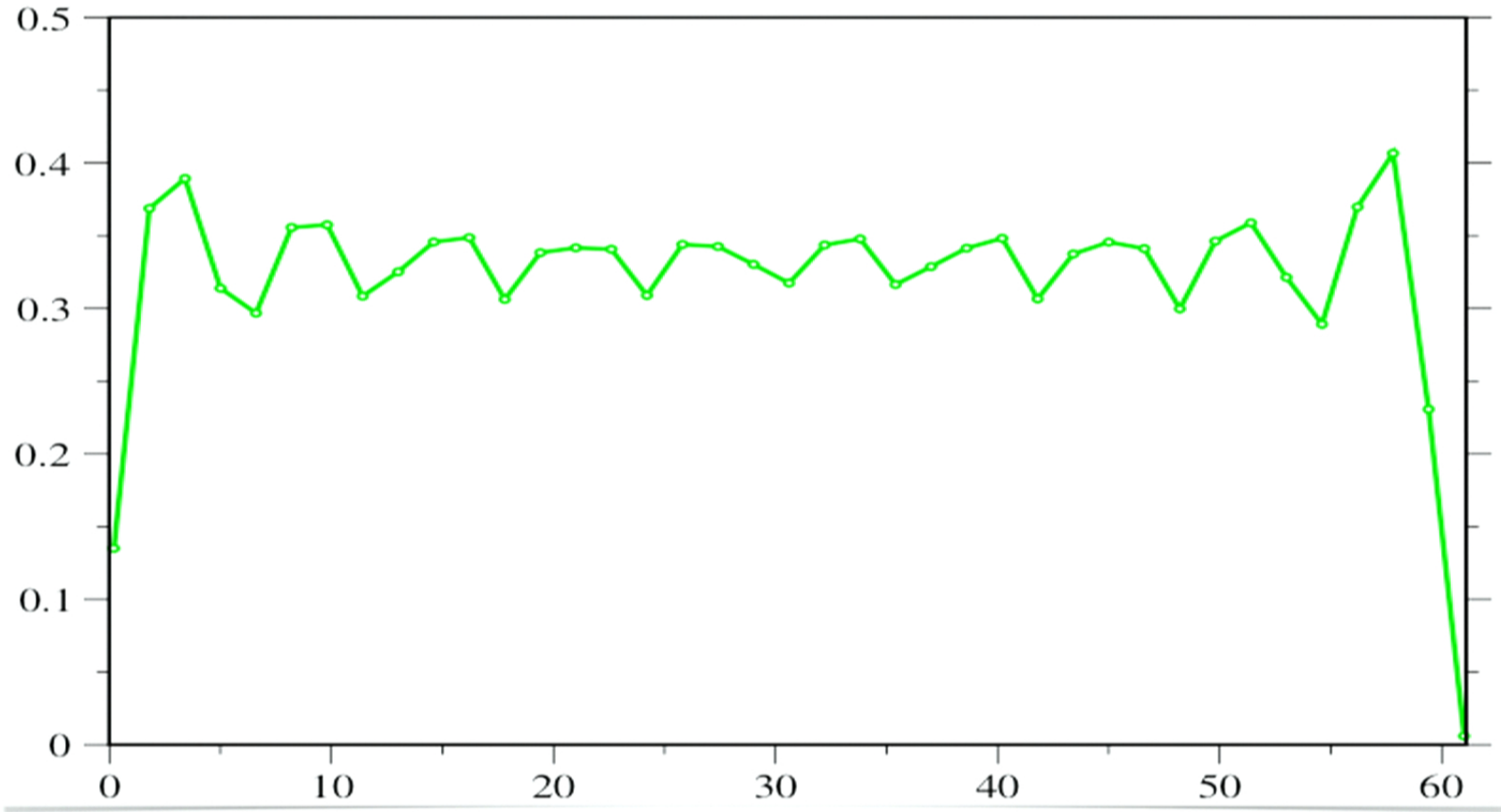
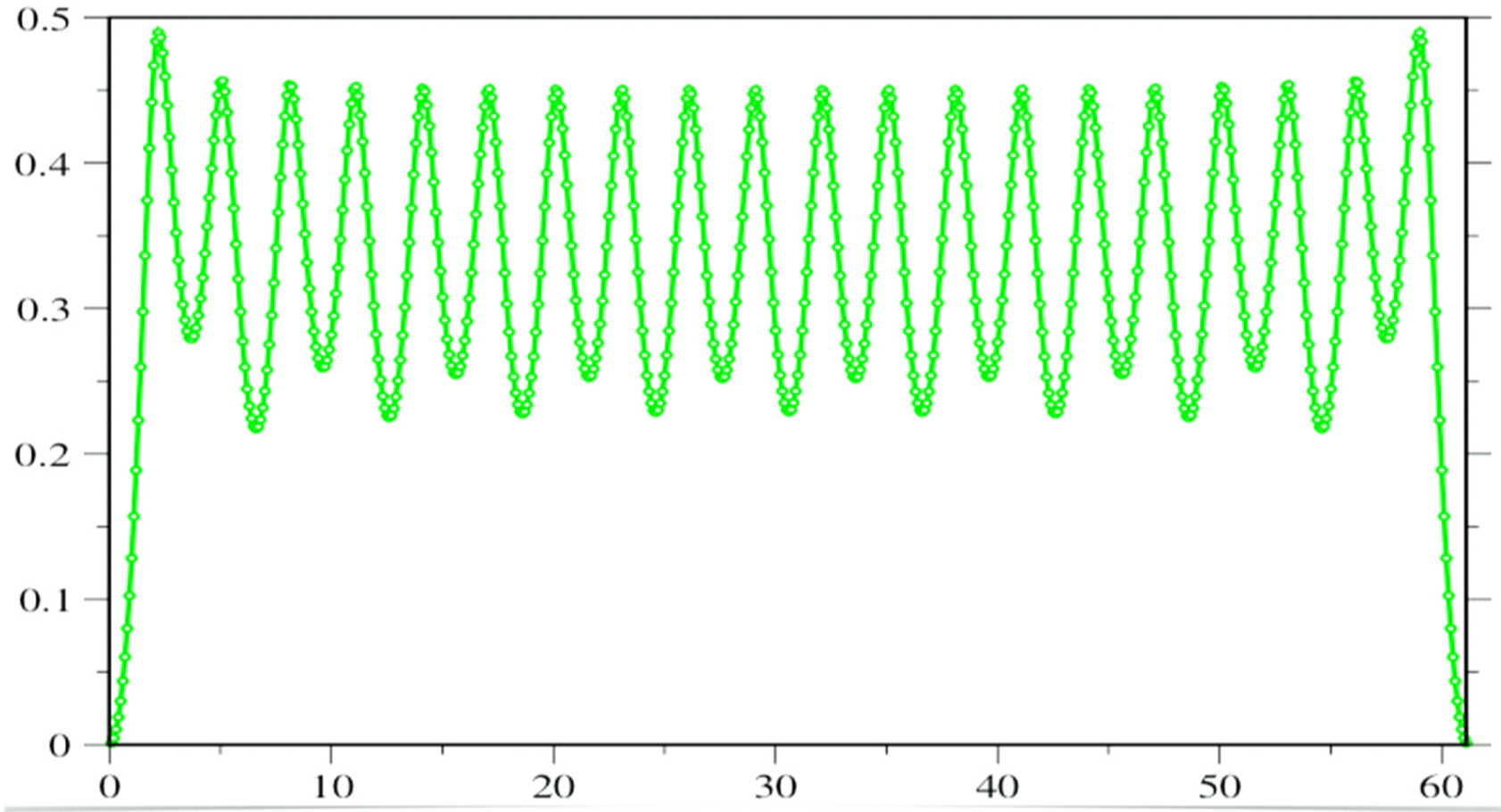


Demonstration: 612 Grid Points



Current Project

Charge Gaps in 1d Atom Chains

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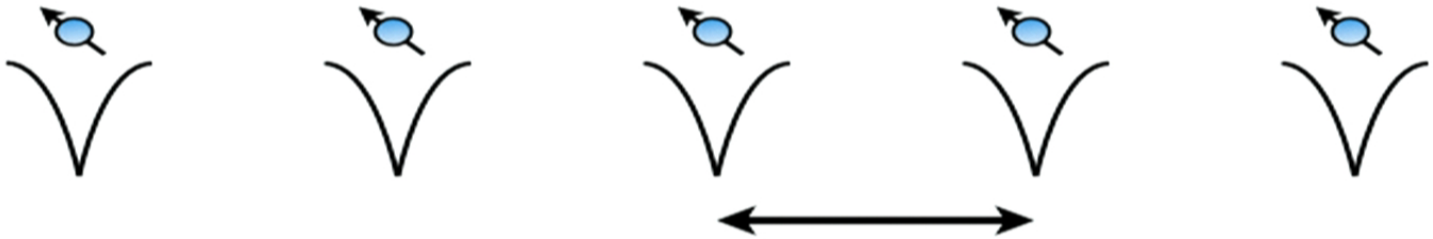
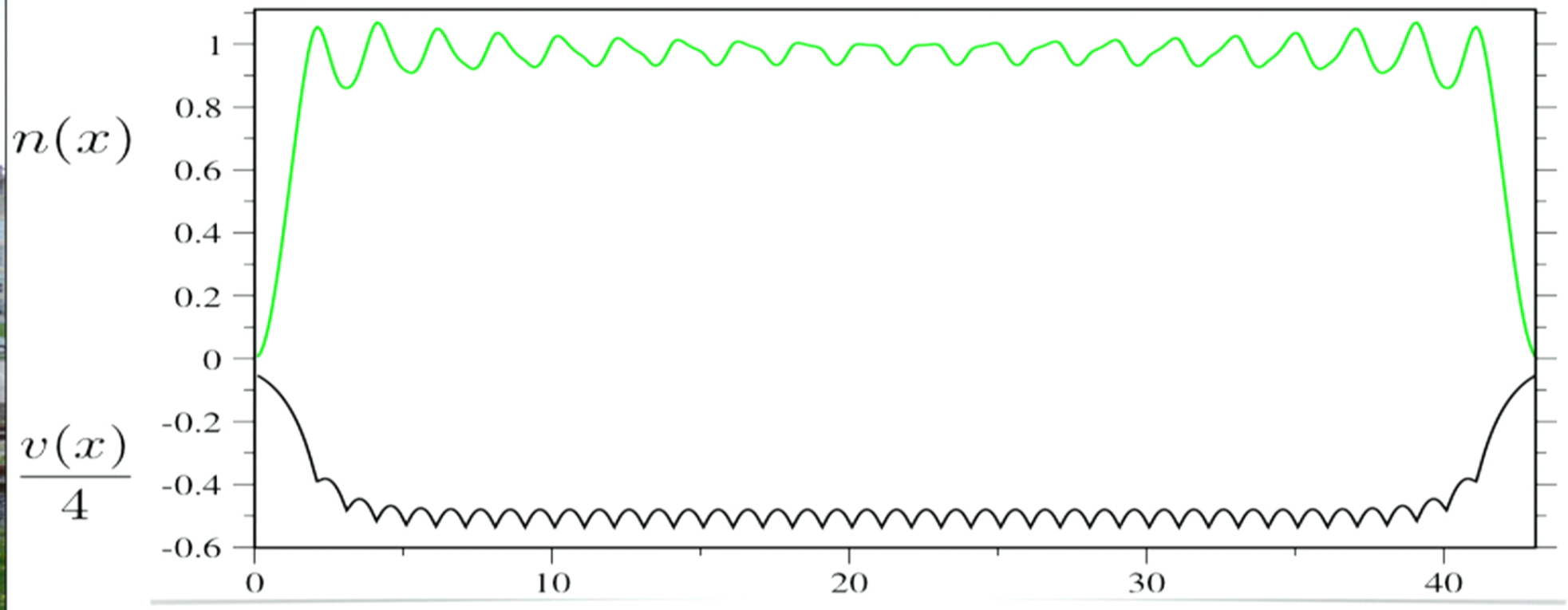
Hydrogen Chains

Simplest system a chain of stretched 1d hydrogen atoms



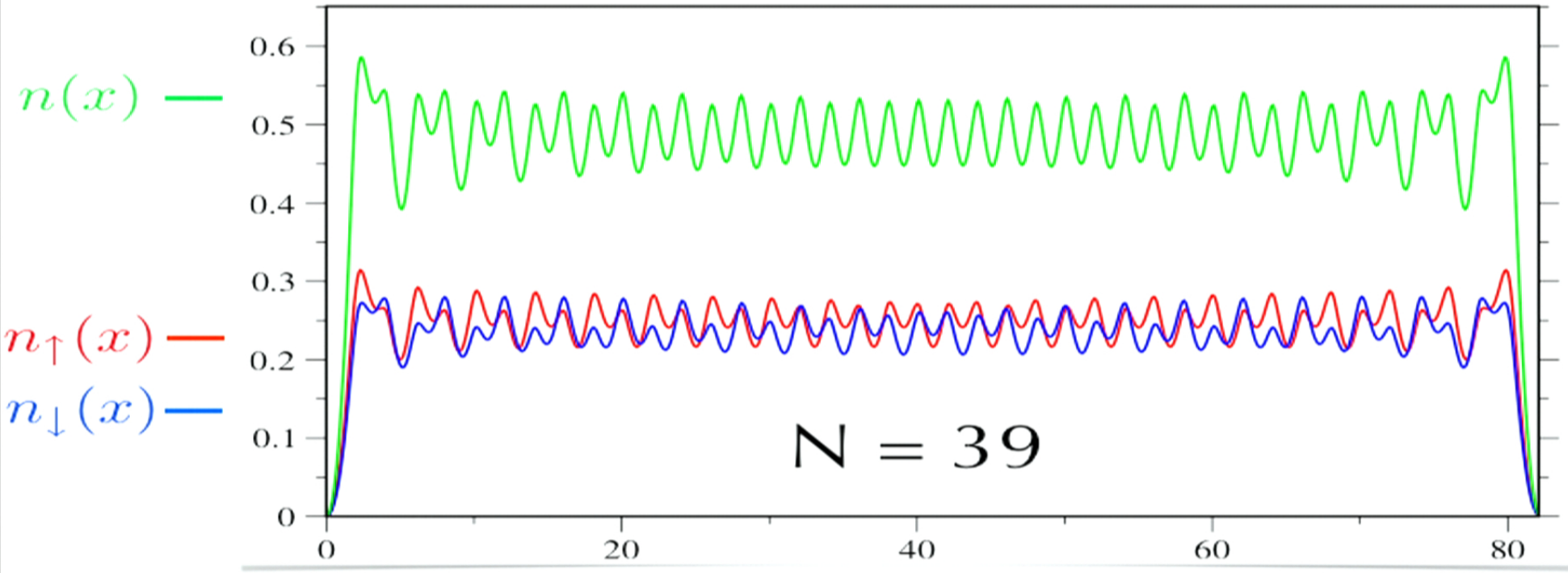
tune bond length "b"

Hydrogen Chains (40 atoms)



b = 1.0

Hydrogen Chains

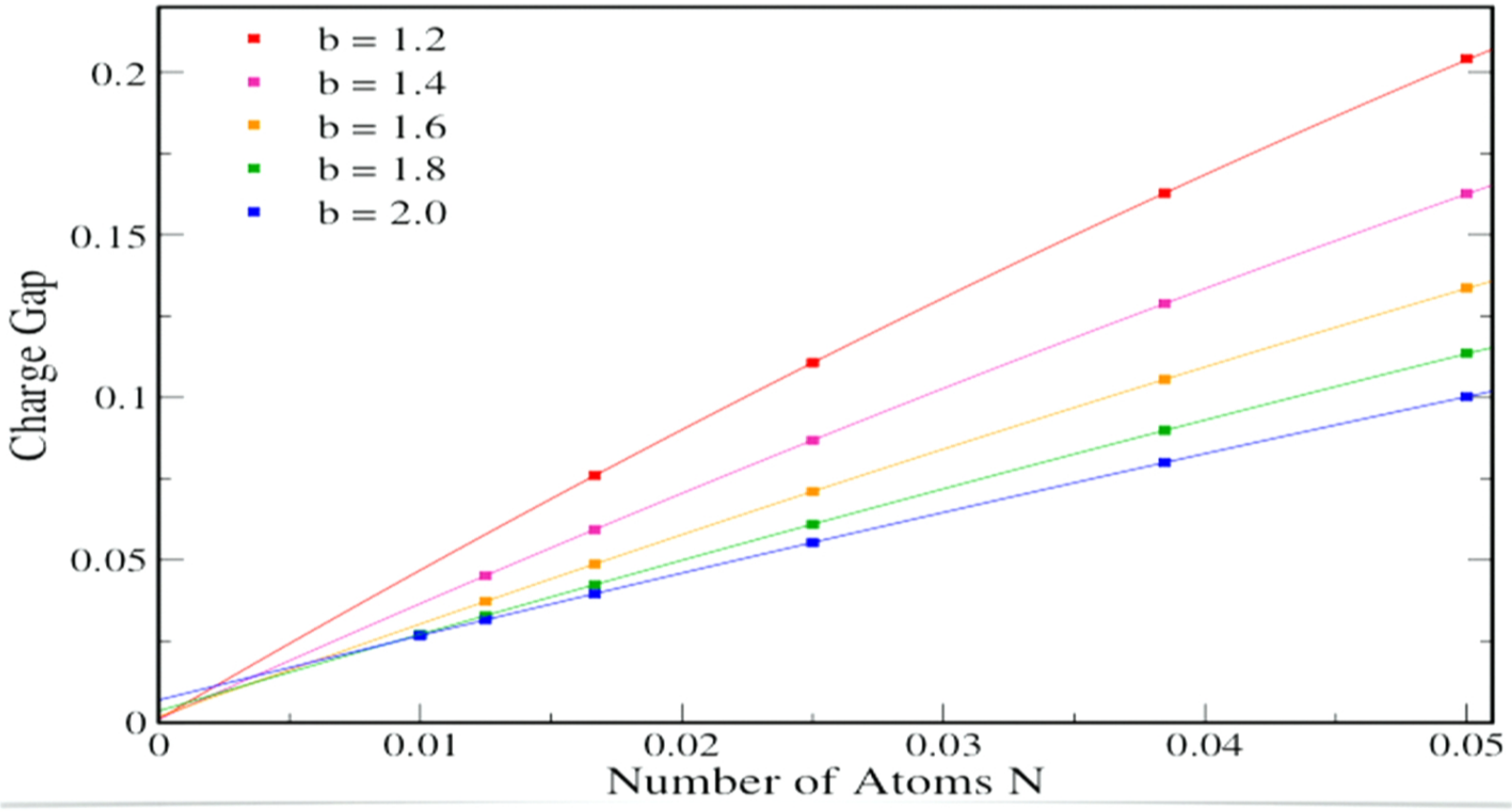


For each, measure charge gap:

$$E_g = E_{N+1} - 2E_N + E_{N-1}$$

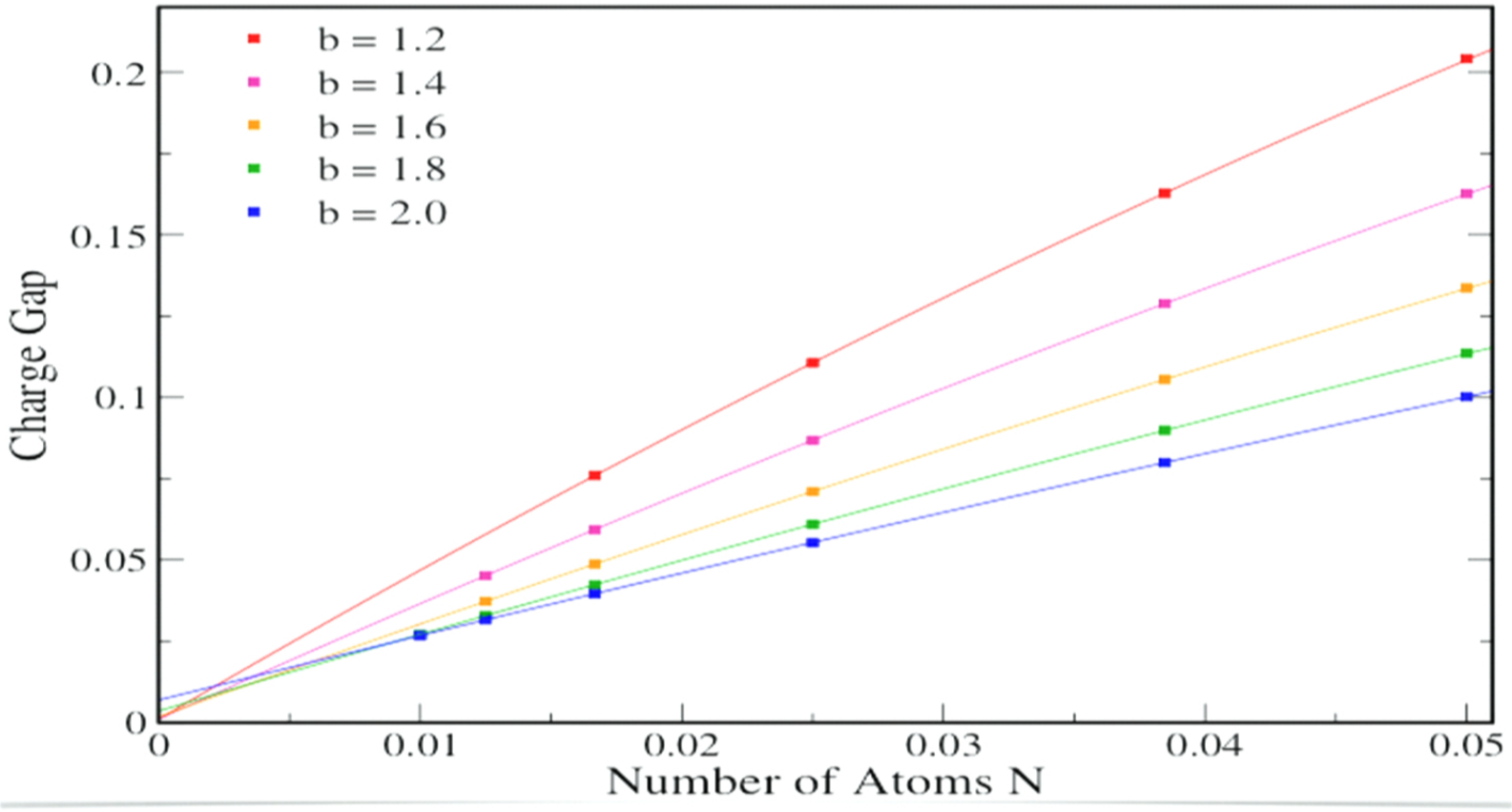
Hydrogen Chains

Extrapolate gaps to thermo. limit



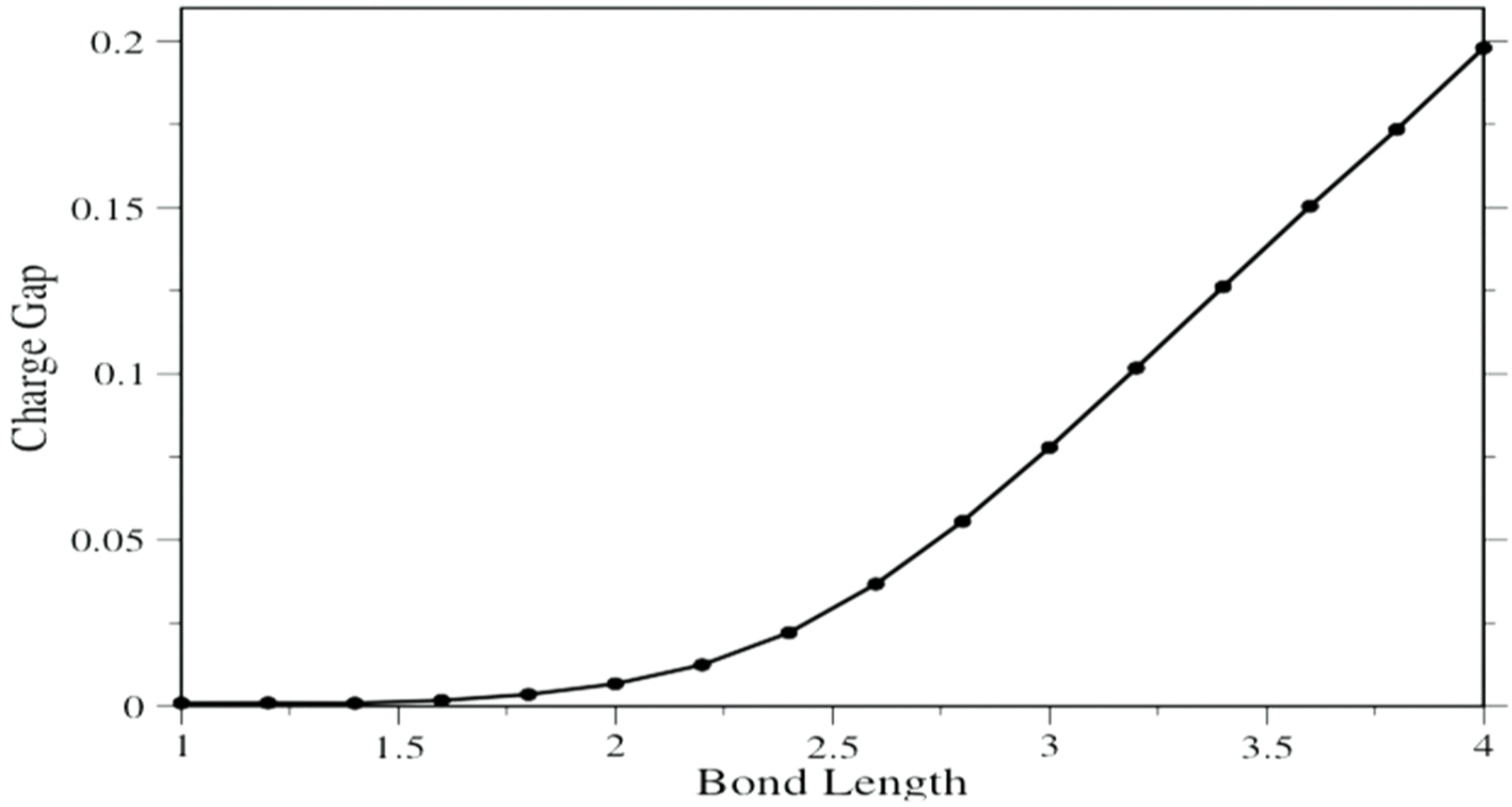
Hydrogen Chains

Extrapolate gaps to thermo. limit



Hydrogen Chains

Some qualitative similarity to 1d Hubbard



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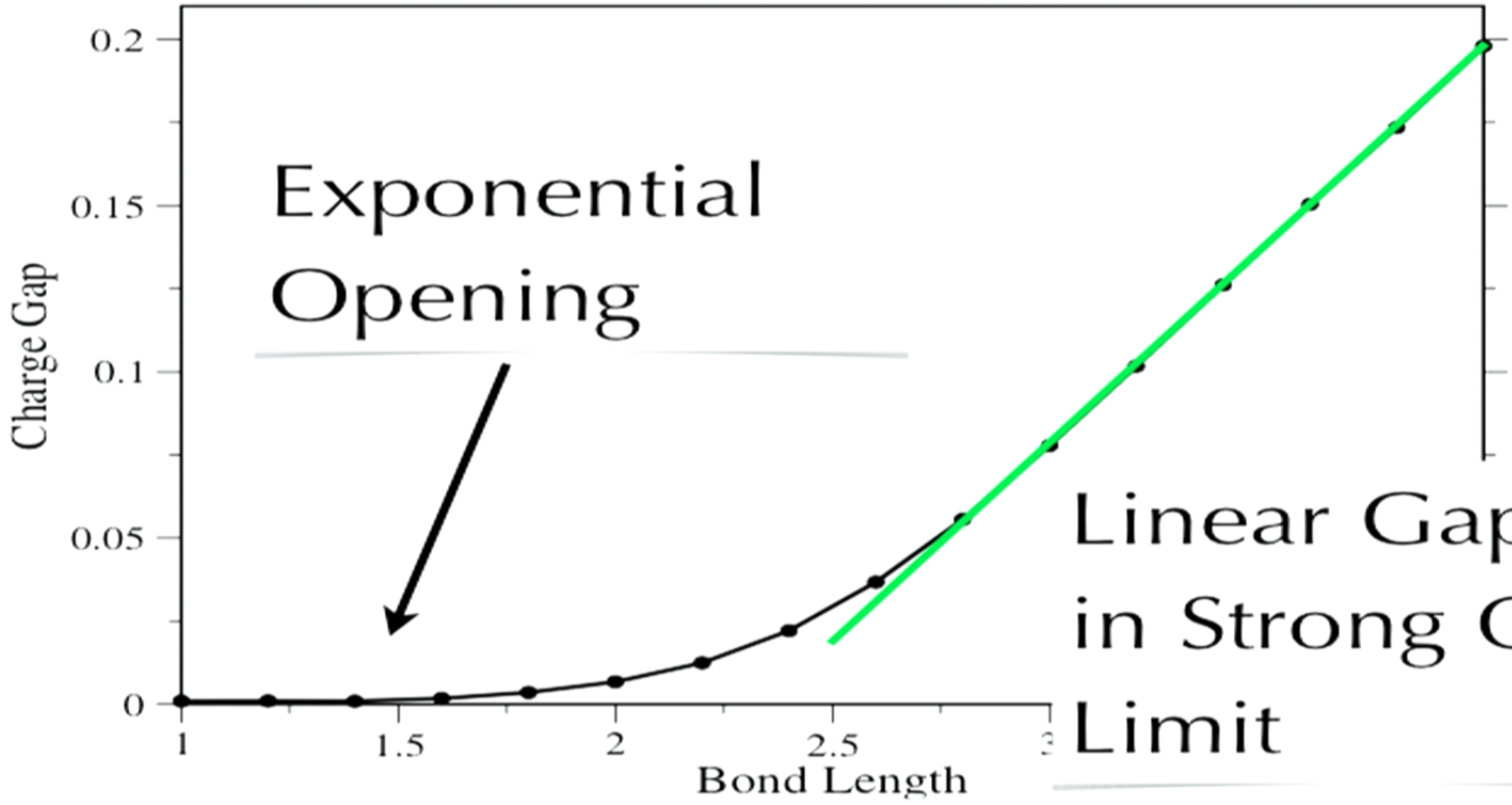
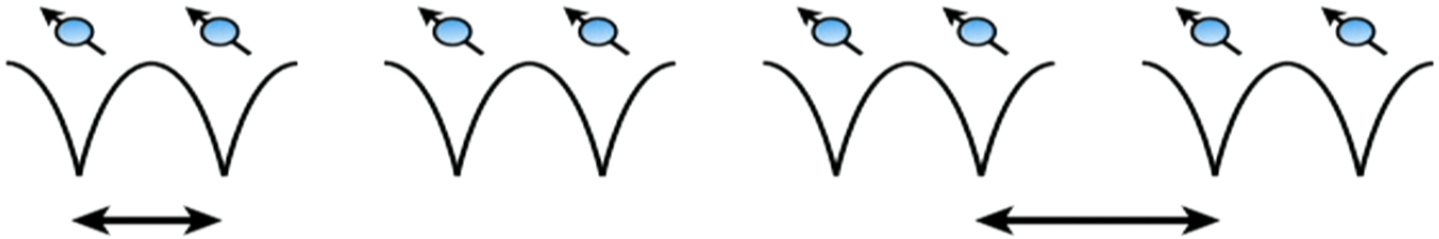


H_2 Chains

Chains of H2 molecules–
simple example of band insulator



fixed H_2 equil length 1.26

tune bond length "b"

H_2 Chains

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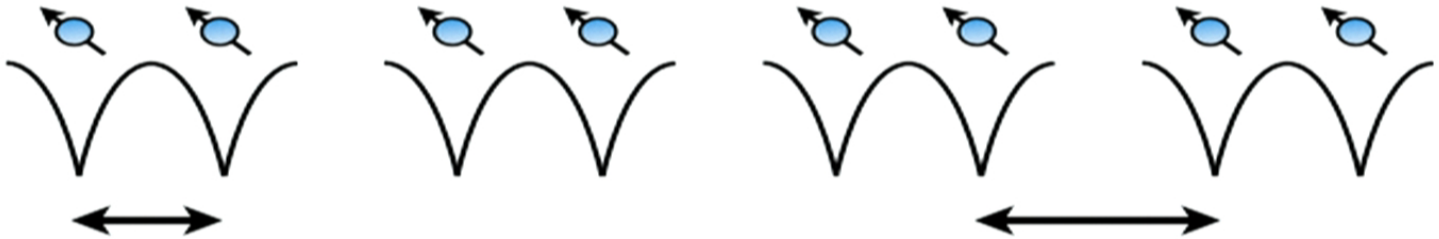

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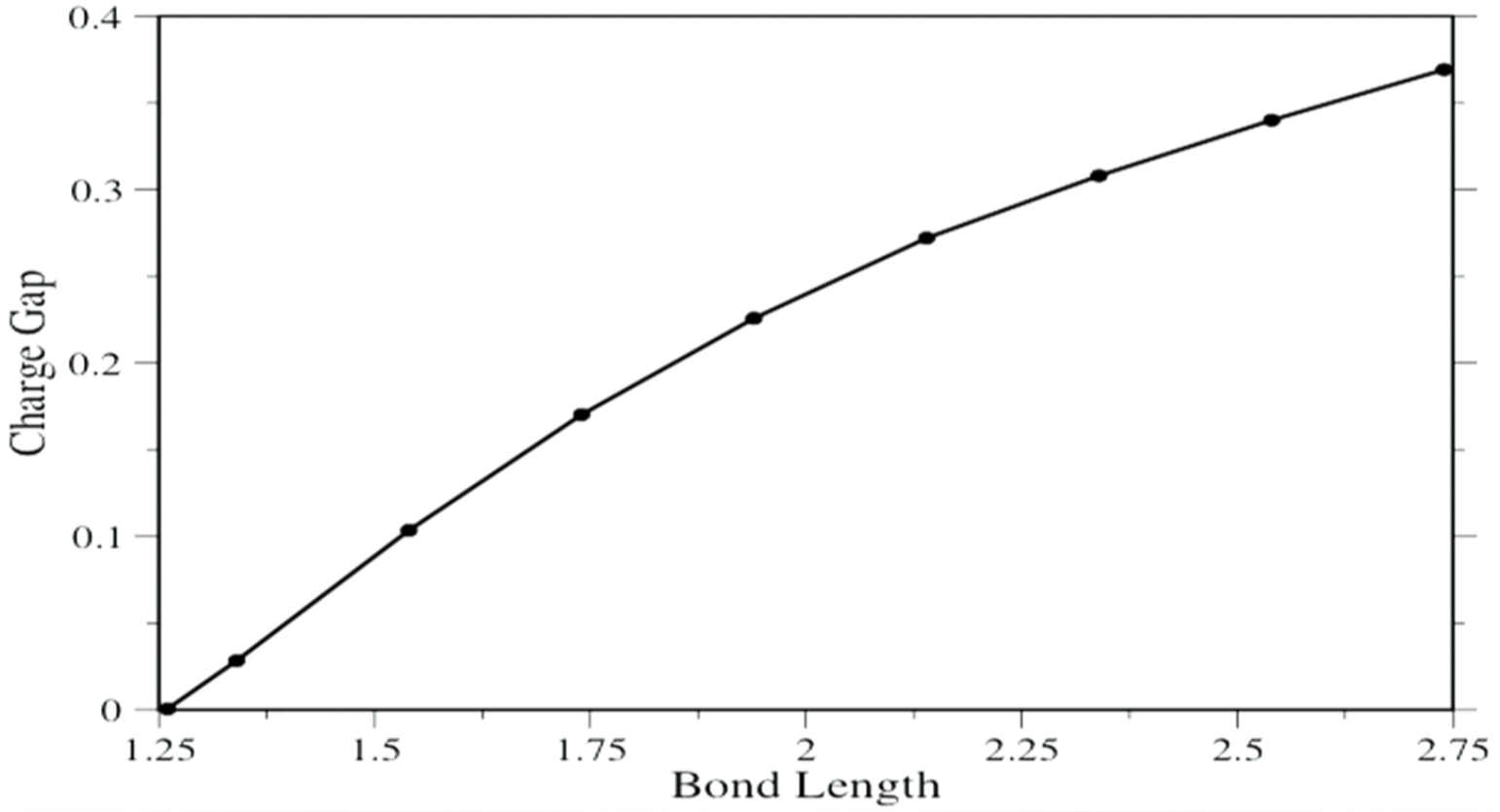
H_2 Chains

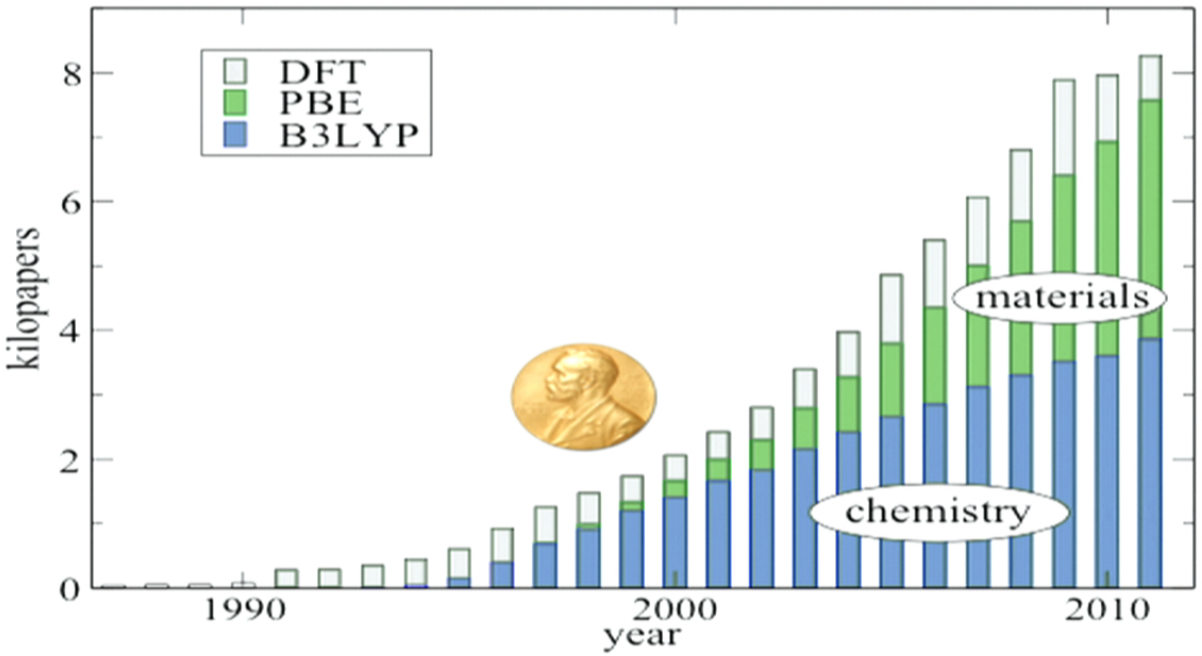
Large gap opens immediately



Exact DFT Band Gaps

How does DFT capture opening of charge gap?

Density functional theory (DFT) is one of the most practical, widely used methods in physics and chemistry



Burke, J. Chem. Phys. **136**, 150901 (2012)

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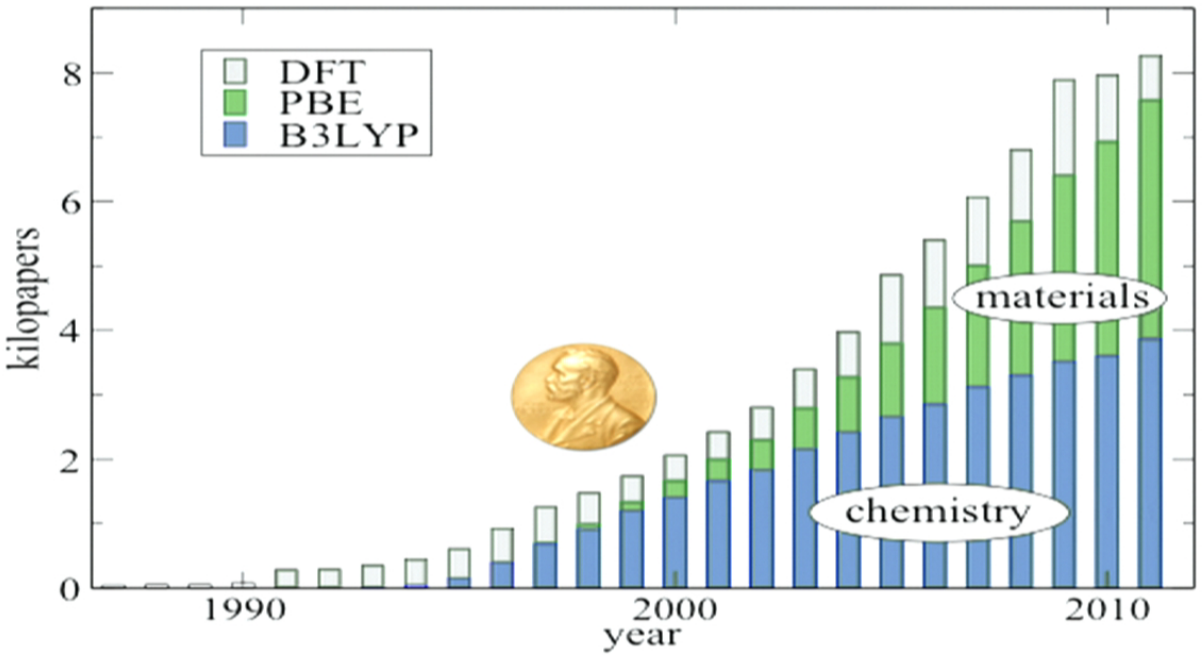


Burke, J. Chem. Phys. **136**, 150901 (2012)

Exact reformulation of quantum mechanics using density, not wavefunction

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

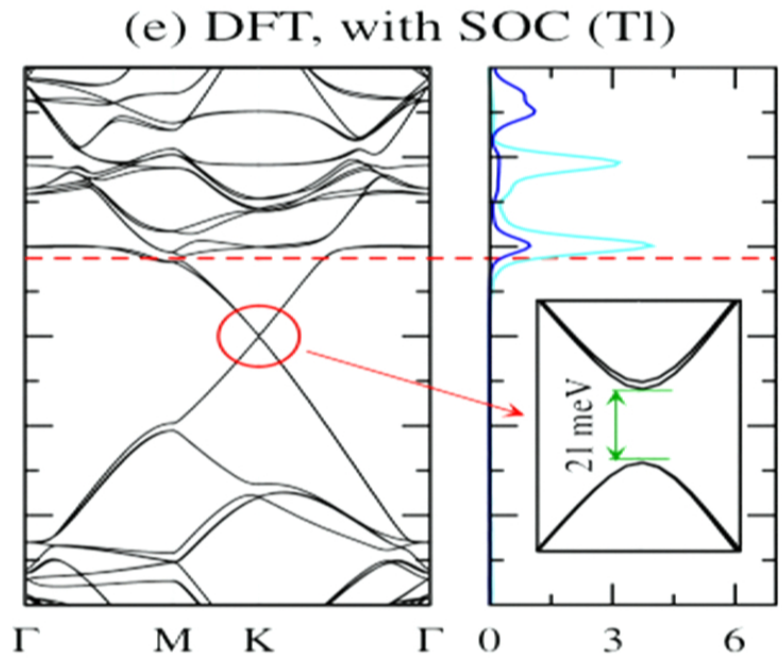
Uses density instead: $E[n]$

"One of the greatest free lunches ever": saves computer time; can study realistic systems

K. Burke, Phys. Rev. Focus **2**, 19 (1998)

Often where "rubber meets the road" in condensed matter physics

Prediction of enhanced T.I. gap in graphene with adatoms deposited:



Weeks, Hu, Alicea, Franz, Wu, PRX **1**, 021001 (2011)

Hohenberg-Kohn Theorem

DFT has a rigorous foundation:

$$\hat{H} = \hat{T} + \hat{V}_{\mathrm{ee}} + \int_x v(x)\,\hat{n}(x)$$

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HK '64

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HK '64

Kohn-Sham DFT

Practical DFT approx's use Kohn-Sham scheme

HK assume fixed interactions
$\Longrightarrow$ *Two* systems correspond to $n(x)$:

$$\hat{H} = \hat{T} + \hat{V}_{\mathrm{ee}} + \int_x v(x)\,\hat{n}(x)$$

$$\hat{H}_s = \hat{T} + \int_x v_s(x)\,\hat{n}(x)$$

$n(x)$

Kohn-Sham DFT

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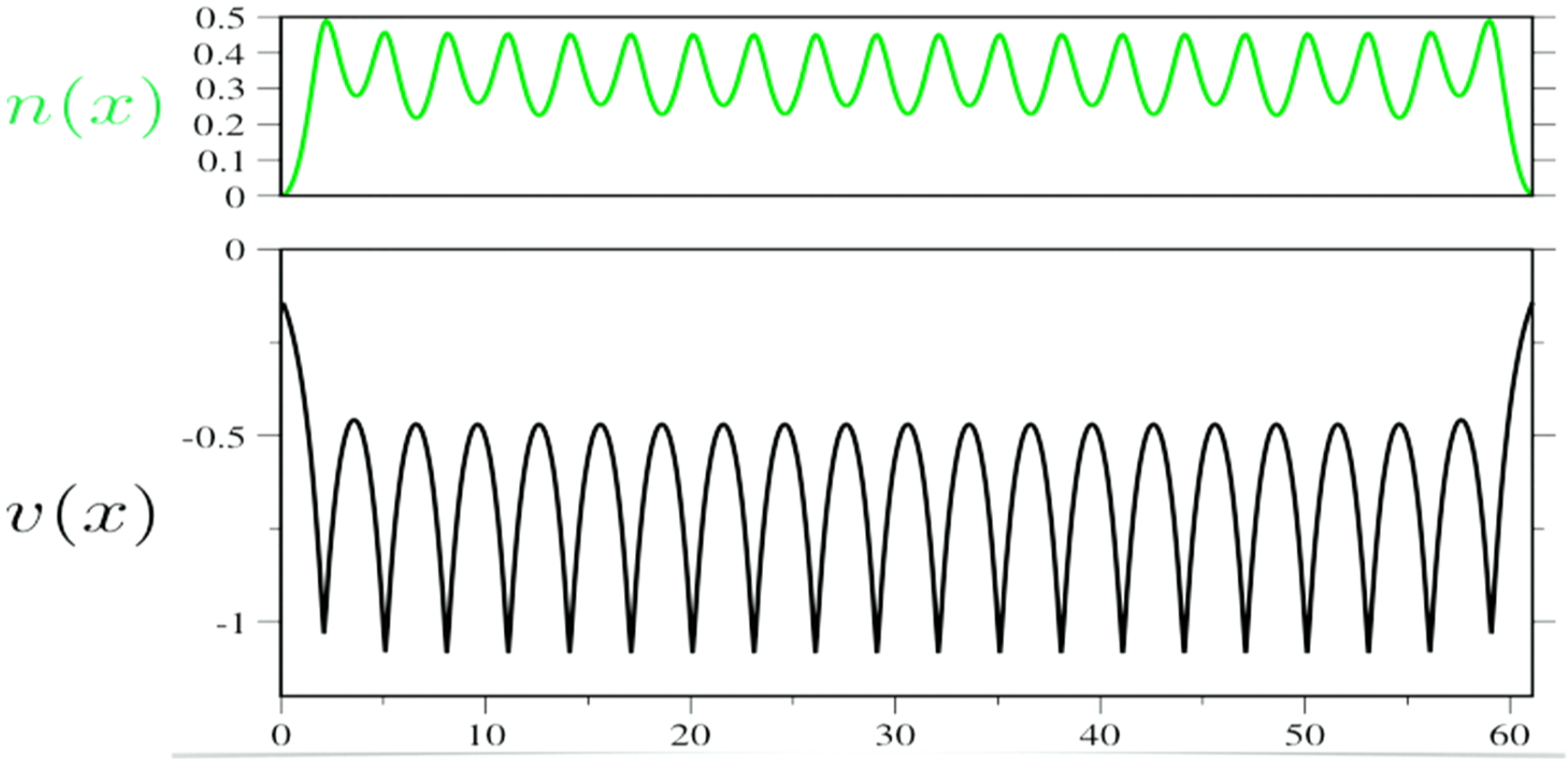
$\Longrightarrow$ *Two* systems correspond to $n(x)$:

$$\hat{H} = \hat{T} + \hat{V}_{\mathrm{ee}} + \int_x v(x)\,\hat{n}(x)$$

$$\hat{H}_s = \hat{T} + \int_x v_s(x)\,\hat{n}(x)$$

$n(x)$

With exact density, can easily compute exact Kohn-Sham potential:



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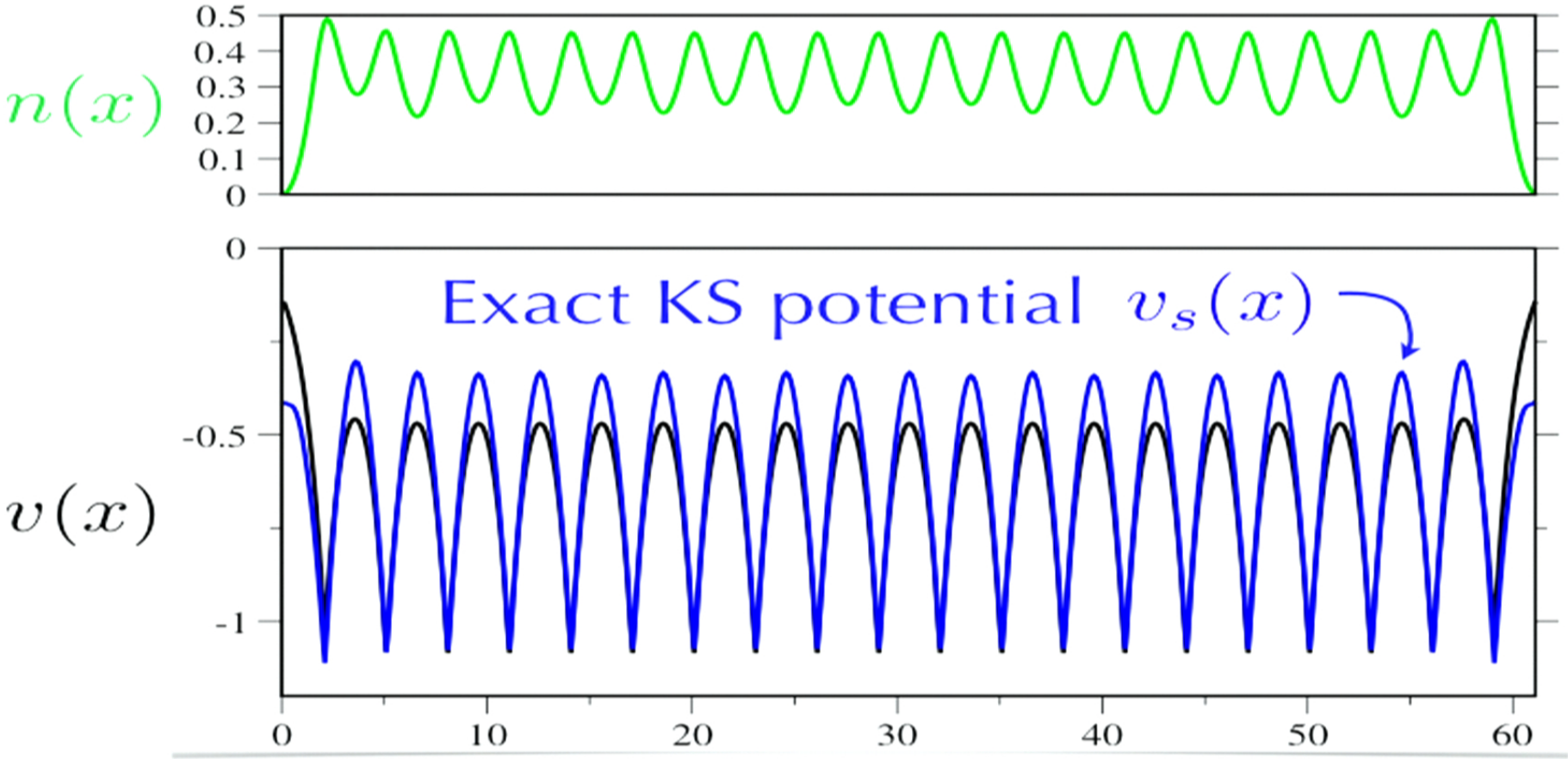


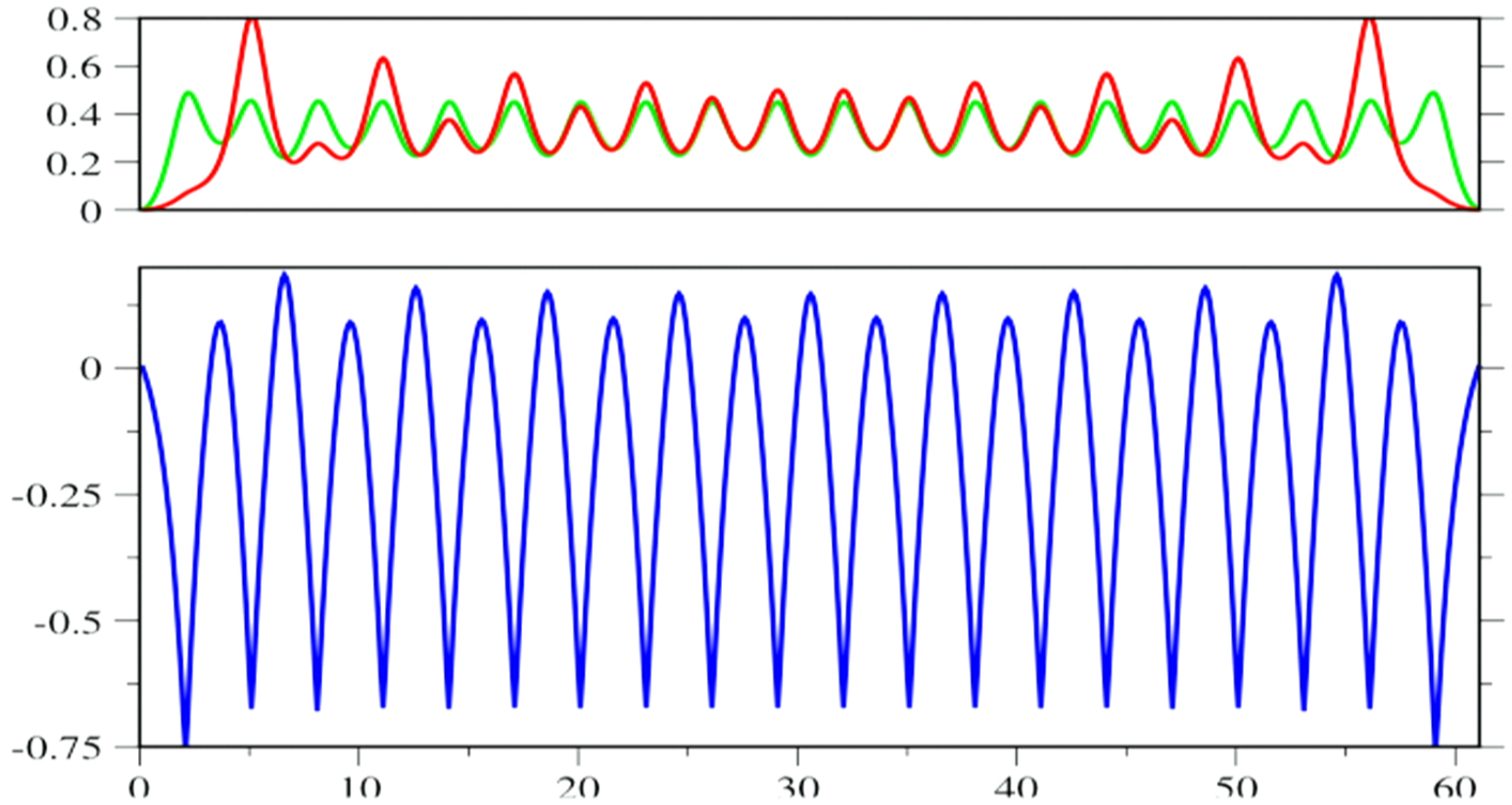
Here's how:

1. Start with guessed Kohn-Sham potential and solve non-interacting problem.

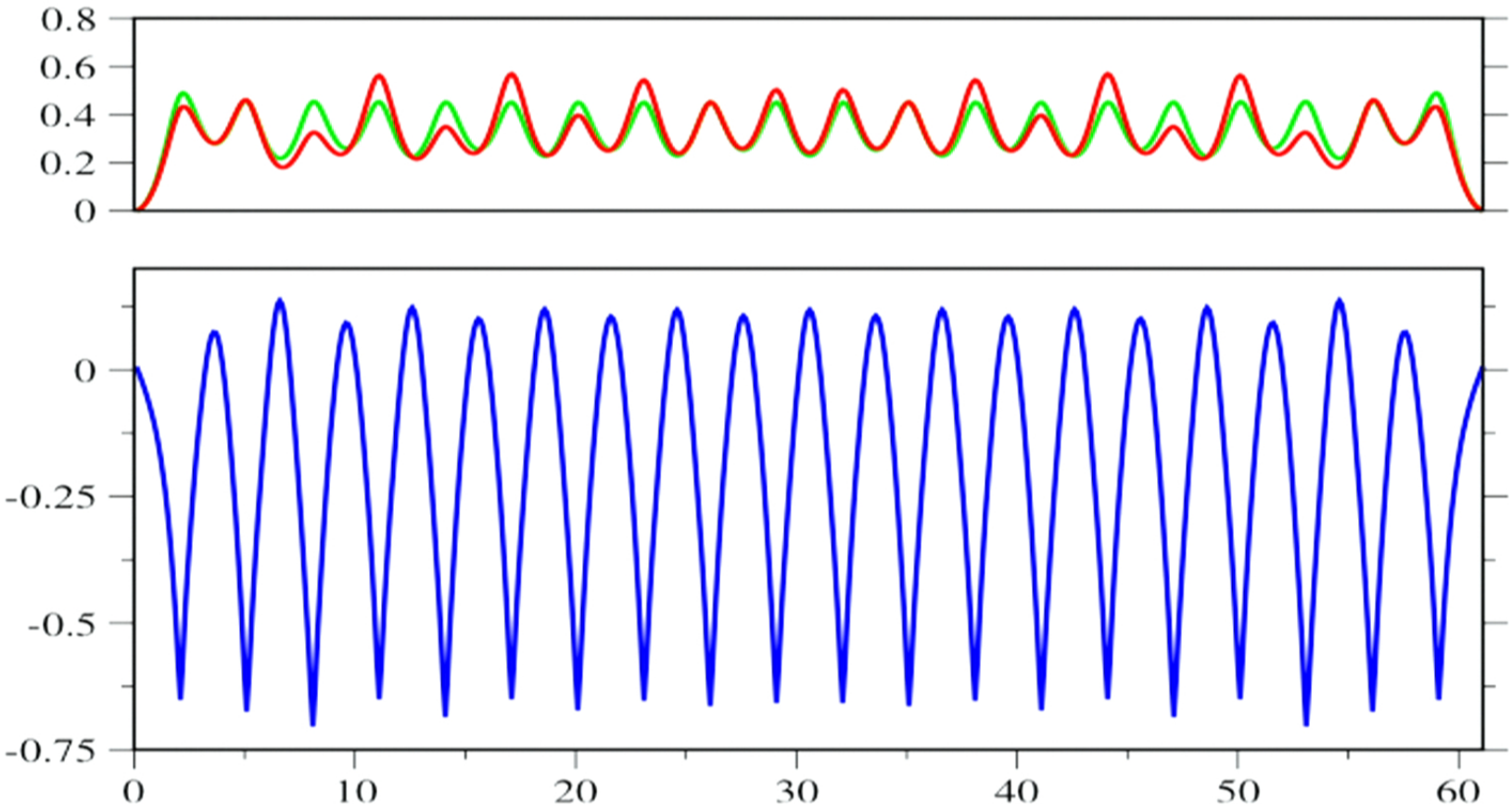
2. Compare resulting density to exact (interacting system) density.

3. Update potential: attempt to reduce $\Delta n(x) = n_{\mathrm{trial}}(x) - n(x)$

Sample Kohn-Sham calculation:



Sample Kohn-Sham calculation:



In practice, divide KS potential into original $v(x)$ plus correction

$$v_s(x) \stackrel{\text{def}}{=} v(x) + v_{\text{HXC}}(x)$$

Mean-field-like picture:

$$\hat{H}_s = \hat{T} + \int_x v_{\text{HXC}}(x)\hat{n}(x) + \int_x v(x)\hat{n}(x)$$

Accounts for missing interactions

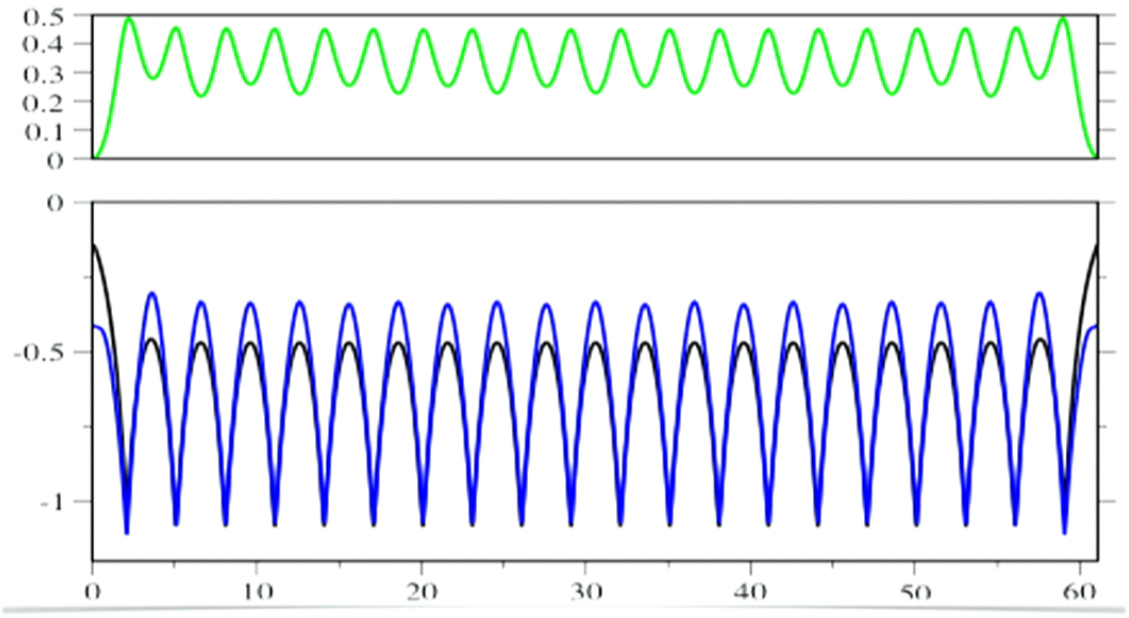
Is DFT a mean-field theory?

No: exact ground-state density and energy
(though approximations used in practice)

Yes: practitioners ask for more (too much?)
by treating band structure as realistic

Is DFT a mean-field theory?

Another key difference:
Mean-field $v_{\mathrm{HXC}}(x)$ reproduces exact density

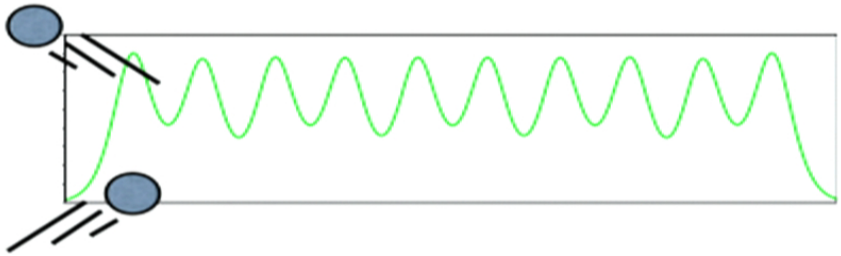


Major issue in DFT:

How good is Kohn-Sham gap for predicting real gap?

Exact Gap

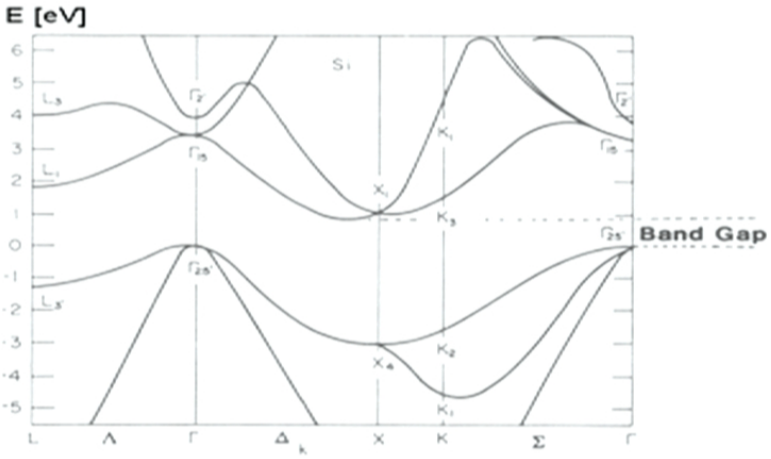
$$E_g = I - A$$



$$I = E_{N-1} - E_N$$

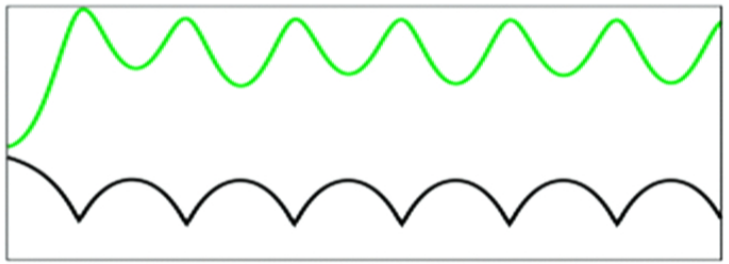
$$A = E_N - E_{N+1}$$

Kohn-Sham Gap

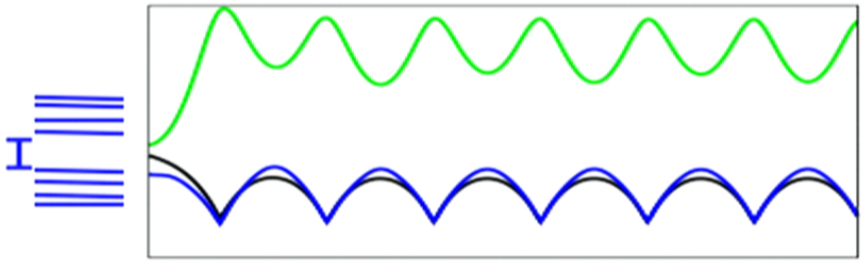


First, hydrogen chains:

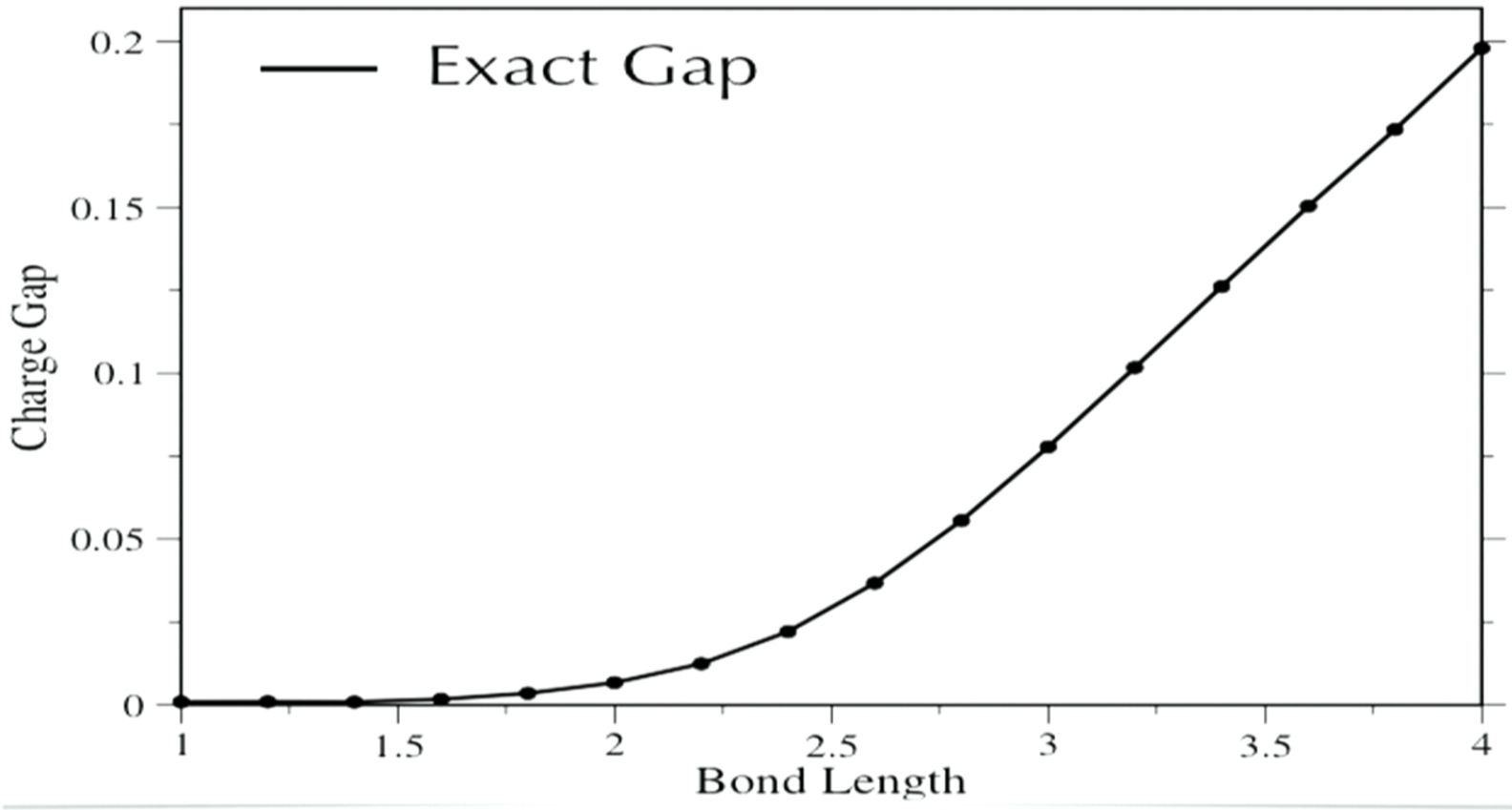
1. Compute exact density of N-electron system.



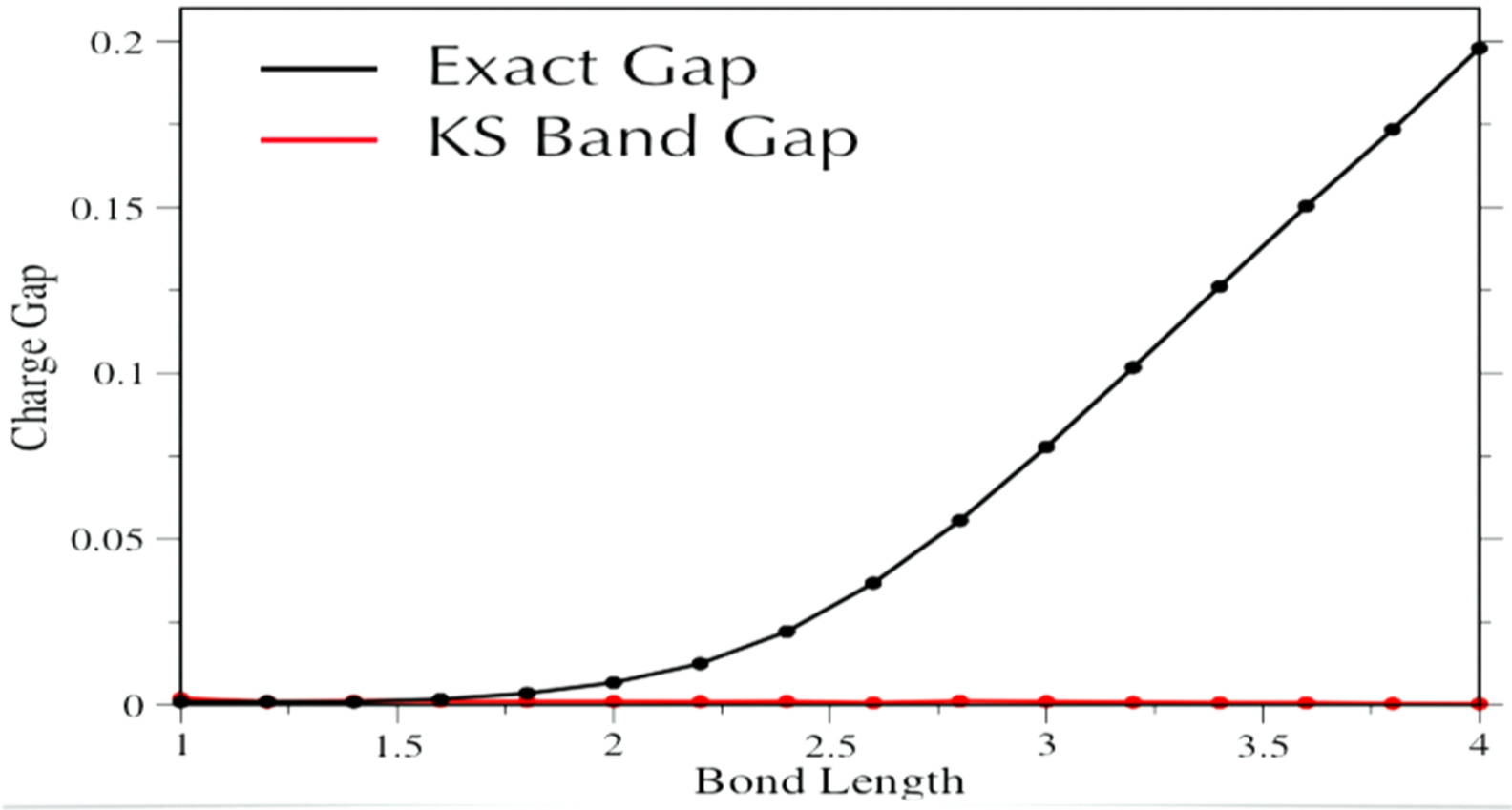
2. Obtain (exact) Kohn-Sham potential and read off Kohn-Sham gap



Resulting Kohn-Sham Band Gaps:



Resulting Kohn-Sham Band Gaps:



How to understand?

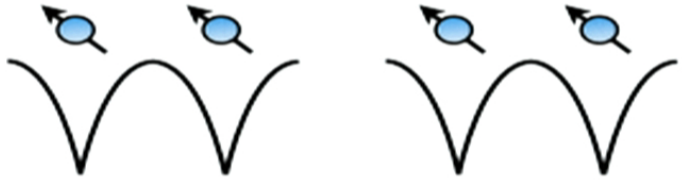
Gapped systems are Mott insulators,
one electron per unit cell

$\Longrightarrow$ lowest band of Kohn-Sham system
is half full

DFT *definition* of a Mott insulator

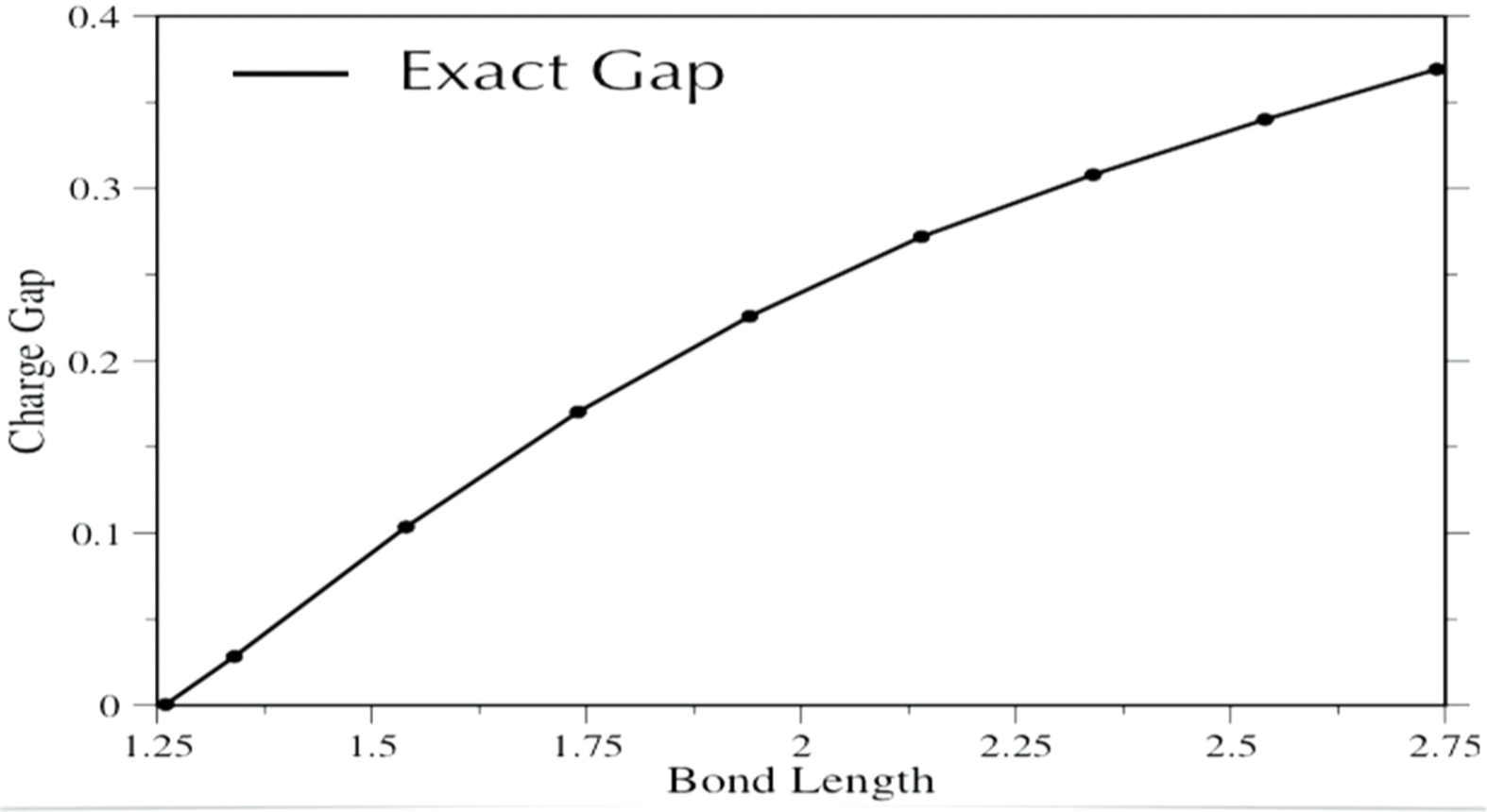
Not a failure of DFT or DFT approx's

Now for H_2 chains, expect Kohn-Sham system can be gapped.

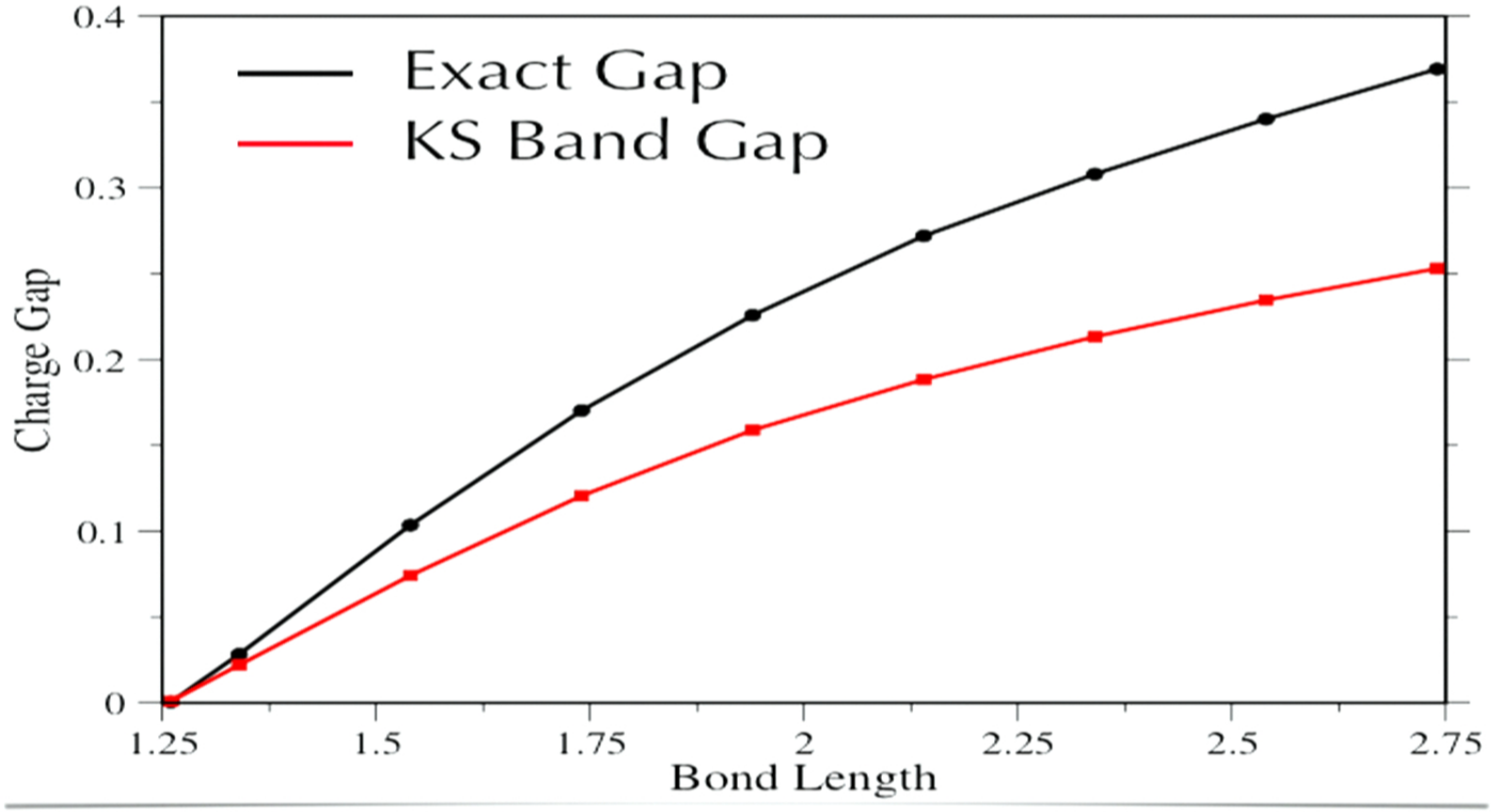


What percent of true gap is KS gap?

H_2 Chain Band Gaps:



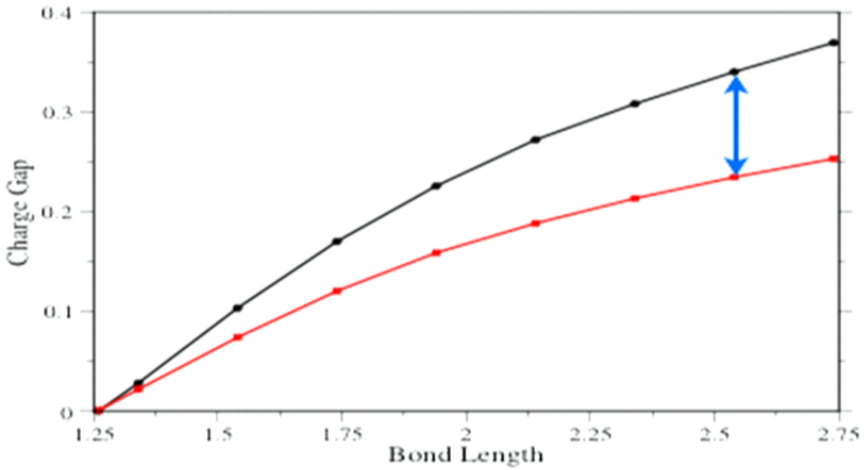
H_2 Chain Band Gaps:



First calculations of this type for extended systems (i.e. matter in thermodynamic limit)

Problem can't be fixed by better approximations alone: inherent to procedure (but not a failure of DFT)

Missing piece known as "derivative discontinuity"; absent from most approximations



Perdew, Parr, Levy, Balduz, PRL **49**, 1691 (1982)

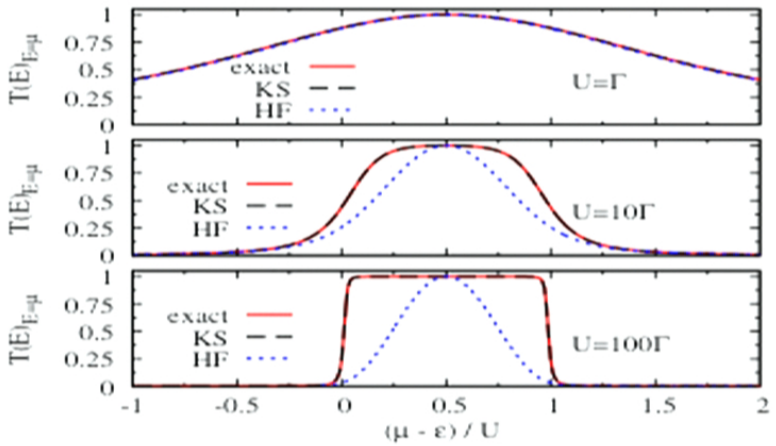
Future Directions

Gaps are an example where *exact* Kohn-Sham system fails to reproduce exact properties.

What about transport?

Common approx: $G(k,\omega) \longrightarrow G^{\mathrm{KS}}(k,\omega)$

Yields exact transport properties of single-impurity Anderson model!



Other models?

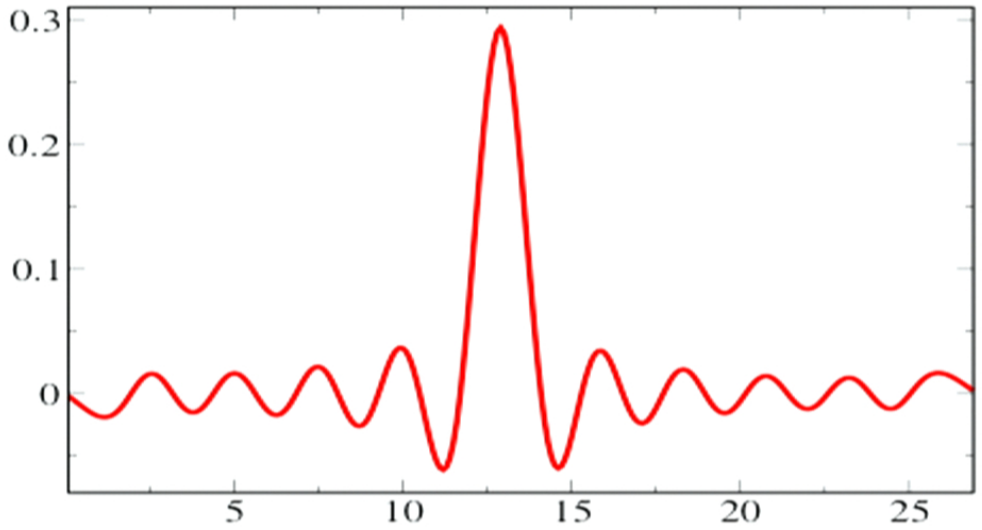
Bergfield et al., Phys. Rev. Lett **108**, 066801 (2012)

Work in progress: exact lattice params

Diagonalize $G_{ij} = \sum_{\sigma} \langle c^{\dagger}_{\sigma i} c_{\sigma j} \rangle$

and localize eigenvectors to form Wannier orbitals

b = 1.2

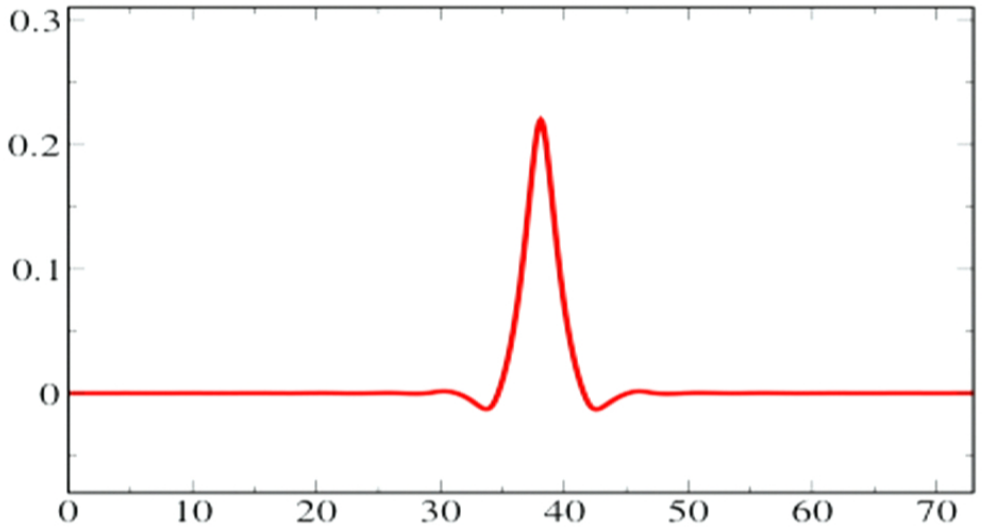


Work in progress: exact lattice params

Diagonalize $G_{ij} = \sum_{\sigma} \langle c^{\dagger}_{\sigma i} c_{\sigma j} \rangle$

and localize eigenvectors to form Wannier orbitals

b = 4.0



Much more to explore:

- DFT approx's such as LDA+U
- Finite-temperature continuum calculations
- Comparison to cold atom experiments