Tailored Density Cumulant Theory

A novel theoretical approach for strongly correlated systems

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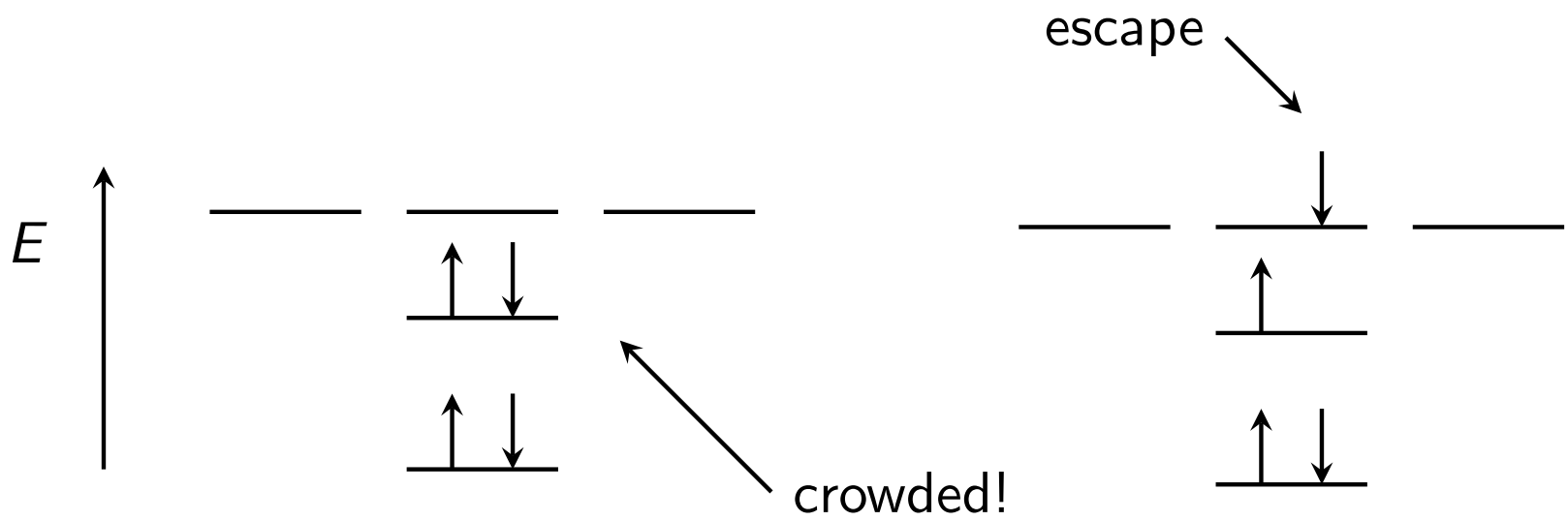
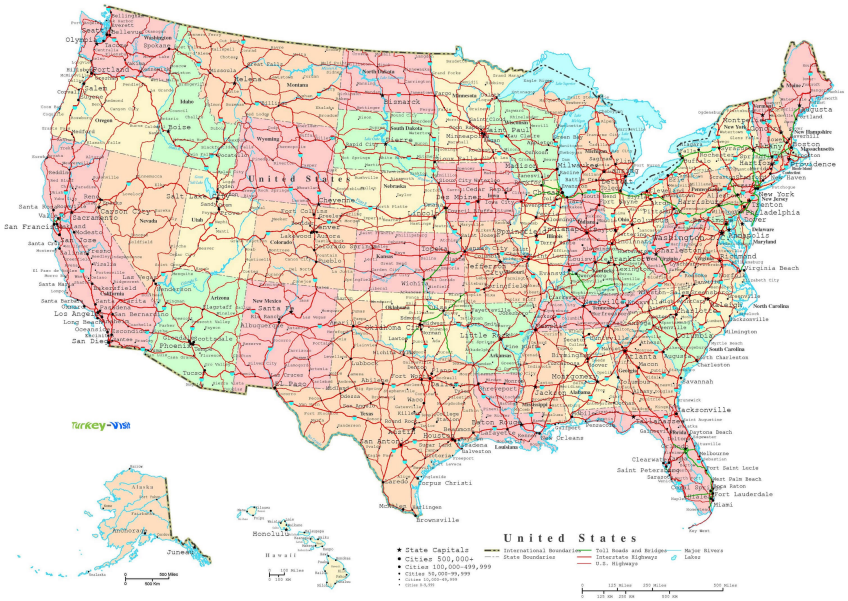
Rule of the game



Electron configurations of Be atom

- Electron correlation is the tendency of electrons to escape from each others.
- Strong correlation occurs when many e^- are likely to be found high up.

A framework based on density cumulant theory



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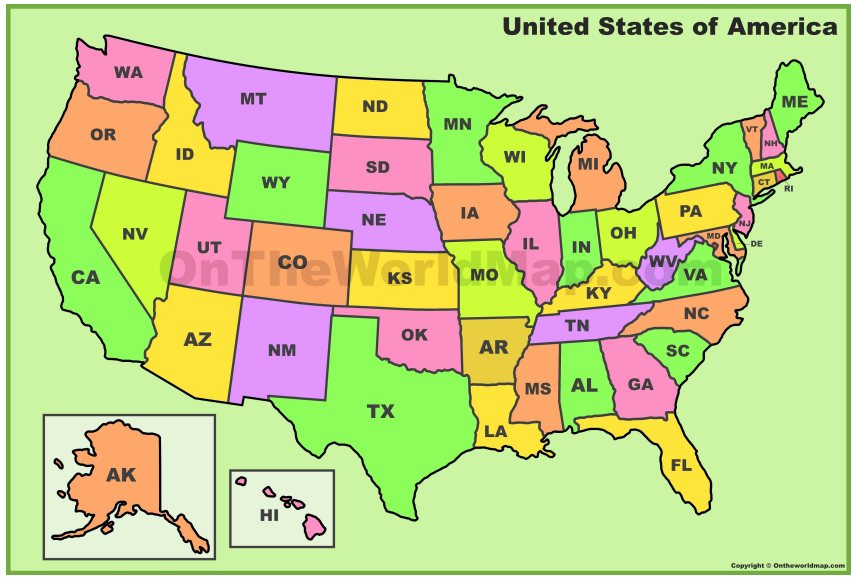

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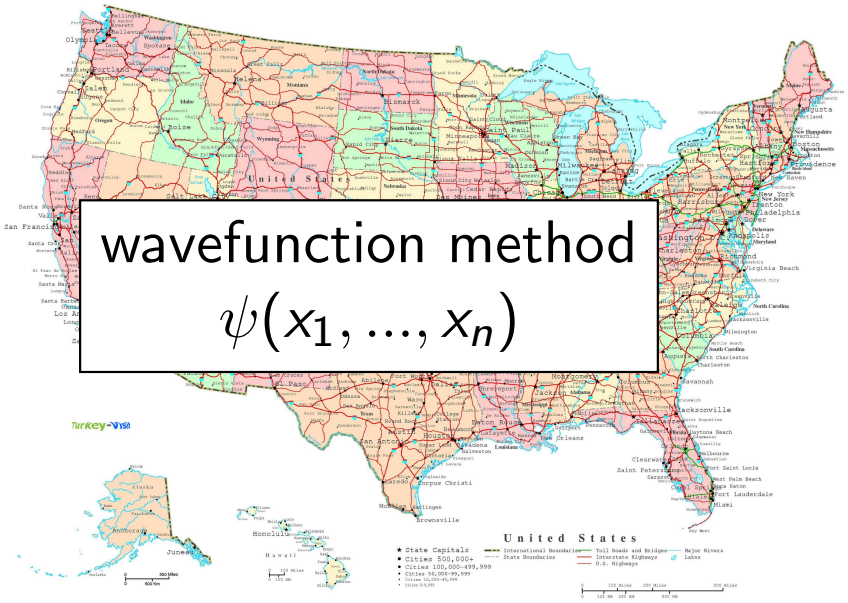
A framework based on density cumulant theory



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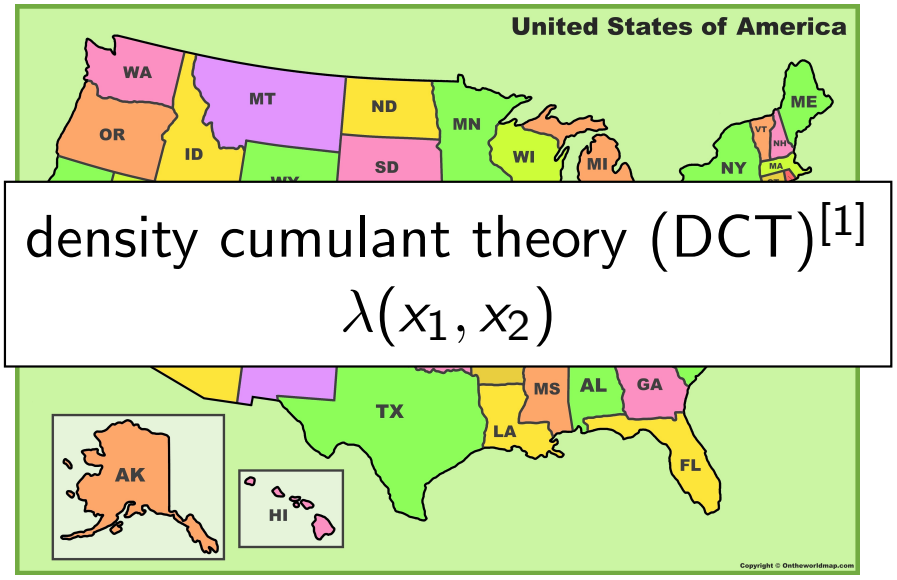

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- DCT is more efficient than existing wavefunction methods.

[1] Werner Kutzelnigg. "Density-cumulant functional theory". J. Chem. Phys. 125, 171101(2006)

DCT breaks down in strong correlation region

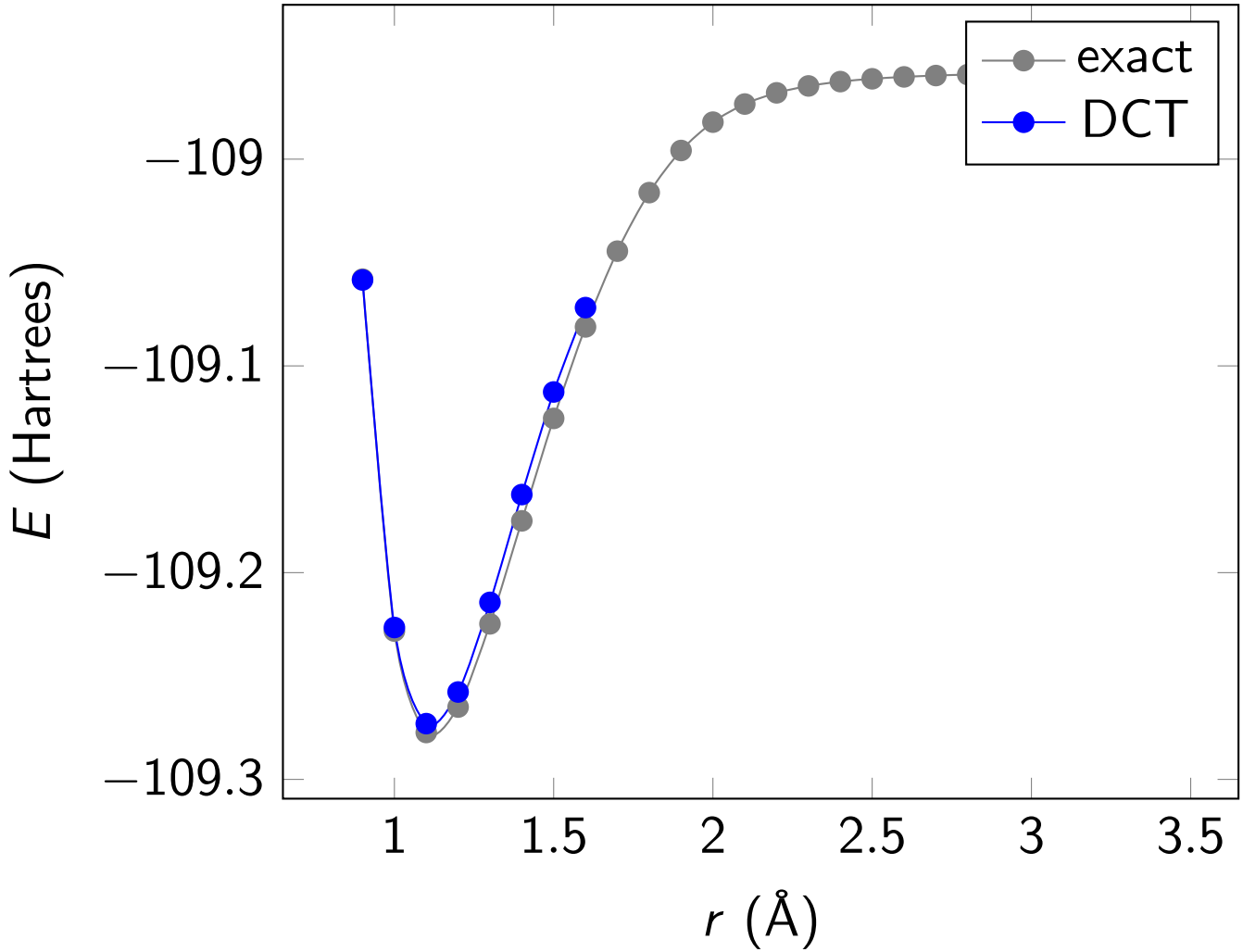


Figure: Energy of N_2 as a function of bond length

DCT breaks down in strong correlation region

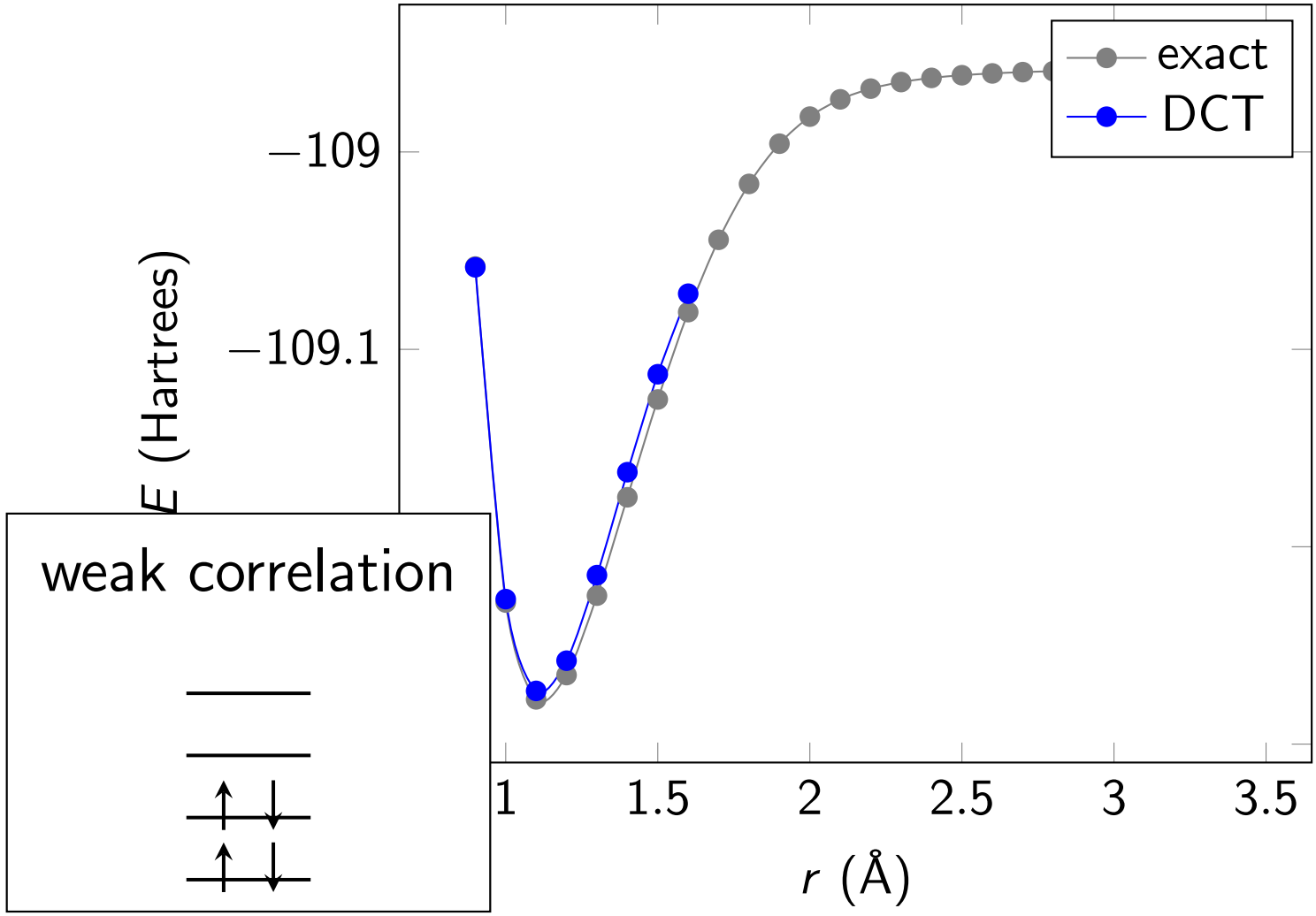


Figure: Energy of N_2 as a function of bond length

DCT breaks down in strong correlation region

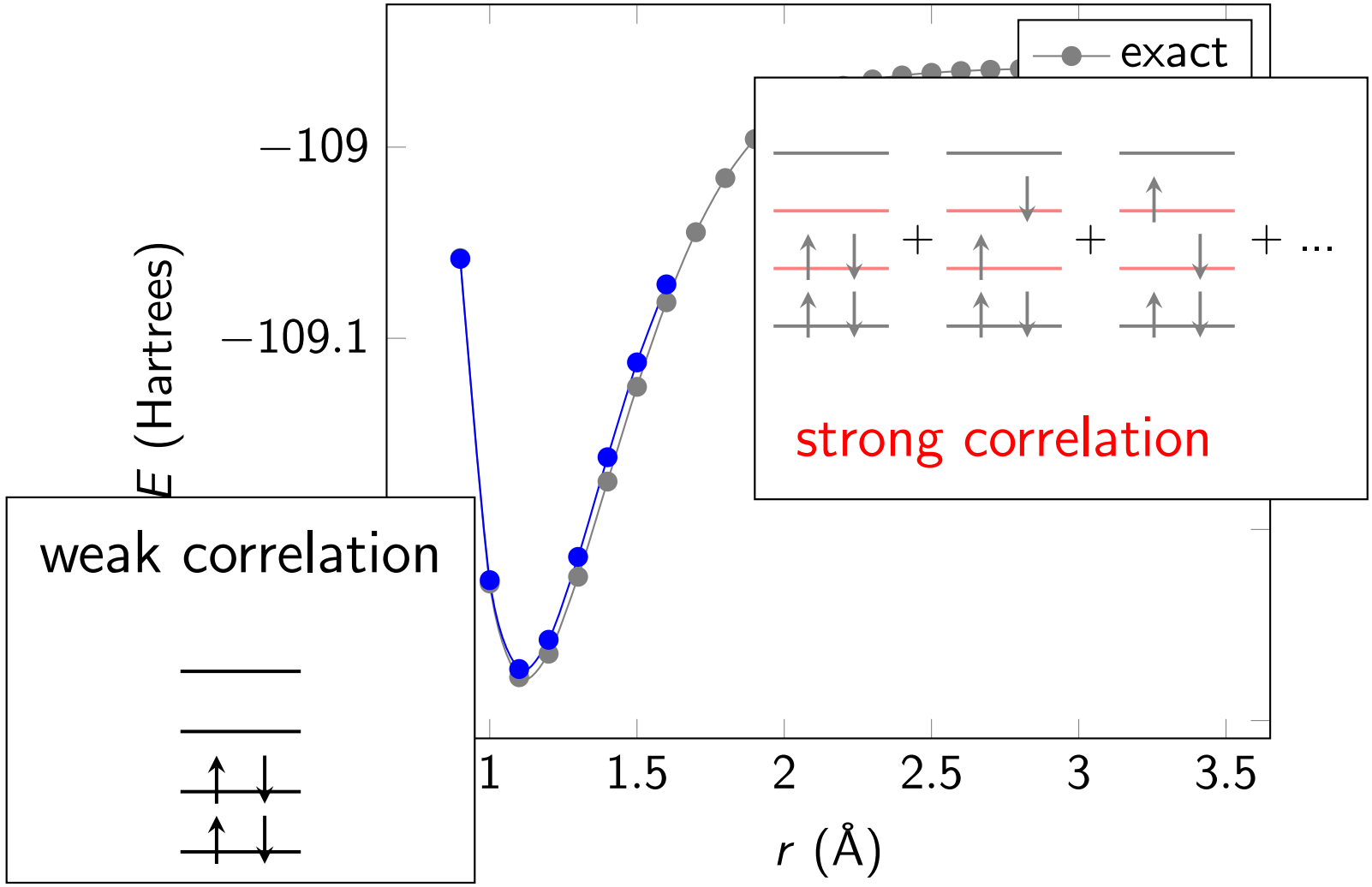
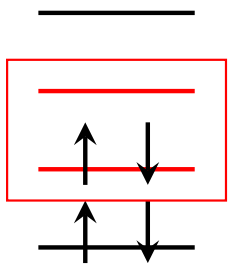
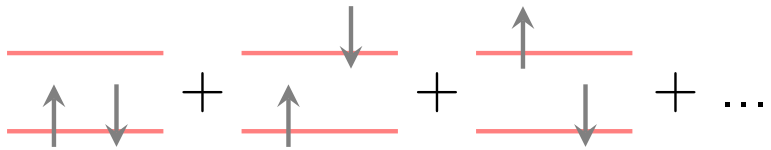


Figure: Energy of N_2 as a function of bond length

Calculated with ccpvdz basis set

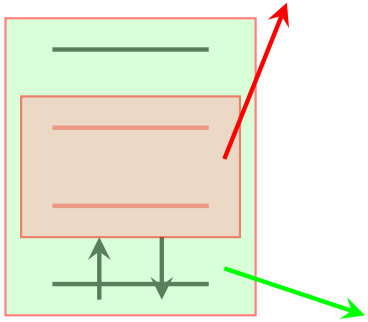
Tailored-DCT algorithm





step 1:
strong correlation using
wavefunction method

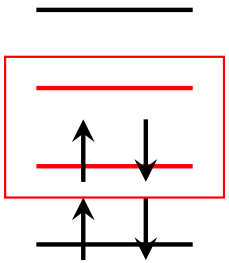
strong correlaton ψ

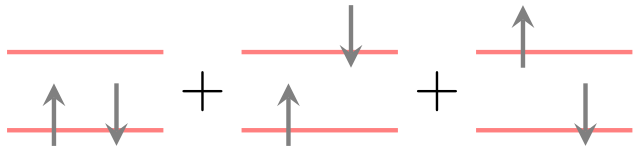


step 2:
additional weak correlation
using DCT

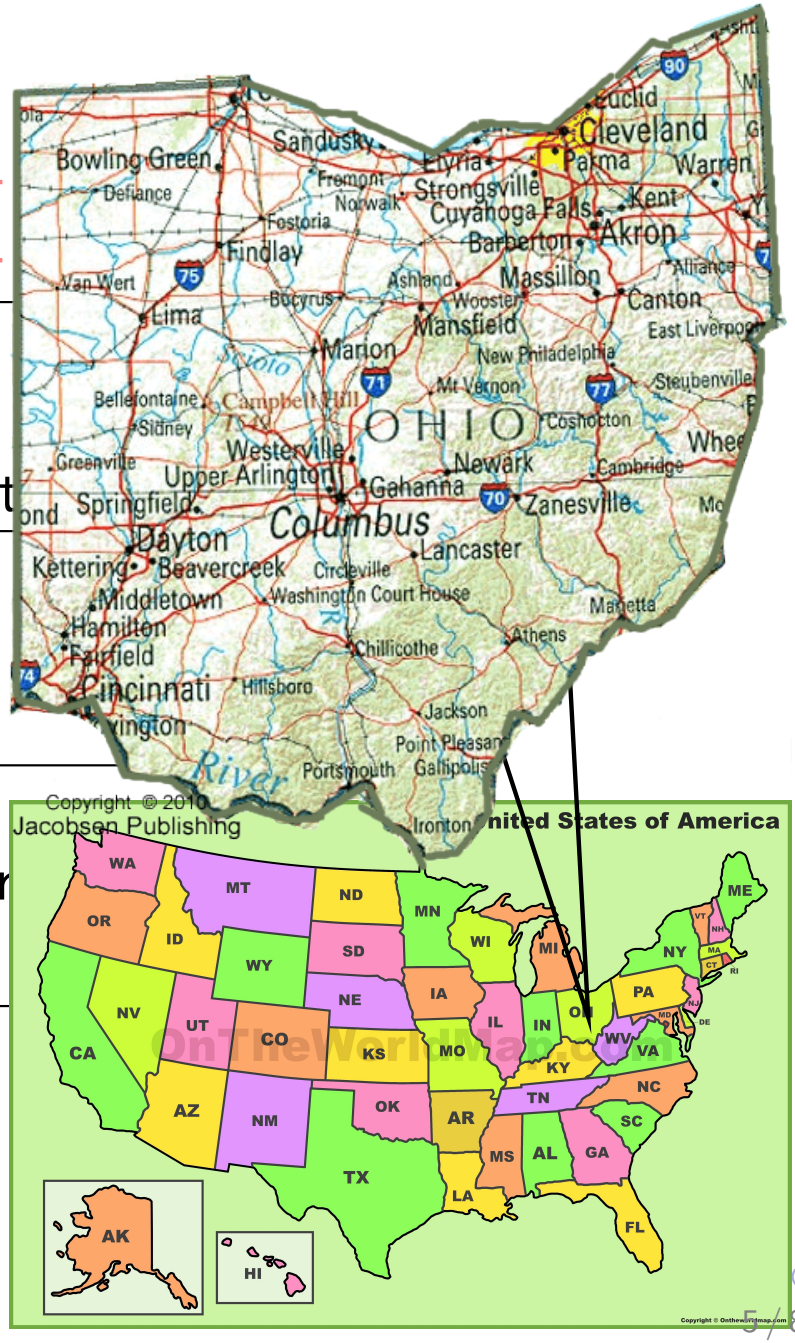
weak correlation λ

Tailored-DCT algorithm



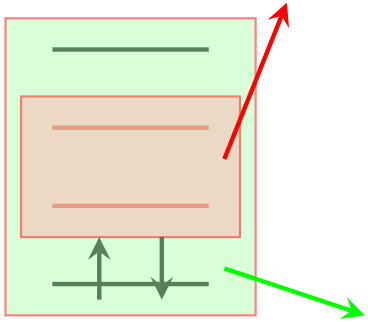


step 1:
strong correlation
wavefunction met



step 2:
additional weak corr
using DCT

strong correlaton ψ



weak correlation λ

Preliminary results and future work

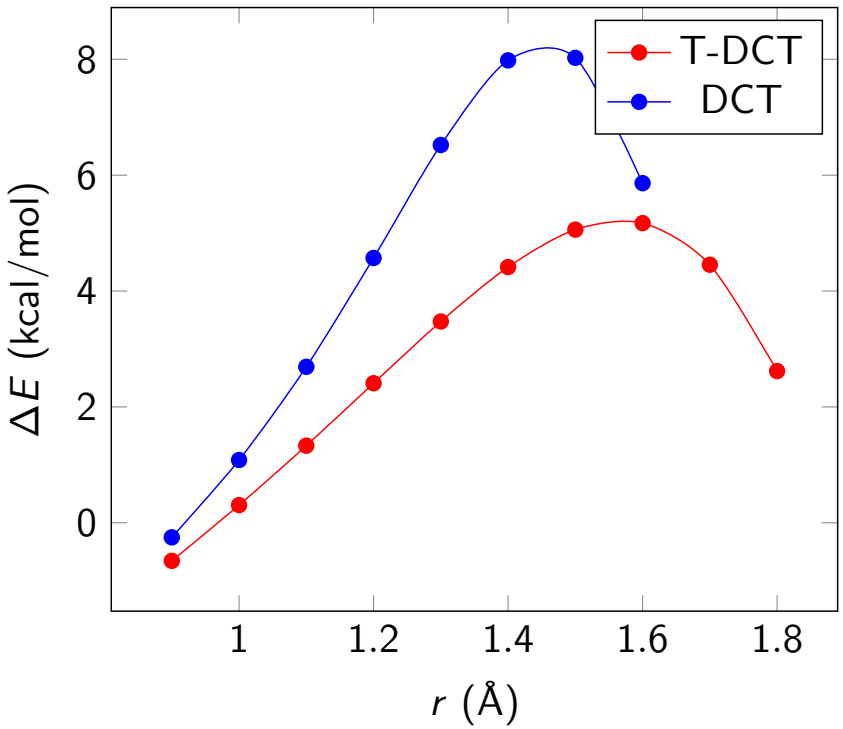


Figure: DCT and T-DCT error for N_2 bond stretching relative to exact energy

- Improvements:
  - reduced energy error.
  - naturally incorporates strong correlation.
- Future work:
  - investigate numerical instability.
  - application to large systems.

Calculated using ccpvdz basis set, 6,6 active space.

Acknowledgment

The Sokolov group

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Ruojing Peng

Computational scheme