Tailored Density Cumulant Theory
A novel theoretical approach for strongly correlated systems

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November 1st, 2018
Rule of the game

Electron configurations of Be atom

- Electron correlation is the tendency of electrons to escape from each other.
- Strong correlation occurs when many $e^-$ are likely to be found high up.
A framework based on density cumulant theory

wavefunction method $\psi(x_1, \ldots, x_n)$
density cumulant theory (DCT)

$\lambda(x_1, x_2)$

DCT is more efficient than existing wavefunction methods.

A framework based on density cumulant theory

- wavefunction method \( \psi(x_1, \ldots, x_n) \)

- density cumulant theory (DCT)\(^1\)
  \[ \lambda(x_1, x_2) \]

▶ DCT is more efficient than existing wavefunction methods.

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 cc-pvdz basis set
Tailored-DCT algorithm

step 1:
strong correlation using wavefunction method

step 2:
additional weak correlation using DCT
Tailored-DCT algorithm

step 1: strong correlation using wavefunction method

step 2: additional weak correlation using DCT

strong correlation $\psi$

weak correlation $\lambda$
Preliminary results and future work

Figure: DCT and T-DCT error for N$_2$ bond stretching relative to exact energy

Calculated using cc-pvdz basis set, 6,6 active space.

- Improvements:
  - reduced energy error.
  - naturally incorporates strong correlation.

- Future work:
  - investigate numerical instability.
  - application to large systems.
Acknowledgment

The Sokolov group

Dr. Alexander Sokolov
Kousik Chatterjee
Samragni Banerjee
Ilia Mazin
Ruojing Peng
Computational scheme

valence-correlated wavefunction

weak correlation between subspaces

relaxation of orbital parameters

recalculate valence strong correlation

valence strong correlation information

converged