

# Outline

- Not a talk about perturbation theory
- Failure of the coupled cluster paradigm
- Understanding the role of symmetry
- Designing solutions based on symmetry restoration
- Alternatives to the exponential ansatz
- Polynomials of excitations that represent PHF
- Polynomial Product States
- Symmetry-projected UCCSD
- CCSD on PHF

## Why is symmetry important ?

- Symmetry implies <u>degeneracy</u> and <u>factorization</u>
- Simplest example: Hydrogen atom spherical symmetry

 $\Psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \varphi), \quad E = E(n), \quad 2n^2 \ degenerate \ states$ 

- Symmetry degeneracy becomes "strong correlation" only when near the Fermi energy; this is flagged by SSB (e.g., UHF atoms down the periodic table)
- Exploiting factorization in electronic structure theory due to symmetry degeneracies (spin, number, point group, etc.) is far from trivial
- This is what we are doing by merging coupled cluster theory with symmetry breaking and restoration ideas
- This talk: progress report on several fronts

# Weak vs Strong Correlation

- Weak correlation :  $|H_1| \rightarrow |H_2|$  (in a loose sense)
  - The mean-field Restricted Hartree-Fock (RHF) picture in the symmetry adapted basis is qualitatively correct.
  - Perturbation theory works (Taylor expansion of the wavefunction).
- Strong correlation :  $|H_1| < |H_2|$ 
  - Physics is determined by the interaction, not the mean-field.
  - **RHF** is bad. Symmetries break spontaneously in **HF**.
  - No good perturbation expansion in **R** basis. Degeneracy rules.
  - Collective behavior becomes important !
  - Range of weak & strong correlations are different
  - In quantum chemistry, the Coulombic repulsive H cannot break number symmetry in mean-field; it does break spin symmetry

# An important remark on HF symmetry breaking

- Stationarity of the HF does not imply a local minimum
- The diagonal of the number conserving (ph-ph) HF instability hessian is instructive:

$$M_{ai,ai}^{t} = \varepsilon_{a} - \varepsilon_{i} - J_{ai} - K_{ai}$$

$$M_{ai,ai}^{c} = \varepsilon_{a} - \varepsilon_{i} - J_{ai} + K_{ai}$$

$$M_{ai,ai}^{s} = \varepsilon_{a} - \varepsilon_{i} - J_{ai} + 3K_{ai}$$

$$J_{ai} > 0$$

$$K_{ai} > 0$$

$$J_{ai} > K_{ai}$$

$$I : occ$$

$$a: unocc$$

- For the hessian to have a negative eigenvalue, a negative diagonal element is sufficient (but not necessary)
- Symmetry breaking can occur with large gaps if J and K are even larger -> strong correlation
- Good example: fullerenes and particularly C<sub>60</sub>

# Weak Correlation Paradigm: Coupled Cluster Theory

CC works very well in weakly correlated situations where symmetries do not break and (symmetry adapted) Restricted Hartree-Fock (RHF) is a good approximation

#### Achieving Chemical Accuracy with Coupled-Cluster Theory

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#### Abstract

Due to formal and computational advances in coupled-cluster theory over the past few years, it is now possible to obtain very accurate molecular geometries, vibrational frequencies, heats of formation, binding energies, and vertical electronic excitation energies. For example, based on statistical analyses of a large number of calculations, it is shown that the CCSD(T)/spdfg level of theory gives  $r_{XH}$ ,  $r_{XY}$  (double bonds), and  $r_{XY}$  (triple bonds) with an average error of 0.0010, 0.0020, and 0.0026 Å, respectively, with the theoretical bond distances usually too long relative to experiment. This level of theory yields bond angle predictions that are too small by 0.21 degrees on average. Fundamental vibrational frequencies predicted at the CCSD(T)/spdfg level of theory are accurate to better than 8.0 cm<sup>-1</sup> on average,

Sometimes referred to as the "gold standard"

# Coupled Cluster theory

 Coupled Cluster theory is based on an exponential ansatz of particle-hole excitations T out of a reference determinant |0>

$$|\Psi\rangle = e^T |0\rangle, \qquad He^T |0\rangle = Ee^T |0\rangle, \qquad T = T_1 + T_2 + T_3 + T_4 + \dots$$

• CC reparametrizes the exact solution (FCI) via an exponential

$$\left| FCI \right\rangle = (1 + C_1 + C_2 + C_3 + C_4 + \dots) \left| 0 \right\rangle = e^{T_1 + T_2 + T_3 + T_4 + \dots} \left| 0 \right\rangle$$

$$C_1 = T_1, \quad C_2 = T_2 + \frac{1}{2!} T_1^2, \quad C_3 = T_3 + T_2 T_1 + \frac{1}{3!} T_1^3$$

$$C_4 = T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{4!} T_1^4$$

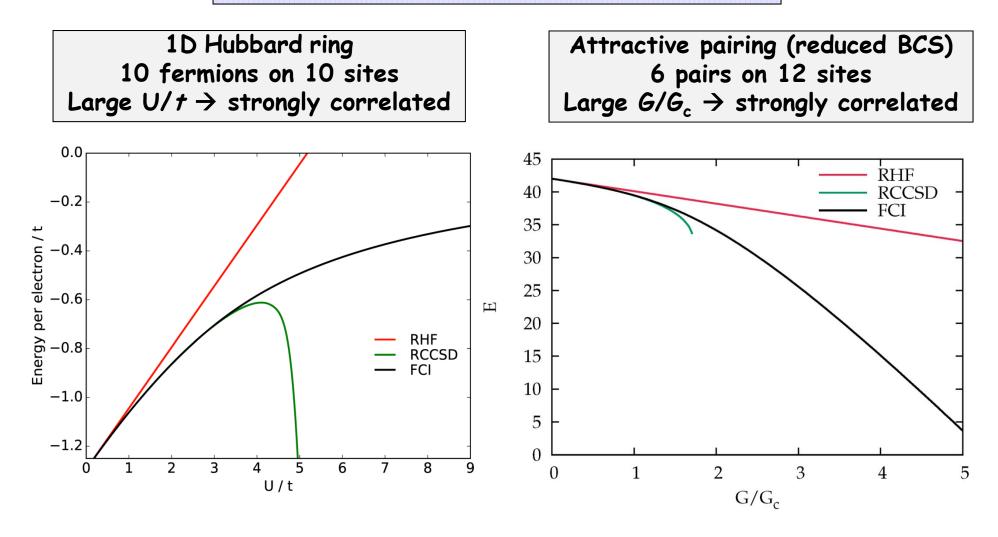
- The Hamiltonian is similarity transformed:  $H = e^{-T} H e^{T}$
- CC yields a set of nonlinear algebraic equations:  $R_n = \langle n | \overline{H} | 0 \rangle = 0$
- To decouple the equations, one neglects high-order connected excitations  $T_{n+1}$  and  $T_{n+2}$  in  $R_n$  ( $T_3$  and  $T_4$  in CCSD)
- Truncated CC retains disconnected higher order excitations.

# **Coupled Cluster theory**

- By retaining disconnected terms, the CC ansatz yields size extensivity, adding terms absent in CI via exponential factorization
- CC computational cost is polynomial as a function of size
- By increasing **n** in  $T_n$ , **CC** yields a series of approximations that <u>eventually</u> gets the right answer for the right reason
- We must truncate  $T_n$  to avoid combinatorial cost and decouple the *CC* algebraic equations
- Truncated CC is not variational

# An incredibly successful theory but...

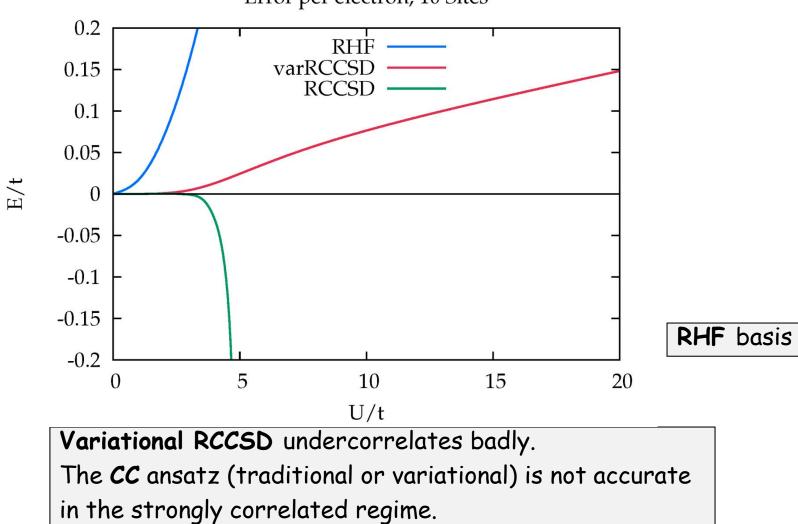
#### **RCC** catastrophic failure



RCCSDT, RCCSDTQ... all fail similarly, except for full CC. Variational RCCSD undercorrelates (next slide; combinatorial cost !)

Variational RCCSD

10x1 Hubbard chain; 10 electrons Error per electron respect to FCI



Error per electron, 10 Sites

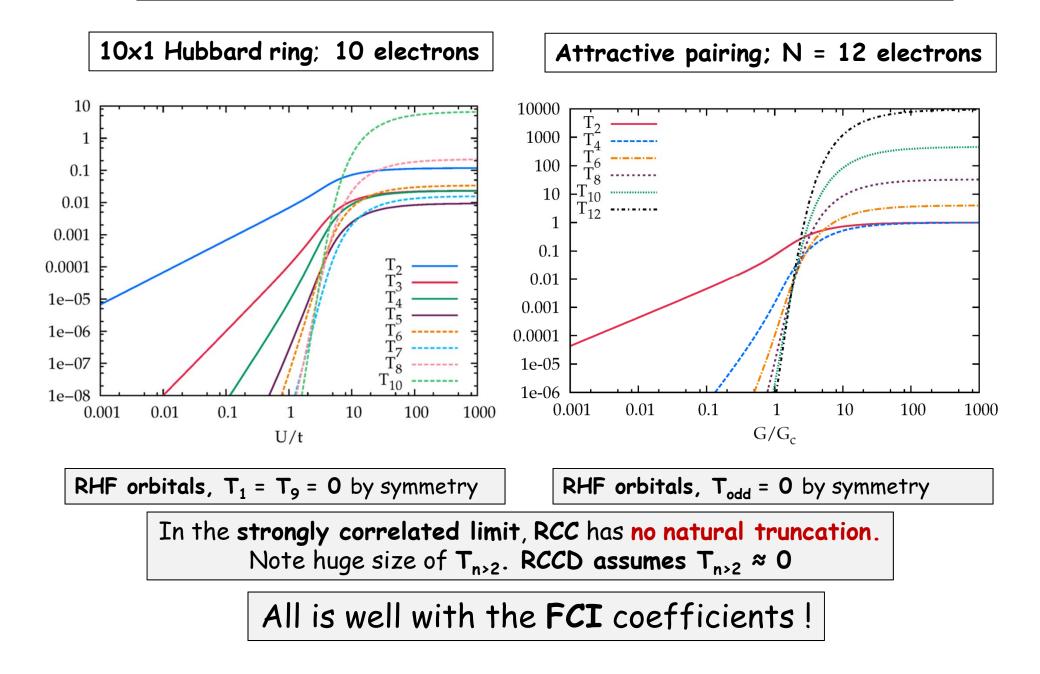
# The problem is to know what the problem is

#### Albert Einstein

The hard part of solving a problem is identifying the problem itself

Why does coupled cluster fail under strong correlation ?

#### RCC reverse-engineered from FCI



Why does coupled cluster fail under SC ?Because decoupling does not work if neglected Tn are largeWhy are the Tn large ?

Because exp[truncated(T)] is a poor approximation to FCI

• Given that the **FCI** coefficients are always small, could there be a better polynomial of excitations?

$$|FCI\rangle = (1 + C_1 + C_2 + C_3 + C_4 + ...)|0\rangle = F(K_1, K_2, K_3, K_4, ...)|0\rangle$$
$$= (1 + K_1 + K_2 + K_3 + K_4 + a_1K_1^2 + a_2K_2^2 + b_2K_3^2 + K_2K_3 + ...)|0\rangle$$

$$C_4 = K_1 + K_2 K_1 + a_2 K_2^2 + a_1 K_2 K_1^2 + a_1^2 K_1^4$$

Where could *F* come from?

- Symmetry collective states because :
- Broken symmetry UCCSD energy is fine
- Strong correlation => symmetry breaking and degeneracy
- Projected HF is exact in SC limit of these model H

## Why is symmetry important?

- Symmetry implies <u>degeneracy</u> and <u>factorization</u>
- Exploiting **factorization** from symmetry (spin, number, point group, etc.) in electronic structure is non trivial
- This is what we are doing via <u>collective states</u>
- In the language of p-h excitations, we have discovered polynomials associated with symmetry projection

## **Reduced BCS Hamiltonian**

$$H = \sum_{p} \varepsilon_{p} N_{p} - G \sum_{pq} P_{p}^{\dagger} P_{q}, \qquad P_{p}^{\dagger} = c_{p\uparrow}^{\dagger} c_{p\downarrow}^{\dagger}, \quad N_{p} = c_{p\uparrow}^{\dagger} c_{p\uparrow} + c_{p\downarrow}^{\dagger} c_{p\downarrow}$$

- In large G limit, PBCS is exact
- Full CC is of course exact but truncated CCD blows up
- The FCI eigenfunction can be rewritten as a non-exp polynomial of <u>only</u> doubles, with factorized amplitudes

$$|FCI\rangle = \exp\left(T_2 + T_4 + T_6 + T_8 + T_{10} + \ldots\right)|RHF\rangle = |F(T_2)|RHF\rangle = |PBCS\rangle$$

$$\begin{split} \left| PBCS \right\rangle &= \widehat{P_N} \left| BCS \right\rangle = \widehat{P_N} \exp Q_1 \left| RHF \right\rangle = \widehat{P_N} \exp \left( \sum_a x^a P_a^{\dagger} \right) \exp \left( \sum_i x_i P_i \right) \left| RHF \right\rangle \\ &= \widehat{P_N} (1 + \sum_i x_i P_i + \frac{1}{2} \sum_{ij} x_i x_j P_i P_j + \dots) (1 + \sum_a x^a P_a^{\dagger} + \frac{1}{2} \sum_a x^a x^b P_a^{\dagger} P_b^{\dagger} + \dots) \left| 0 \right\rangle \\ &= \left( 1 + T_2 + \frac{1}{4} T_2^2 + \dots \right) \left| 0 \right\rangle = F(T_2) \left| RHF \right\rangle, \qquad T_2 = \sum_{ia} x_i x^a P_a^{\dagger} P_i \end{split}$$

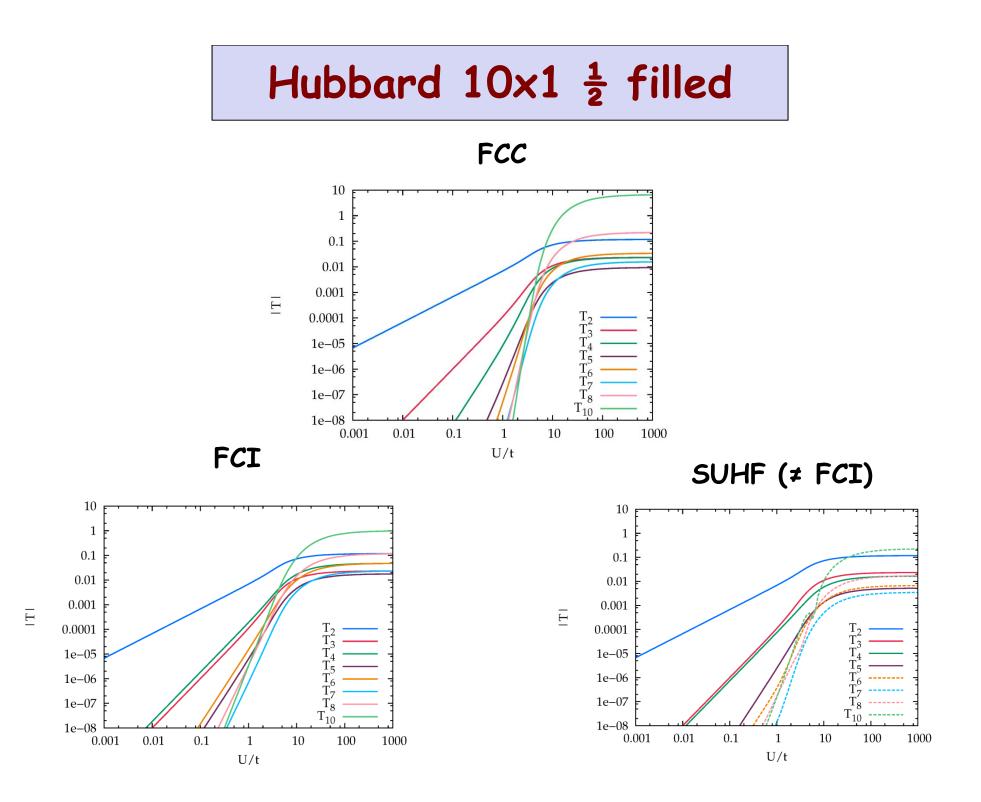
M. Degroote, T. M. Henderson, J. Zhao, J. Dukelsky, and G. E. Scuseria, Phys. Rev. B 93,125124 (2016)

$$\begin{aligned} & \left| SUHF \right\rangle = \widehat{P_s} \left| \phi \right\rangle = \widehat{P_s} e^{\mathcal{Q}_{1s}} \left| 0 \right\rangle = F_s \left| 0 \right\rangle = (1 + K_{2s} + \frac{3}{10} K_{2s}^2 + ...) \left| 0 \right\rangle \\ & \mathcal{Q}_{1s} = \sum_{ia} q_i^a \left( c_{a\uparrow}^{\dagger} c_{i\uparrow} - c_{a\downarrow}^{\dagger} c_{i\downarrow} \right), \qquad K_{2s} = -\frac{1}{6} \sum_{ijab} \left( q_i^a q_j^b + 2q_i^b q_j^a \right) E_a^i E_b^j \\ & \left| E_a^i = c_{a\uparrow}^{\dagger} c_{i\uparrow} + c_{a\downarrow}^{\dagger} c_{i\downarrow} \right| \end{aligned}$$

 $|\phi\rangle$  is broken symmetry,  $|0\rangle$  is symmetry adapted  $Q_{1S}$  breaks spin symmetry and transforms RHF into UHF Symmetry projection is here done analytically  $K_{2S}$  factorizes.  $E_a^{\ i}$  are symmetry adapted (totally symmetric)

SUHF has  $a_2 = 3/10$ , PBCS has  $a_2 = \frac{1}{4}$ , CC has  $a_2 = \frac{1}{2}$  (fails under SC) The change in  $a_2$  with interaction regime is a renormalization effect. These results can be used to merge CC with Projected HF

M. Degroote, T. M. Henderson, J. Zhao, J. Dukelsky, and G. E. Scuseria, *Phys. Rev.* B 93,125124 (2016).
Y. Qiu, T. M. Henderson, and G. E. Scuseria, *J. Chem. Phys.* 146, 184105 (2017).
T. M. Henderson and G. E. Scuseria, *Phys. Rev.* A 96, 022506 (2017).



#### Spin Polynomial Similarity Transformation

• SPoST is an interpolation between CCSD and SUHF

$$\mathbf{F}(T_2) = 1 + T_2 + a_2 T_2^2 + a_3 T_2^3 + \dots$$

Hamiltonian is similarity transformed

$$\overline{H} = F^{-1}(T_2)H F(T_2)$$

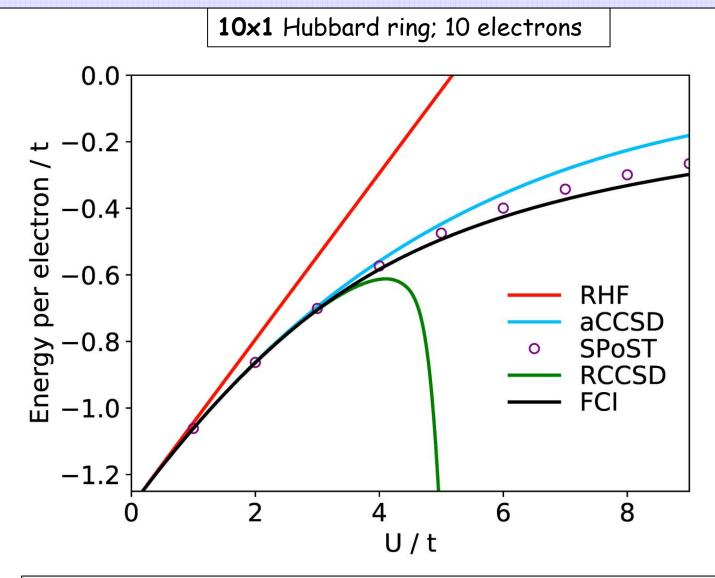
•  $a_2$  and  $T_2$  are optimized using CC-like equations

- **aCCSD** identifies collective mode(s) by diagonalizing  $T_2 = K_2 + S_2$
- The largest eigenvalue mode  $(K_2)$  is treated with the symmetry polynomial  $F(K_2)$  while the rest of the modes uses  $exp(S_2)$

$$\overline{H} = e^{-S_2} \mathbf{F}^{-1}(K_2) H \mathbf{F}(K_2) e^{S_2}$$

J. A. Gomez, M. Degroote, J. Zhao, Y. Qiu, and G. E. Scuseria, *Phys. Chem. Chem. Phys.* **19**, 22385 (2017). J. A. Gomez, T. M. Henderson, and G. E. Scuseria, *Mol. Phys.* **115**, 2673 (2017).

### Merging spin collective states with CCSD



**Proof of Principle: aCCSD** and **SPoST** are qualitatively correct (and symmetry adapted)

#### Polynomial Product States

- Consider an ansatz composed of products of polynomials of particlehole excitations that preserve (T) or break (Q) symmetries
- Symmetry-project broken-symmetry terms

$$\widehat{P}(e^{Q_1+Q_2+\dots}) = F(K) = I + K + a_2K^2 + a_3K^3 + \dots$$

• Similarity-transform

$$\overline{H} = \mathbf{F}^{-1}(K)e^{-T}H e^{T}\mathbf{F}(K)$$

Solve via CC-like equations

$$E = \langle 0 | \overline{H} | 0 \rangle, \quad 0 = \langle n | \overline{H} | 0 \rangle$$

More general than attenuated CC or PoST



- **PPS** are size extensive and different from **CC**
- In TDL only linked diagrams (CC) survive but the CC weight gets renormalized by F(K)
- PPS carry "rank-n extensivity" associated with the 'n' in  $Q_n$

## Take II: broken symmetry

#### • Smoking gun:

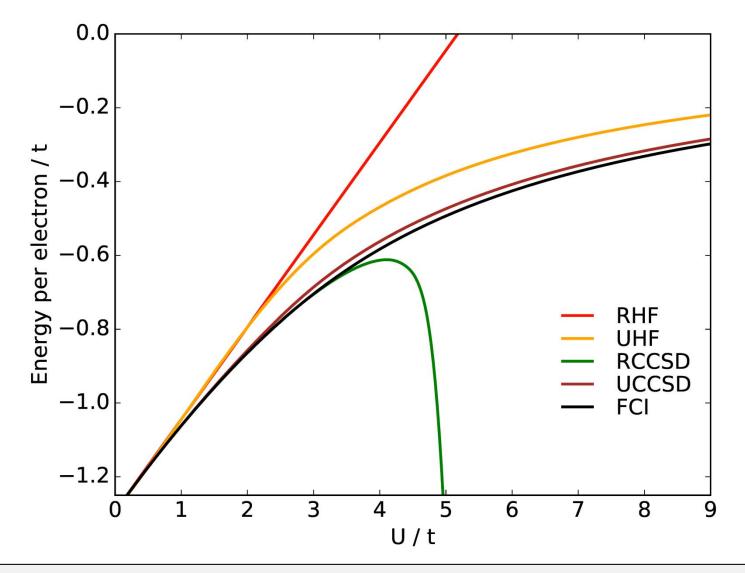
If we allow spin symmetry to break (RHF  $\rightarrow$  UHF) the UHF energy is fine and even better at the UCC level .

- But the wave function has wrong quantum numbers!
- Symmetry dilemma:

Symmetries can be broken to improve the energy but the road to eigenfunctions can be full of obstacles

- Close connection among symmetry breaking, degeneracy & strong correlation
- Let's see what happens in the broken symmetry basis

#### Broken spin symmetry picture



UHF and UCCSD energies are fine but we lose good quantum numbers Inspection of  $U_3$ ,  $U_4$ , etc., shows that they are small

# S<sup>2</sup> projection: SUHF

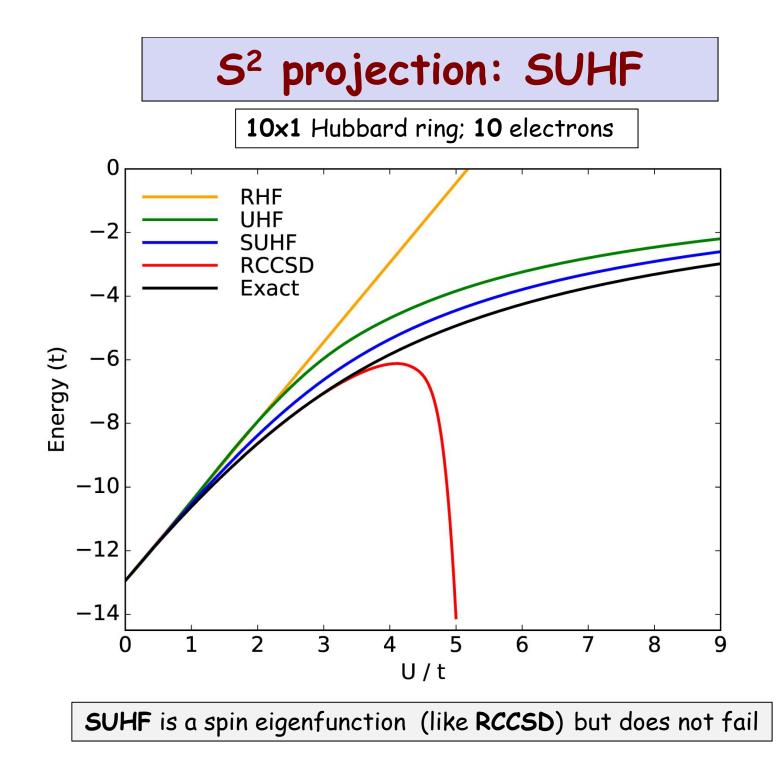
• Spin restoration is done imposing rotational invariance in spin space using a projection operator  $\hat{P}$  acting over broken symmetry determinants  $e^{i\beta\hat{S}_{y}}|\phi\rangle$   $\left|SUHF\rangle = \hat{P}|\phi\rangle = \int_{0}^{\pi} d\beta \sin\beta e^{i\beta\hat{S}_{y}}|\phi\rangle$ 

• SUHF  $\rightarrow$  non-orthogonal determinants in the broken symmetry basis  $\rightarrow$  collective excitations in symmetry adapted basis.

$$\left\langle \phi \right| e^{i\beta \hat{S}_{y}} \left| \phi \right\rangle = \left\langle \phi \right| \beta \right\rangle \neq 0$$

- Spin projection has a long history (Löwdin 1955) but never took off
- Our work on symmetry breaking and restoration :
  - Number and Spin (both  $S^2$  and  $S_z$ ) (continuous)
  - Complex Conjugation and Point Group (discrete)
  - Linear Momentum and Space Group in periodic systems

J. Chem. Phys. 135, 124108 (2011), J. Chem. Phys. 136, 164109 (2012), J. Chem. Phys. 139, 204102 (2013).



#### Spin Projected UCCSD

$$H\widehat{P}e^{U_1+U_2}|\phi\rangle = E\widehat{P}e^{U_1+U_2}|\phi\rangle \qquad \widehat{P} = \int_0^{\pi} d\beta \sin\beta e^{i\beta\hat{S}_y}$$

The merge seems simple but there is a fundamental language barrier:

- CC is built from orthogonal p-h excitations
- Symmetry projection uses **non-orthogonal** determinants

#### Main result of our work: disentangled cluster formalism

$$e^{i\beta\hat{S}_{y}}e^{U_{1}+U_{2}}|\phi\rangle = e^{W_{0}(\beta)}e^{W_{1}(\beta)+W_{2}(\beta)+W_{3}(\beta)+\dots}|\phi\rangle$$

 $W_0(\beta)$  is a constant. The  $W_n(\beta)$  are purely excitation operators. They restore symmetry.

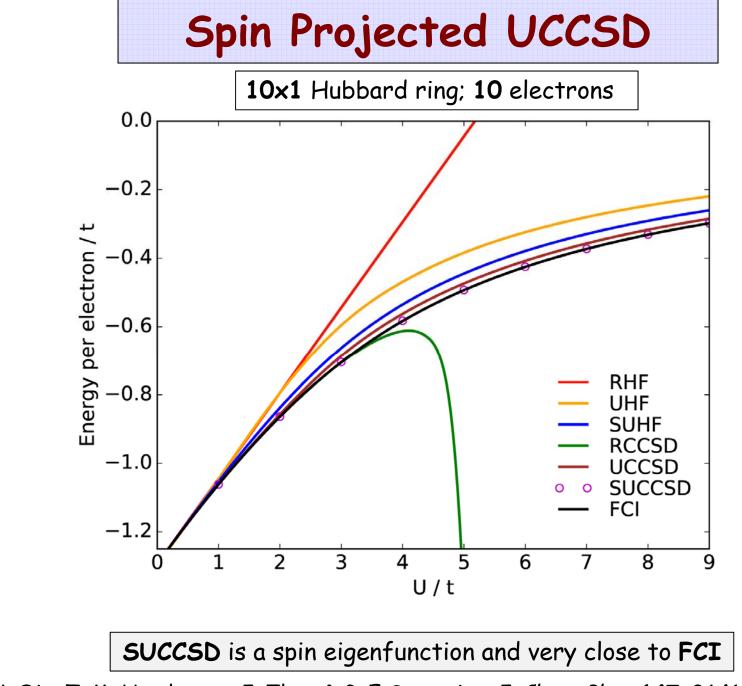
They afford truncation in the spirit of UCC theory.

At  $\beta = 0 \implies W_1(0) = U_1, \quad W_2(0) = U_2, \quad W_{n>2}(0) = 0$ 

 $W_n(\beta)$  are obtained solving differential equations in su(2)

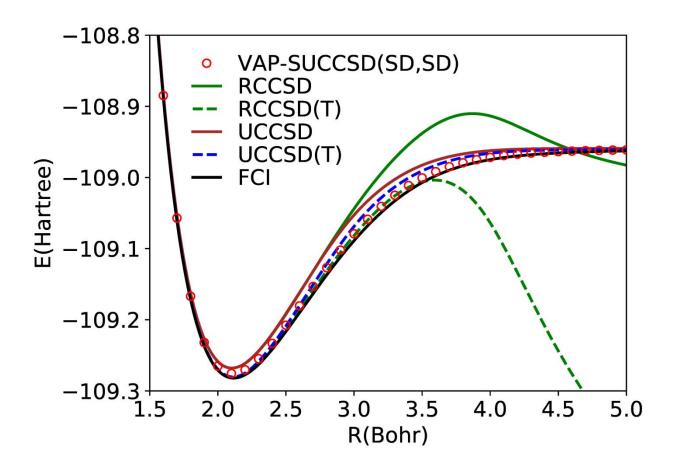
T. Duguet, J. Phys. G 42, 025107 (2015)

Y. Qiu, T. M. Henderson, J. Zhao & G. E. Scuseria, J. Chem. Phys. 147, 064111 (2017)



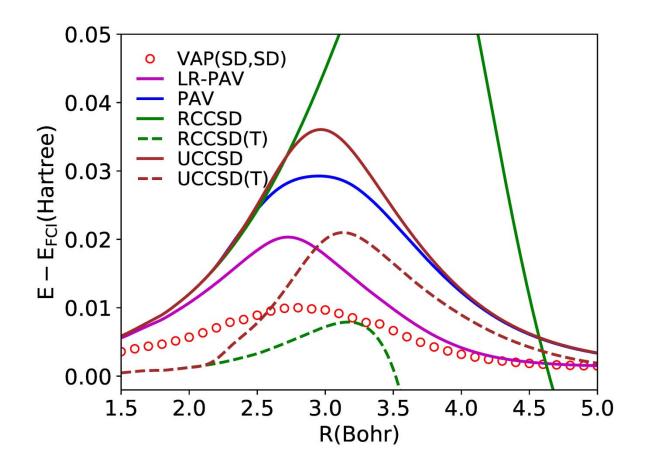
Y. Qiu, T. M. Henderson, J. Zhao & G. E Scuseria, J. Chem. Phys. 147, 064111 (2017)

# N<sub>2</sub> dissociation cc-pvdz



Y. Qiu, T. M. Henderson & GES, work in progress

# N<sub>2</sub> dissociation cc-pvdz



Y. Qiu, T. M. Henderson & GES, work in progress

### Take III: CCSD on PHF

$$E = \frac{\langle SUHF | (1+Z)e^{-T}He^{T} | SUHF \rangle}{\langle PHF | PHF \rangle}$$
$$0 = \langle SUHF | \widehat{T}^{\dagger}e^{-T} (H-E)e^{T} | SUHF \rangle$$
$$|SUHF \rangle = \widehat{P} | \phi \rangle = \int_{0}^{\pi} d\beta \sin\beta e^{i\beta \widehat{S}_{y}} | \phi \rangle$$

- SUHF is done variationally and CCSD non-variationally
- Conceptually the simplest model but SUHF 6-rdm is scary!
- Requires grid integration over rotated states
- Not implemented until recently, after *drudge* was born

# CCSD on PHF by drudge\*

When robots do the algebra and write the code, the **6-rdm** is no longer intimidating.

Algebraic manipulators can be instrumental in implementing algebraic involved theories.

\* Jinmo Zhao & GES (unpublished)

 $\underset{p \in L}{\succeq} 2 \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{\underset{p \in L}{2}} \xrightarrow{\alpha \text{ or renormal }} \underset{p \in L}{2} \xrightarrow{\alpha \text{ or renorm$  $\sum_{p \in L} \frac{G}{2} u_{p_2}^2 v_{p_2}^2 v_{p_2}^2 v_{p_2} t_{p_2} t_{p$  $\sum_{p \in L} 2Gu_{p_1}^2 u_{p_2}^3 v_{p_1}^4 u_p v_{p_2} t_{p_1,p} t_{p_1,p_2} t_{p_1,p_2} t_{p_1,p_2} t_{p_2,p_1} t_{p_1,p_1} t_{p_2,p} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^4 v_{p_2}^4 u_p u_{p_2} v_{p_1} t_{p_2,p_1} t_{p_2,p_1} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^4 v_{p_2}^4 u_{p_2} v_{p_1} t_{p_1,p_1} t_{p_2,p_1} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^4 v_{p_2}^2 u_{p_2} v_{p_1} t_{p_1,p_1} t_{p_2,p_1} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^4 v_{p_2}^2 u_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^4 v_{p_2}^2 u_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_2}^4 v_{p_2}^2 u_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_2}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_2}^2 v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_2} v_{p_2} v_{p_2} v_{p_2} v_{p_1} t_{p_2,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_2} v_{p_2}$  $\sum_{p \in L} 2Gu_{p_1}^2 u_{p_2}^2 v_{p_2}^4 u_{p_1} v_{p_2} v_{p_3} t_{p_{2p}} t_{p_{2p}} t_{p_{2p}} t_{p_1} v_{p_2} v_{p_1} t_{p_{2p}} v_{p_1} t_{p_{2p}} v_{p_1} t_{p_{2p}} v_{p_1} t_{p_{2p}} t_{p_$  $+ 2Gu_{p_1}^2v_{p_1}^2v_{p_2}^2t_{p_1,p_1}^2 + 2Gu_{p_1}^2v_{p_1}^2t_{p_1,p_2} + 2Gu_{p_2}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1}^2 + 2Gu_{p_2}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_2}^2 + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2t_{p_1,p_1}^2 + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1}^2v_{p_1}^2t_{p_1,p_1} + 3Gu_{p_1}^4v_{p_1}^2v_{p_1$  $-\frac{G}{2}u_{\mu}^{2}u_{\mu}^{5}v_{\mu}^{2}t_{\mu_{1},\mu_{1}}t_{\mu_{2},\mu_{2}}t_{\mu_{2},\mu_{2}} - \frac{1}{2}u_{\mu}^{2}v_{\mu}^{2}t_{\mu_{2},\mu_{2}}t_{\mu_{2},\mu_{2}}t_{\mu_{1},\mu_{1}}t_{\mu_{2},\mu_{1}}t_{\mu_{1},\mu_{1}}t_{\mu_{2},\mu_{1}}t_{\mu_{1},\mu_{1}}t_{\mu_{2},\mu_{2}}t_{\mu_{2},\mu_{2}}t$  $\sum_{q \in L} \frac{G}{4} \delta_{p_1 p_2} u_{p_1}^2 u_{q}^2 v_{p}^2 v_{p_1}^2 u_{q}^2 v_{p}^2 v_{p_1}^2 u_{p_1}^2 u_{q}^2 v_{p}^2 v_{p_1} u_{q_1} u_{p_1}^2 u_{p_2}^2 u_{p_2}^2 u_{p_1}^2 u_{p_1}^2 u_{p_2}^2 u_{p_1}^2 u_{p_1}^2$  $\sum_{q \in L} Gu_p^2 u_p^2 v_p^2 v_p^2 u_q u_q t_{p,p_1} t_{p_2 p} + \sum_{p \in L} Gu_p^2 v_p^2 v_p^2 v_p^2 u_q^2 u_q t_{p,p_1} t_{p,p_2} + \sum_{p \in L} G\delta_{p,p_2} u_p^4 u_p^2 v_p^2 u_q^2 u_q t_{p,q} t_{p,p_1} + \sum_{p \in L} \sum_{q \in L} G\delta_{p,p_2} u_p^4 u_p^2 u_q v_{p,q} t_{p,q_1} t_{p,p_1} + \sum_{p \in L} \sum_{q \in L} G\delta_{p,p_2} u_p^4 u_p^2 u_q v_{p,q_1} t_{p,q_1} + \sum_{p \in L} \sum_{q \in L} G\delta_{p,p_2} u_q^4 u_p^2 u_{p,q_1} t_{p,q_1} t_{p,q_1} + \sum_{p \in L} \sum_{q \in L} G\delta_{p,p_2} u_p^4 u_p^2 u_{p,q_1} t_{p,q_1} t_{p,q_1} + \sum_{p \in L} \sum_{q \in L} G\delta_{p,p_2} u_p^4 u_p^2 u_{p,q_1} t_{p,q_1} t_{p$  $\sum_{q \in L} \frac{G}{2} u_{p}^{2} u_{p}^$  $\sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} v_p^{2} u_q^{3} u_q^{2} v_p t_{p_1 p_1} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{2} u_q v_{p_1} v_q t_{p_2 p_1} t_{p_1 p_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} u_q^{2} v_{p_1} v_q t_{p_2 p_1} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} u_q^{2} v_{p_1} v_q t_{p_2 p_1} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} u_q^{2} v_{p_1} v_q t_{p_2 p_1} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} u_q^{2} v_{p_1} v_q t_{p_2 p_1} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} u_q^{2} v_{p_1} v_q t_{p_2 p_1} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_p^{3} u_q^{2} v_{p_1} v_{p_1} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} v_{p_1 q_2} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_1 q_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_1 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_p^{4} u_{p_2 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_{p_2} t_{p_2 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} t_{p_2 q_2} t_{p_2 q_2} + \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_{p_2} t_{p_2 q_2} t_{p_2 q$  $\sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^5 u_p u_{p_1} v_p t_{p,q} t_{p,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^3 v_{p_2}^5 u_p u_{p_1} v_p t_{p,q} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_p v_p v_q t_{p,q} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} v_{p_1} v_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} v_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} v_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} v_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} v_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} v_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} u_{p_1} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} u_{q,q} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} u_{q,q} t_{q,q} - \sum_{p \in L} \sum_{q \in L} \frac{G}{4} u_q^4 v_{p_1}^5 v_{p_2}^2 u_{p_1} u_{p_1} u_{p_1} u_{p_1} u_{p_2} u_{p_1} u_{p_2} u_{p_1} u_{p_1} u_{p_2} u_{p_1} u_{p_2} u_{p_1} u_{p_2} u_{p_1} u_{p_2} u_{p_2} u_{p_1} u_{p_2} u_{p_2} u_{p_1} u_{p_2} u_{p_2} u_{p_2} u_{p_1} u_{p_2} u_{p$  $\sum_{acL} \frac{G}{4} v_{p_1}^2 v_{p_2}^2 v_{q_1}^2 v_{p_2}^2 v_{q_1}^2 u_{p_2} v_{p_1} t_{q_2} v_{p_2} v_{q_1} v_{p_1} v_{q_1} v_{p_1} v_{q_1} t_{p_2,p_1} - \sum_{acL} \frac{G}{4} v_{p_1}^2 v_{p_2}^2 u_{q_2}^2 v_{q_1} t_{p_1,p_2} + \sum_{acL} \frac{G}{4} u_{p_1}^4 u_{p_1}^2 u_{q_2}^2 u_{q_2} v_{q_2} v_{q_1} t_{p_1,p_2} + \sum_{acL} \frac{G}{4} u_{p_1}^4 u_{p_1}^2 u_{q_2}^2 u_{q_2} v_{q_2} v_{q_1} t_{p_2,p_2} t_$  $\sum_{q \in L} G\delta_{p_l p_2} u_{p_1}^{\delta} v_{p_1}^{2} u_{p_2} u_{p_1} v_{p_1}^{2} u_{p_1} v_{p_1} u_{p_2} v_{p_2} v_{p_2} u_{p_2} v_{p_2} v_{p_2} u_{p_2} v_{p_2} u_{p_2} v_{p_2} u_{p_1} v_{p_1} u_{p_2} v_{p_1} u_{p_1} v_{p_1} u_{p_2} v_{p_1} u_{p_1} v_{p_1} u_{p_2} v_{p_1} u_{p_2} v_{p_2} u_{p_2} v_{p_1} u_{p_1} v_{p_1} u_{p_2} v_{p_2} v_{p_2} u_{p_2} v_{p_2} v$  $-\sum_{p \in L} \sum_{q \in L} 2G \delta_{p_1 p_2} u_p^2 u_p^2 v_p^2 v_p^2 u_{p_1} u_{p_1} t_{p_1 p_2} + \sum_{p \in L} \sum_{q \in L} 2G \delta_{p_1 p_2} u_p^2 u_p^2 v_p^2 v_{p_1} u_q v_q t_{p_2 p_1} t_{p_2} + \sum_{p \in L} \sum_{q \in L} 2G \delta_{p_1 p_2} u_p^2 u_p^2 v_p^2 u_q^2 v_q t_{p_2 p_1} u_{p_2} u_{p_2} t_{p_2 q_2} + \sum_{p \in L} \sum_{q \in L} 2G \delta_{p_1 p_2} u_p^2 u_p^2 u_{p_2} u_{p_2} u_{p_2} u_{p_2} u_{p_2} t_{p_2 q_2} + \sum_{p \in L} \sum_{q \in L} 2G \delta_{p_1 p_2} u_p^2 u_{p_2} u_{p_2}$  $\sum_{q \in L} \frac{G}{2} u_{p_1}^2 u_{p_2}^2 v_{p_2}^2 u_{p_2} u_{q_2} v_{p_2} v_{p_1} t_{p_1 p_2} t_{p_1 p_2} t_{p_2 p_2} t_{p_1 p_2} e_{p_1} - \sum_{p \in L} \frac{1}{4} u_{p_1}^4 u_{p_2}^2 v_{p_1}^2 t_{p_2 p_2} t_{p_1 p_2} e_{p_2} - \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_1 p_2} e_{p_2} - \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_1 p_2} e_{p_2} - \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_1 p_2} e_{p_2} - \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_1 p_2} e_{p_2} - \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} e_{p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} e_{p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_{p_2 p_2} t_{p_2 p_2} + \sum_{p \in L} \frac{G}{4} u_{p_1}^2 v_{p_2}^2 t_{p_2 p_2} t_$  $\sum_{p \in L} \frac{G}{4} u_{p_2}^2 v_p^4 v_{p_1}^6 t_{p_2 p_1} t_{p_1 p_1} - \sum_{p \in L} \frac{G}{4} u_{p_2}^2 v_p^2 v_{p_1}^2 t_{p_2 p_1} t_{p_2 p_2} t_{p_2 p_1} t_{p_2 p_1} t_{p_2 p_1} t_{p_2 p_2} t_{p_2 p_2$  $\sum_{n \in L} \frac{G}{2} u_p^{b} u_p^{2} v_p^{2} t_{p_2} t_{p_2} t_{p_2} t_{p_2} t_{p_2} t_{p_2} t_{p_1} t_{p_1} t_{p_1} t_{p_1} t_{p_2} t_$  $+\sum_{p\in L} 2G\delta_{p_{1}p_{2}}u_{p}^{5}v_{p}^{5}t_{p}^{2}u_{p_{1}}u_{p_{1}}v_{p} + \sum_{p\in L} 2G\delta_{p_{1}p_{2}}u_{p}^{5}v_{p}^{5}t_{p}^{2}u_{p}v_{p}v_{p}^{5}t_{p}^{2}u_{p}v_{p}v_{p} + \sum_{p\in L} 2G\delta_{p_{1}p_{2}}u_{p}^{5}v_{p}^{2}v_{p}^{2}u_{p}v_{p}v_{p}t_{p}t_{p}v_{p}t_{p} + \sum_{p\in L} 2G\delta_{p_{1}p_{2}}u_{p}^{5}v_{p}^{2}t_{p}^{2}u_{p}^{2}v_{p}^{2}v_{p}^{2}t_{p}^{2}u_{p}^{2}v_{p}^{2}v_{p}^{2}t_{p}^{2}u_{p}^{2}v_{p}^{2}v_{p}^{2}u_{p}^{2}v_{p}^{2}v_{p}^{2}v_{p}^{2}u_{p}^{2}v_{p}^{2}v_{p}^{2}u_{p}^{2}v_{p}^{2}v_{p}^{2}u_{p}^{2}v_{p}^$  $\sum_{p \in L} 2G \delta_{p_1 p_2} v_{p_1}^{b} u_p u_{p_1} v_p t_{p_1 p_1} + \sum_{p \in L} 3G \delta_{p_1 p_2} v_{p_1}^{b} t_{p_1 p_1}^{b} u_{p_1} v_p + \sum_{p \in L} 4G \delta_{p_1 p_2} u_{p_1}^{b} v_{p_1}^{b} u_{p_1}^{b} v_{p_1}^{b} u_{p_1}^{b} v_{p_1}^{b} v_{p_2}^{b} t_{p_1 p_2} t_{p_1 p_2} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_1}^{b} v_{p_1}^{b} v_{p_2}^{b} t_{p_2} t_{p_1 p_1} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_1}^{b} v_{p_2}^{b} v_{p_2}^{b} t_{p_2} t_{p_2 p_1} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_1}^{b} v_{p_2}^{b} v_{p_2}^{b} t_{p_2} t_{p_2} t_{p_2} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_1}^{b} v_{p_2}^{b} v_{p_2}^{b} t_{p_2} t_{p_2} t_{p_2} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_1}^{b} v_{p_2}^{b} v_{p_2}^{b} t_{p_2} t_{p_2} t_{p_2} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_1}^{b} v_{p_2}^{b} v_{p_2}^{b} t_{p_2} t_{p_2} t_{p_2} + \sum_{p \in L} \frac{3G}{4} u_p^{b} u_{p_2}^{b} v_{p_2}^{b} t_{p_2} t_{p_2$  $\sum_{w:L} \frac{3G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{4} t_{p,p}^{2} t_{p,p} t_{p,p} + \sum_{w:L} \frac{5G}{2} \delta_{p,p_2} u_{p}^{4} u_{p}^{2} v_{p}^{2} t_{p,p} t_{p,p$  $\sum_{u \in L} G \delta_{p_1 p_2} u_p^3 u_p^3 v_p^3 v_{p_1 p_2} v_{p_2 p_3} v_{p_1 p_2 p_3} v_{p_2 p_3} v_{p_1 p_2 p_3} v_{p_1 p$  $\sum_{w:L} \frac{G}{2} u_{\mu}^{2} u_{\mu}^{2} v_{\nu}^{2} v_{\mu}^{2} v_{\mu}^{2} t_{\mu} v_{\mu} t_{\mu,\nu} t_{\mu,\mu} t_{\mu,\nu} t_{\mu,\nu} t_{\mu,\nu} t_{\mu,\nu} t_{\mu,\nu} t_{\mu,\nu$  $\sum_{p \in L} Gu_p^4 u_p^3 u_{p_2}^3 u_{p_2} v_{p_1} t_{p_1, p_2} t_{p_1, p_2} - \sum_{p \in L} Gu_p^4 u_{p_1}^3 v_{p_1}^3 u_{p_1} v_{p_2} t_{p_1, p_2} t_{p_1, p_2} t_{p_1, p_1} - \sum_{p \in L} Gu_p^5 u_{p_2}^3 v_{p_1}^3 u_{p_1} v_{p_2} t_{p_1, p_2} t_{p_2, p_2} t_{p_1, p_2} t_{p_2, p_2}$  $\sum_{p \in L} Gu_p^5 v_p^3 v_{p_2}^2 u_{p_1} v_{p_2} t_{p_1 p_1} t_{p_2 p_1} t_{p_2} u_p^4 u_p^2 v_p^2 v_{p_1} t_{p_2 p_1} t_{p_2 p_2} t_{p_2 p_2} t_{p_2 p_1} t_{p_2 p_2} t_{p_$  $\sum_{p \in L} 4G \delta_{p_1 p_2} u_{p_1}^2 v_{p_2}^2 u_{p_1}^2 v_{p_2}^2 u_{p_2} v_{p_1 p_2} u_{p_1}^2 v_{p_1}^2 u_{p_2} v_{p_1 p_2} u_{p_1}^2 u_{p_2}^2 u_{p_2}^2$  $-\sum_{p \in L} \frac{3G}{2} u_p^2 u_{p1}^2 v_{p2}^2 v_{p1}^2 v_{p2}^2 v_{p1} t_{p1} t_{p2} t_{p2} - \sum_{p \in L} \frac{3G}{2} u_{p2}^2 u_{p2}^2 v_{p2}^2 v_{p2}^2 t_{p2} v_{p1} t_{p1} t_{p1} t_{p2} - \sum_{p \in L} \frac{G}{2} u_{p2}^2 v_{p1}^2 u_{p1} v_{p1} t_{p2} t_{p$  $\sum_{v \in L} \frac{G}{2} u_{p_1}^3 v_{p_1}^4 u_p v_{p_2} t_{p_1, p_2} t_{p_2, p_1} - \sum_{v \in L} \frac{1}{2} u_{p_2}^4 v_{p_1}^3 u_p u_{p_1} v_{p_1, p_2} t_{p_2, p_1} \epsilon_{p_2} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^2 u_p u_{p_1} v_{p_1, p_2} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_p u_{p_1} v_{p_1, p_2} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_p u_{p_1} v_{p_1, p_2} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_p u_{p_1} v_{p_1, p_2} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1, p_2} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_1}^3 u_{p_2} v_{p_1} t_{p_2, p_1} - \sum_{v \in L} \frac{G}{2} u_{p_2}^5 v_{p_2}^5 u_{p_2} t_{p_2, p_2} t_{p_2,$  $\sum_{p \in L} 2Gu_{p_1}^4 u_{p_2}^3 v_{p_1}^2 u_p v_{p_2} t_{p_1,p}^2 t_{p_1,p_2} t_{p_1,p_2} t_{p_1,p_2} t_{p_2} v_{p_2} t_{p_1,p_1} t_{p_2,p} - \sum_{p \in L} 2Gu_{p_1}^4 v_{p_2}^2 v_{p_2}^2 u_p u_{p_2} v_{p_1} t_{p_2,p_1} - \sum_{p \in L} 2Gu_{p_1}^4 v_{p_1}^2 v_{p_1}^2 u_{p_1} v_{p_1} t_{p_1,p_2} - \sum_{p \in L} 2Gu_{p_1}^4 v_{p_2}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} - \sum_{p \in L} 2Gu_{p_1}^4 v_{p_2}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} - \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} + \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} + \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} + \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} u_{p_1} v_{p_1} t_{p_1,p_2} + \sum_{p \in L} 2Gu_{p_1}^2 v_{p_1}^2 u_{p_1} u_{p_1} u_{p_1} u_{p_1} u_{p_2} u_{p_2} u_{p_2} u_{p_1} u_{p_2} u_{p_2}$  $\sum_{v \in L} 2Gu_{p_1}^2 v_{p_1}^2 v_{p_2}^4 u_p u_{p_1} v_p t_{p_1,p_1} t_{p_2,p_1} - \sum_{v \in L} 2Gu_{p_2}^4 v_{p_1}^2 v_{p_1,p_2} t_{p_1,p_2} - \sum_{v \in L} 2Gu_{p_1}^4 v_{p_2}^2 v_{p_2}^2 u_p u_{p_1} v_p t_{p_2,p_2} - \sum_{v \in L} \frac{1}{2} u_{p_1}^2 u_{p_1}^2 v_{p_1}^2 u_{p_1} v_{p_1} t_{p_1,p_2} t_{p_2,p_2} t_{p_1,p_2} t_{p_1,p_2} t_{p_1,p_2} t_{p_1,p_2} t_{p_1,p_2} t_{p_2,p_2} t_{p_1,p_2} t_{p_2,p_2} t_{p_1,p_2} t_{p_2,p_2} t_{p_1,p_2} t_{p_2,p_2} t_{p_1,p_2} t_{p_2,p_2} t_{p_1,p_2} t_{p_2,p_2} t_$  $+ 3Gu_{p_2}^{4}v_{p_1}^{2}v_{p_2}^{2}t_{p_2p_2}^{2} - \frac{G}{2}u_{p_1}^{2}v_{p_1}^{10}t_{p_1,p_2}t_{p_2,p_2} - \frac{1}{2}u_{p_1}^{4}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_2}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{2}v_{p_1}^{10}t_{p_1,p_1}t_{p_2,p_1} - \frac{1}{2}u_{p_2}^{4}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{1}{2}u_{p_2}^{4}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_2} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_1,p_2}t_{p_2,p_1} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_2,p_2}t_{p_2,p_2} - \frac{G}{2}u_{p_1}^{6}v_{p_2}^{6}t_{p_2,p_2}t_{p_2,p_2} - \frac{G}{2}u_{p_2}^{6}v_{p_1}^{6}t_{p_2,p_2}t_{p_2,p_2} - \frac{G}{2}u_{p_2}^{6}v_{p_2}^{6}t_{p_2,p_2}t_{p_2,p_2} - \frac{G}{2}u_{p_2}^{6}v_{p_2}^{6}t_{p_2,p_2}t_{p_2,p_2}t_{p_2,p_2} - \frac{G}{2}u_{p_2}^{6}v_{p_2}^{6}t_{p_2,p_2}t_{p_2,p$  $+Gu_{p_1}^2u_{p_2}^2v_{p_3}^2t_{p_1,p_2}t_{p_2,p_2}+Gu_{p_1}^2u_{p_2}^4v_{p_3}^4t_{p_1,p_2}t_{p_2,p_1}+\frac{7G}{2}u_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_3}^4t_{p_2,p_1}^2+Gu_{p_1}^2u_{p_2}^2v_{p_3}^5v_{p_1,p_1,p_1,p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_1,p_1,p_1,p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_1,p_1,p_1,p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2,p_1}+Gu_{p_1}^2u_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{p_2}^2v_{p_2}^2v_{p_1}^2v_{p_2}^2v_{$  $+Gu_{p_1}^2v_{p_2}^2u_{p_2}t_{p_1,p_1}t_{p_2,p_1}t_{p_2,p_1}+Gu_{p_2}^2v_{p_2}^2u_{p_1}t_{p_1,p_2}t_{p_2,p_2}t_{p_1,p_2}t_{p_2,p_2}+\frac{1}{2}u_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_2}t_{p_2,p_2}\epsilon_{p_1}+\frac{1}{2}u_{p_1}^4u_{p_2}^2v_{p_1}^2v_{p_2}^2t_{p_1,p_1}t_{p_2,p_1}\epsilon_{p_2}-u_{p_1}^2u_{p_2}^2v_{p_1}^2v_{p_1}t_{p_2,p_1}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_1}^2v_{p_1}^4u_{p_2}v_{p_1}^2t_{p_2,p_1}\epsilon_{p_1,p_1}t_{p_2,p_1}\epsilon_{p_2,p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_1}^2v_{p_2}^4u_{p_2}v_{p_1}^2t_{p_2,p_1}\epsilon_{p_2,p_1}\epsilon_{p_2,p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_1}t_{p_2,p_1}\epsilon_{p_2,p_2}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_1}\epsilon_{p_2,p_2}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_2}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_2}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_2}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_1}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_2}\epsilon_{p_1}+\sum_{p\in L}Gd_{p_1p_2}u_{p_2}^3v_{p_2}^2u_{p_2}^2t_{p_2,p_2}\epsilon_{p_2}+\sum_{p\in L}Gd_{p_1p_2}u_{p_2}^2u_{p_2}^2t_{p_2,p_2}^2t_{p_2,p_2}\epsilon_{p_2}+\sum_{p\in L}Gd_{p_1p_2}u_{p_2}^2u_{p_2}^2t_{p_2,p_2}t_{p_2,p_2}\epsilon_{p_2}+\sum_{p\in L}Gd_{p_1p_2}u_{p_2}^2t_{p_2,p_2}t_$  $\sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, p_1, p_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 u_{q_1, p_1, p_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1, p_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1}^3 v_{q_1}^4 u_p v_p t_{p_1, q_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1} v_{p_1} v_{p_1, q_1, q_1} + \sum_{p \in L} \sum_{q \in L} G \delta_{p_1 p_1} u_{p_1} v_{p_1} v_{p_1}$  $\sum_{q \in L} \frac{G}{2} u_p^3 u_{p_1}^2 v_{p_2}^2 u_{q_1} v_{q_1} v_{p_1 p_1} + \sum_{p \in L} \sum_{q \in L} \frac{G}{2} u_p^3 u_{p_2}^2 v_{p_2}^2 v_{p_1}^2 u_{q_1} v_{q_1} v_{p_1} + \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_1} u_{p_1}^2 v_{p_1}^2 u_{q_1} v_{p_1} v_{p_1 p_1} v_{p_1} v_{p_1}$  $\sum_{q \in L} \frac{G}{2} u_p^2 u_{p_1}^2 v_{p_2}^2 u_{q_1} v_{p_2} u_{q_1} v_{p_2} t_{p_3} t_{p_4} - \sum_{p \in L} \frac{G}{q \in L} \frac{2}{2} u_{p_1}^2 v_{p_2}^2 v_{p_1} u_{q_1} v_{p_2} t_{p_3} u_{q_1} v_{p_2} u_{p_2} v_{q_1} u_{q_2} v_{p_3} u_{q_1} t_{p_3} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} u_{p_1}^2 v_{p_2}^2 v_{p_3} u_{q_1} v_{q_2} t_{p_3} u_{q_1} v_{p_2} t_{p_3} u_{q_1} v_{p_2} t_{p_3} u_{q_1} v_{p_2} t_{p_3} u_{q_1} v_{p_2} u_{q_1} v_{p_2} v_{q_2} u_{q_1} v_{q_2} u_{q_2} v_{q_2} u_{q_2} u_{q_2} v_{q_2} u_{q_2} u_$  $\sum_{q \in L} \frac{G}{2} u_{p_1}^2 v_{p_2}^2 u_{p_1} u_{q_2} v_{q_1} v_{q_2} t_{p_1, p_2} - \sum_{p \in L} \sum_{q \in L} \frac{G}{2} u_{p_1}^2 u_{p_2}^4 u_{q_2}^2 v_{q_1} v_{p_1, q_1} + \sum_{p \in L} \sum_{q \in L} \frac{G}{2} \delta_{p_1 p_2} u_{p_1}^2 v_{p_1}^2 v_{q_1} u_{p_2, q_1} v_{p_1, q_1} + \sum_{p \in L} \sum_{q \in L} \frac{G}{2} u_{p_1}^2 u_{p_2}^2 u_{q_2}^2 v_{q_1} v_{p_2}^2 v_{q_1} v_{p_2} v_{q_1} v_{q_2} v_{q_1} v_{q_1} v_{q_2} v_{q_1} v_{q_2} v_{q_1} v_{q_1} v_{q_2} v_{q_1} v_{q_2} v_{q_1} v_{q_1} v_{q_2} v_{q_1} v_{q_1} v_{q_2} v_{q_1} v_{q_1} v_{q_2} v_{q_1} v_$  $\sum_{a \in L} \frac{G}{4} u_{p}^{b} u_{p}^{2} u_{q}^{b} v_{p}^{2} u_{q} v_{p} v_{q} t_{p,p} t_{p,p} + \sum_{u \in L} \sum_{a \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,p} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{p}^{2} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} v_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{p}^{2} u_{p}^{2} u_{p} u_{q} v_{q} t_{p,p} t_{p,q} + \sum_{u \in L} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{p}^{2}$  $\sum_{acL} \frac{G}{4} u_{p}^{2} u_{p}^{2} u_{q}^{2} v_{p}_{1} v_{p}^{2} u_{q} v_{p,1} v_{q} t_{p,p,1} t_{p,1,q} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,p,q} t_{p,1,p} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,1,q} t_{p,1,p} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,1,q} t_{p,1,p} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,1,q} t_{p,1,q} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,1,q} t_{p,1,q} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,1,q} t_{p,1,q} t_{p,1,q} + \sum_{wcL,wcL} \frac{G}{4} u_{p}^{4} u_{p}^{2} u_{q}^{2} v_{p,1} v_{q} t_{p,1,q} t_{p,1$ 

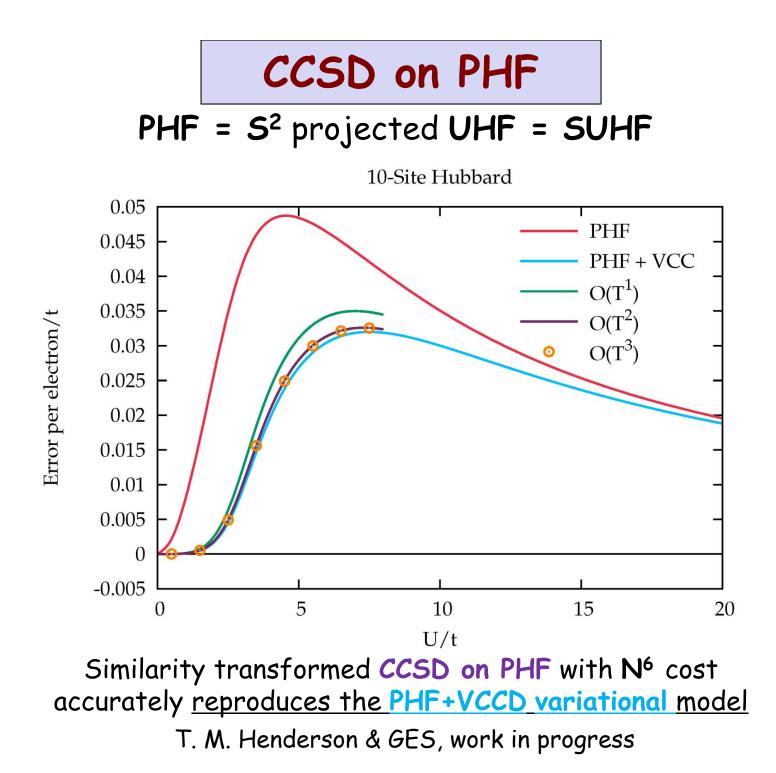


Resulting residual:

$$\begin{split} R^{ab}_{ij} \approx n_i \, n_j \, \bar{n}_a \, \bar{n}_b \left\{ \bar{v}^{ab}_{ij} + f^b_c \, t^{ac}_{ij} + f^a_c \, t^{cb}_{ij} - f^k_i \, t^{ab}_{kj} - f^k_j \, t^{ab}_{ik} \right. \\ & \left. + \frac{1}{2} \, \left( 1 - n_c - n_d \right) \, \bar{v}^{ab}_{cd} \, t^{cd}_{ij} - \frac{1}{2} \, \left( 1 - n_k - n_l \right) \, \bar{v}^{kl}_{ij} \, t^{ab}_{kl} \right. \\ & \left. + \frac{1}{4} \, \left[ -1 + n_k + n_l + \left( n_c + n_d \right) \, \left( 1 + n_k + n_l \right) \right] \, \bar{v}^{cd}_{cd} \, t^{ab}_{kl} \, t^{cd}_{ij} \right. \\ & \left. - \frac{1}{2} \, \left[ n_d \, \left( 1 - n_k - n_l \right) + n_k \, n_l \right] \, \bar{v}^{kl}_{cd} \, \left( t^{bd}_{kl} \, t^{ac}_{ij} + t^{ad}_{kl} \, t^{cb}_{ij} \right) \right. \\ & \left. - \frac{1}{2} \, \left[ n_l \, \left( 1 - n_c - n_d \right) + n_c \, n_d \right] \, \bar{v}^{kl}_{cd} \, \left( t^{cd}_{jl} \, t^{ab}_{ik} + t^{cd}_{il} \, t^{ab}_{kj} \right) \right. \\ & \left. + \mathcal{P}_{ij} \, \mathcal{P}_{ab} \, \left( n_k - n_c \right) \, \bar{v}^{bk}_{jc} \, t^{ac}_{ik} \\ & \left. + \left( n_k - n_c \right) \, \left( n_l - n_d \right) \, \bar{v}^{kl}_{cd} \, \left( t^{ac}_{ik} \, t^{db}_{lj} - t^{cb}_{ik} \, t^{ad}_{lj} \right) \right\} \end{split}$$

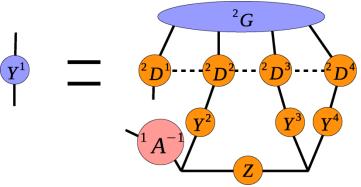
cf. spin-orbital CCD equations in JCP 139, 104113 (2013) (three quadratic channels: ladders, rings & xrings)

Two interesting limits:  $n_{occ} = 1$ ,  $n_{unocc} = 0$  (RCCSD),  $n_{occ} = n_{unocc} = \frac{1}{2}$  (maximum entanglement)



# **Tensor Decomposition**

- Using tensor hypercontraction and canonical polyadic decomposition, we break down both the interaction (V) and CCSD amplitudes (T) into matrices
- We next demand energy stationarity with respect to T decomposition factors :



 Solving for the factors above yields an O(N<sup>4</sup>) procedure with sub-millihartree accuracy

**Details**: Tensor-structured coupled cluster theory, R. Schutski, J. Zhao, T. M. Henderson, and G. E. Scuseria, *J. Chem. Phys.* **147**, 184113 (2017).

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