Bogoliubov coupled cluster theory

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Motivation: computing near-degenerate finite Fermi systems

- Ab initio methods have been developed
  - CC, IM-SRG, SCGF, CI
- Establish techniques to provide reliable predictions for experimental measurements
  - Include assessment of uncertainty from many-body method
  - Expansion techniques are ideal, if contributions are smaller at higher orders
  - Access to other observable properties beyond energy of strong interest
  - Expansion on top of Slater determinant breaks down for open-shell systems
- Three different philosophies to extend to near-degenerate systems
  1. Multireference (MR-CC, MR-IM-SRG)
  2. Effective interaction (from CC, NCSM, IM-SRG)
  3. Symmetry breaking (BCC, Gorkov Green's function methods)
- Possibility to cross-check results beyond current experimentally known region
- Comparison of multiple methods useful (especially single- vs. multi-reference)
- In nuclear physics, require accurate treatment of forces to reproduce experiment
  - Known issues with current forces on the market
  - Ab initio calculations of nuclei provide feedback on accuracy of potentials
  - In fact, probe new aspects of the bare nuclear potentials

Spontaneous symmetry breaking methods

- Extensions beyond closed-shell systems exist via multi-reference methods (e.g., particle-attached equation-of-motion CC)
  - Computationally demanding as more particles are added
  - Formally complicated as well
- Reference state explicitly breaking symmetry can account for superfluid nature
- Build CC techniques around Bogoliubov vacuum
  - K. Emrich and J.G. Zabolitzky, Phys. Rev. B **30**, 2049 (1984)
  - W.A. Lahoz and R.F. Bishop, Z. Phys. B **73**, 363 (1988)
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- Maintain single reference nature (formal and computational simplicity)
- Difficulties
  - Quasiparticle basis- rewrite Hamiltonian normal-ordered wrt HFB vacuum
  - Diagrammatic techniques- rules (e.g. from Shavitt and Bartlett) need modification
  - Additional constraint equation- average particle number
  - Computational aspect- less expedient scaling

$$n_p^i n_h^j \text{ in CC} \rightarrow (n_p + n_h)^{i+j} \text{ in BCC}$$

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Bogoliubov algebra

- Bogoliubov transformation

$$\beta^\dagger_\alpha = \sum_p U_{p\alpha}\, c^\dagger_p + V_{p\alpha}\, c_p \qquad \beta_\alpha = \sum_p U^*_{p\alpha}\, c_p + V^*_{p\alpha}\, c^\dagger_p$$

- Bogoliubov vacuum $|\Phi\rangle \equiv \mathcal{C} \prod_\alpha \beta_\alpha |0\rangle$
- Natural extension from particle-hole language
- Simplifies some aspects of standard CC theory (all lines in one direction)
- Rewrite Hamiltonian, i.e. normal order with respect to $|\Phi\rangle$
  - Derived including three-body interactions (to include implicit two-body component)
  - In terms of components H^{ij} with $i(j)$ quasiparticle creation(annihilation) operators

$$\begin{aligned} H &= H^{00} + H^{11} + H^{20} + H^{02} + \dots \\ &= \tilde{H}^{00} + \sum_{k_1 k_2} \tilde{H}^{11}_{k_1 k_2} \beta^\dagger_{k_1} \beta_{k_2} + \frac{1}{2!} \sum_{k_1 k_2} \left\{ \tilde{H}^{20}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2} + \tilde{H}^{02}_{k_1 k_2} \beta_{k_2} \beta_{k_1} \right\} + \dots \end{aligned}$$

- Each matrix element $\tilde{H}^{ij}_{k_1 \dots k_i k_{i+1} \dots k_{i+j}}$ is:
  1. antisymmetric for all $k_1 \dots k_i$ and $k_{i+1} \dots k_{i+j}$
  2. can be written as a function of NN, NNN, U, V

Bogoliubov coupled cluster theory

- Hamiltonian replaced by grand canonical potential $\Omega = H - \lambda A$
- Solution for nucleus with A_0 particles given by

$$\Omega|\Psi\rangle = \Omega_0|\Psi\rangle$$

- Constraint equation $A_0 = \frac{\langle\Psi|A|\Psi\rangle}{\langle\Psi|\Psi\rangle}$
- Exponential ansatz $|\Psi\rangle = e^{\mathcal{T}}|\Phi\rangle$
- Quasiparticle cluster operator $\mathcal{T} = \mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3 + \ldots$

$$\mathcal{T}_1 = \frac{1}{2!}\sum_{k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2} \beta^\dagger_{k_1} \beta^\dagger_{k_2}$$

$$\mathcal{T}_2 = \frac{1}{4!}\sum_{k_1 k_2 k_3 k_4} \tilde{\mathbf{t}}_{k_1 k_2 k_3 k_4} \beta^\dagger_{k_1} \beta^\dagger_{k_2} \beta^\dagger_{k_3} \beta^\dagger_{k_4}$$

- Similarity transformed grand canonical potential $\bar{\Omega}$

Extension of standard coupled cluster theory

- Motivated by procedure in standard coupled cluster theory
  - Produce eigenvalue equation $\bar{\Omega}|\Phi\rangle = \Omega_0|\Phi\rangle$
  - Utilize Baker-Campbell-Hausdorff expansion
  - Truncate to four $\mathcal{T}$ operators (six with explicit three-body contribution)
  - Limit to connected terms only
  - Only quasiparticle creation operators in $\mathcal{T} \to \Omega$ to the left

$$\bar{\Omega} = \Omega + \left(\Omega\mathcal{T}\right)_C + \frac{1}{2!}\left(\Omega\mathcal{T}\mathcal{T}\right)_C + \frac{1}{3!}\left(\Omega\mathcal{T}\mathcal{T}\mathcal{T}\right)_C + \frac{1}{4!}\left(\Omega\mathcal{T}\mathcal{T}\mathcal{T}\mathcal{T}\right)_C = (\Omega e^{\mathcal{T}})_C$$

- Subtract reference energy for convenience $\Omega_N = \Omega - \langle\Phi|\Omega|\Phi\rangle$
- Produce energy and amplitude equations

$$\langle\Phi|\bar{\Omega}_N|\Phi\rangle_C = \Delta\Omega_0$$
$$\langle\Phi^{\alpha\beta\cdots}|\bar{\Omega}_N|\Phi\rangle_C = 0$$

- Solve under constraint of average particle number

$$A_0 = \frac{\langle\Phi|e^{\mathcal{T}^\dagger}Ae^{\mathcal{T}}|\Phi\rangle}{\langle\Phi|e^{\mathcal{T}^\dagger}e^{\mathcal{T}}|\Phi\rangle} = \langle\Phi|e^{\mathcal{T}^\dagger}Ae^{\mathcal{T}}|\Phi\rangle_C = \langle\Phi|(1+\Lambda)e^{-\mathcal{T}}A_N e^{\mathcal{T}}|\Phi\rangle_C$$

Current status of ab initio BCC theory

- Formalism
  - Derivation of BCCSDT complete, evaluated equivalently in multiple ways
  - Can recover standard CC in Slater determinant limit
    - Produce more general extended coupled cluster method in straightforward limit
  - Can evaluate one- and two- body operators
- Implementation
  - Utilize *NN* interactions from chiral potential (+RG)
  - Bogoliubov vacuum from solution of HFB equations
    - *m*-scheme version of HFB code
    - Utilizes symmetry properties (subblock matrices in most reduced form)
  - BCCSD derived and coded in *m*-scheme with intermediates
    - BCCSD energy and amplitude equations contain 27 diagrams
    - Intermediates reduce computational time and formal complexity
    - Slight issues remaining in comparison to benchmark calculations
- Illustration using BCCD
  - Truncation to $\mathcal{T} = \mathcal{T}_2$
  - Should include most important effects at lowest order (two-body potential)
  - Singles contribution corresponds to Thouless theorem; HFB solution used
  - Does not provide convergence- triples required at least perturbatively

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Proof-of-principle calculations: Methodology

- Comparison to CC results in closed-shell nuclei
  - HFB solution formally collapses to HF solution
  - BCCSD equations in Slater determinant limit contain correlations beyond CCSD
  - In practice, CC results for closed-shell nuclei are reproduced exactly
- Comparison to CC results beyond closed-shell nuclei
  - HFB reference state is constrained to correct particle number on average
  - BCC equations are iterated with Lagrange constraint on particle number (Z and N)
  - Computation of particle number via Λ method is valid at 1st order
  - Extensions of CC, e.g. EOM-CC, provide comparison to BCC
- Allocated time on supercomputing machines for calculations (e.g. TITAN)
- Caveats
  - Intrinsic Hamiltonian treated approximately since HFB solution breaks symmetry
  - Very small model spaces used for preliminary calculations- results are not converged
  - Computational limit reached at $N_{\max} = 8$ oscillator shell (re-coding necessary)
- Parameters of the calculation
  - Bare $\mathrm{NNLO}_{\mathrm{opt}}$ from A.Ekström et al., PRL **110**, 192502 (2013)
  - Spherical harmonic oscillator single particle basis defined by $\hbar\omega$
  - Ground states of ^{16,18,20}O, ^{18}Ne, ^{20}Mg calculated in $N_{\max} = 6$ model space

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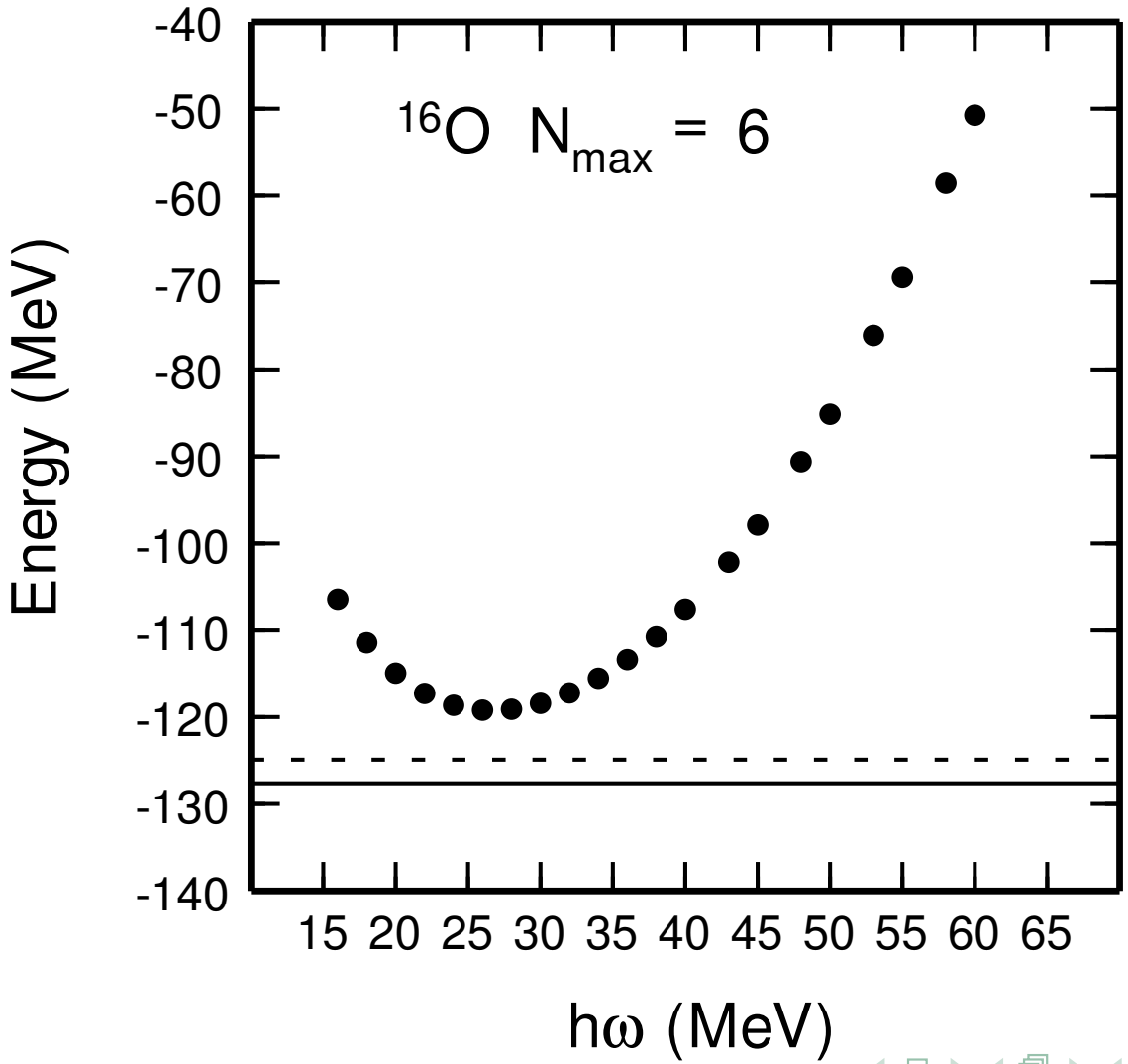
^{16}O: Energies and extrapolations

CCSD energy as a function of $\hbar\omega$

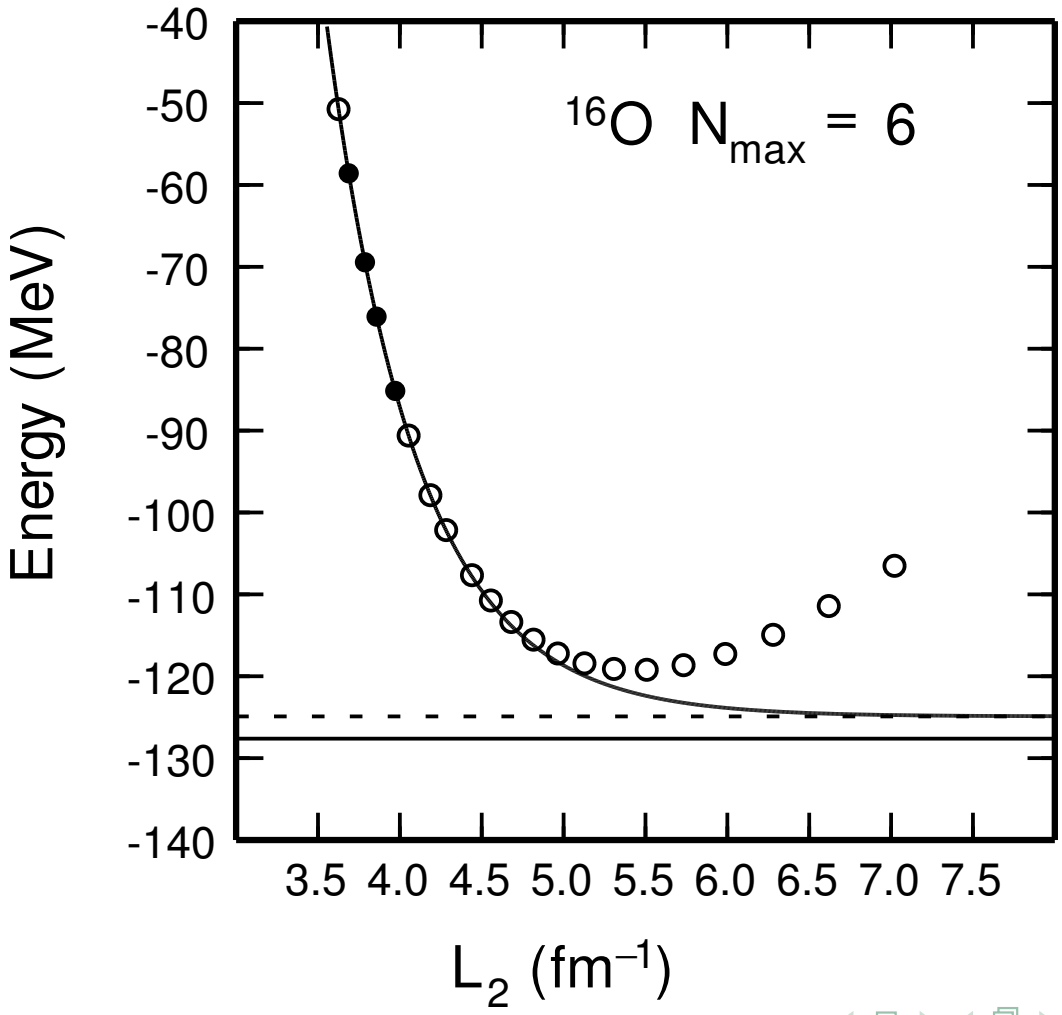


^{16}O: Energies and extrapolations

CCSD energy as a function of effective size of basis L_2

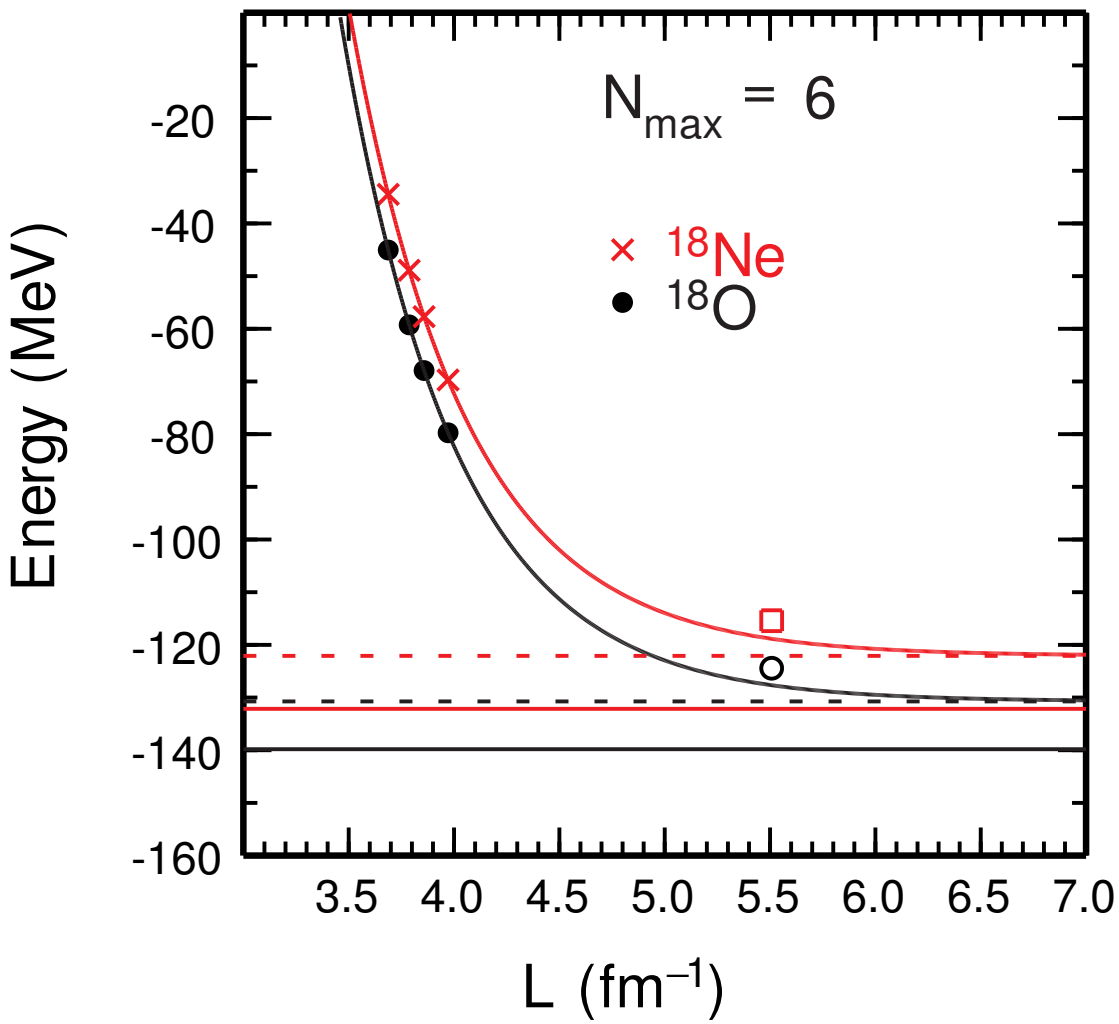
Infrared extrapolation based on Dirichlet boundary condition

Reliable if ultraviolet contamination is small



Open shell nuclei: Energies and extrapolations

$$E(L) = E_\infty + A_\infty e^{-2k_\infty L} \qquad L = L_2 = \sqrt{2(N+3/2+2)}\sqrt{\hbar/(M\omega)}$$



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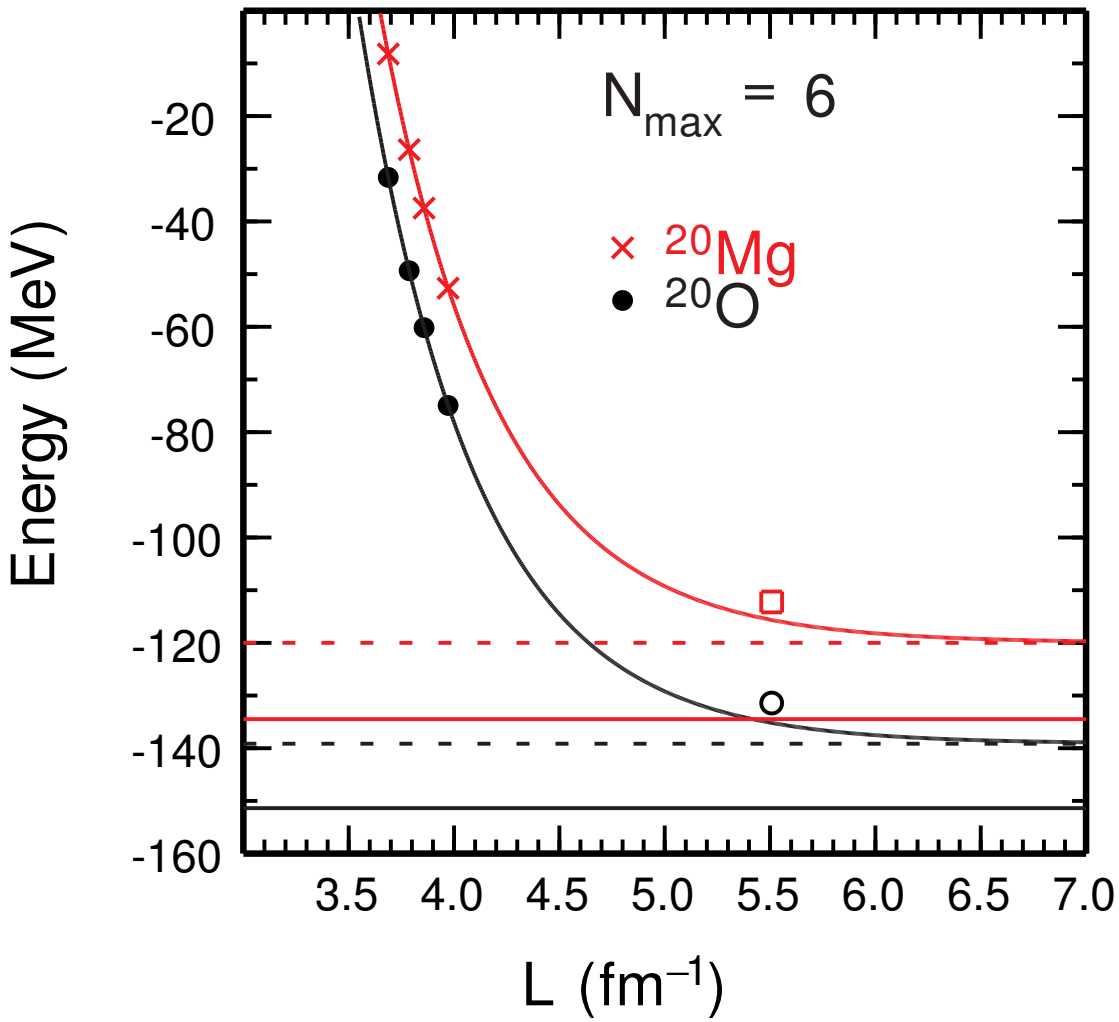

Compiled results of *sd*-shell nuclei

Nucleus	$E^{\mathrm{BCC}}_{N_{\max}=6}$	$E^{\mathrm{CC}}_{N_{\max}=6}$	E_∞	$E^{\mathrm{CC}}_{N_{\max}=12}$	E^{exp}
^{16}O	-119.110	-119.110	-124.821	-123.453	-127.619
^{18}O	-124.440	-126.476	-130.738	-132.990	-139.808
^{20}O	-131.428	n/a	-139.144	n/a	-151.371
^{18}Ne	-115.413	-117.927	-122.089	-124.850	-132.143
^{20}Mg	-112.237	n/a	-119.996	n/a	-134.480

- BCCD extrapolated results given by E_∞
- CCD results
  - For ^{16}O, standard CCD calculation
  - For ^{18}O, ^{18}Ne, two-particles-attached equation-of-motion CCSD with $\hbar\omega = 26$ MeV
  - Future comparison of computational aspects of BCC and EOM-CC necessary
  - For this interaction, ≈ 7 MeV gained by going to Λ-CCSD(T)

Assessing symmetry breaking

- Evaluation of particle number via one-body density matrix
  - Constrained in BCC system of equations to correct number on average
  - Interested in evaluating conservation of symmetry upon solution
- HFB reference state
  - Separately constrained to produce right particle number on average
  - Variance $\sigma_A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$ relates amount of symmetry breaking
  - For closed shell nuclei, HFB equations reduce exactly to HF result ($\sigma_A = 0$)
- BCC results
  - In exact result ($Ap - Ah$ excitations), physical symmetries restored
  - For BCCD in small model spaces, this is far from maintained
  - Amount of symmetry breaking on par with initial HFB state
  - Local fluctuations present ($A = 20$ mirror nuclei differ significantly)

Nucleus	HFB	BCCD
^{16}O	0.000	0.000
^{18}O	1.666	1.677
^{20}O	1.699	1.843
^{18}Ne	1.663	1.662
^{20}Mg	1.691	1.596

Can we project good quantum numbers?

Conclusions

- Open-shell systems within reach with ab initio techniques
  - Extensions via symmetry-breaking (BCC, Gorkov-Green's function methods)
  - Extensions to multi-reference states (MR-IM-SRG)
  - Via shell model with effective interactions derived from bare nuclear forces
  - Explore new aspects (pairing), assess deficiencies of forces from χEFT
- General formalism
  - BCC energy and amplitude equations derived up to BCCSDT
  - Diagrammatic technique developed, reproduces algebraic result
  - Single-reference even for open-shell (superfluid) nuclei, requires constraint on A
  - Microscopic two-body and three-body interactions can be treated
- Implementation in m-scheme
  - HFB, BCCD, linear BCCSD codes are fully operational
  - Results benchmarked for closed-shell nuclei to standard CC results
  - Fewer correlations than two-particle-attached equation-of-motion CC
  - Only microscopic two-body interactions incorporated thus far
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Outlook

- Utilize deformed basis in BCC
  - Advantage of *m*-scheme implementation compared to *J*-coupled scheme
  - Currently, spherical single particle basis and spherical BCS solution employed
  - Permits treatment of doubly-open-shell nuclei
  - HFB *m*-scheme code reproduces deformed HF result, but is not internally consistent
- Evaluation of potential energy surfaces (^{24}Mg) ab initio
  - Implement constraint on deformation
- Go beyond $N_{\max} = 8$ oscillator shell in BCC calculations
  - Distribution of $\mathcal{T}_2$ amplitudes required
  - Further optimization of code desirable
  - Alternatively, implement BCC equations in *J*-scheme
    - Significant improvement due to reduction of dimensions
    - Only requires projection of $U(1)$ symmetry to restore physical quantum numbers

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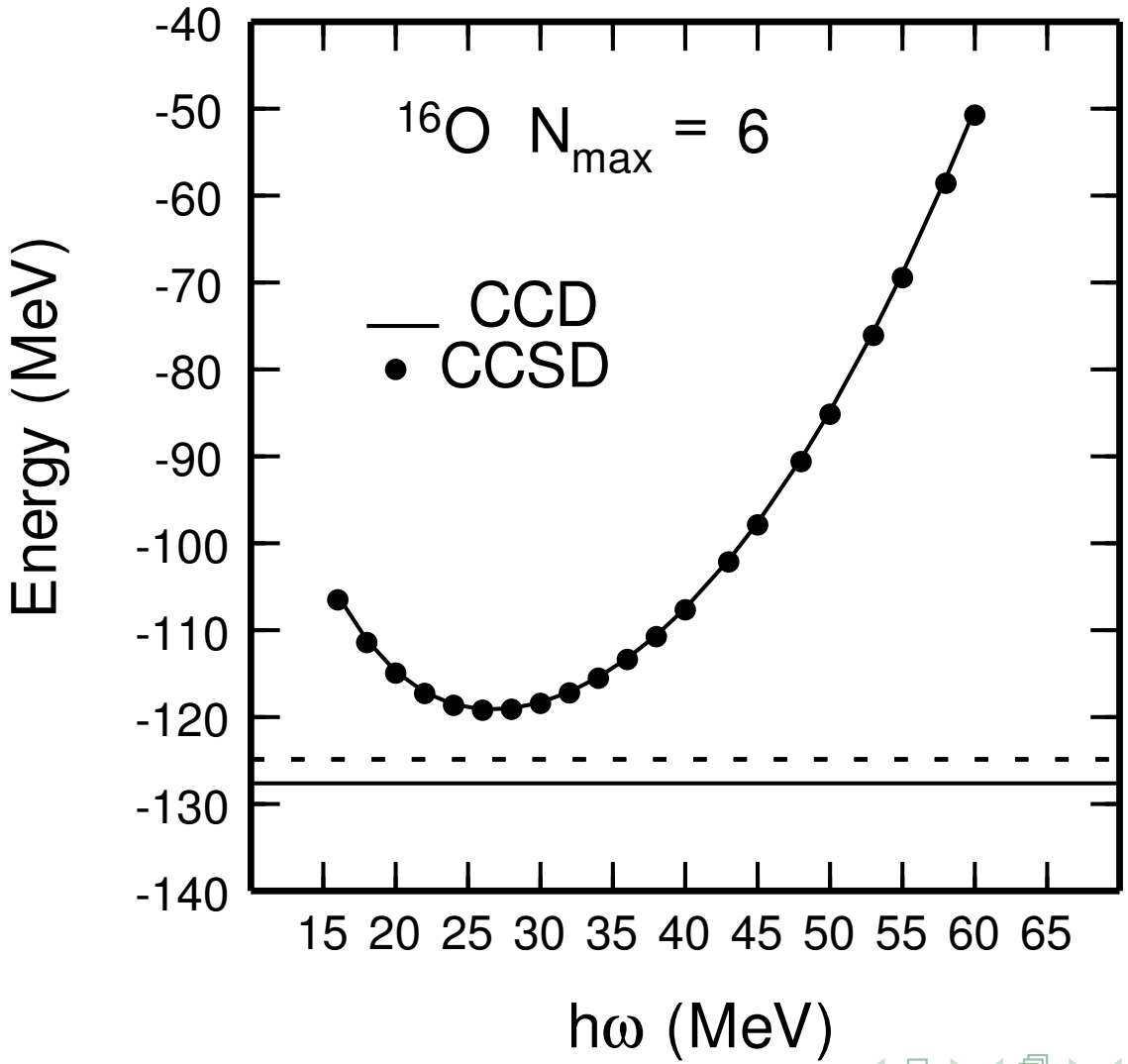
Outlook (including long-term goals)

- Extend to equation-of-motion BCC
  - Equation-of-motion BCC enables the computation of odd nuclei and excited states
  - One-particle attached/removed suffices since all even-even nuclei can be accessed
  - Treatment of one- and two-body operators already in place
  - Computation of observables, e.g. B(E2), for comparison to experiment
- Projection of good quantum numbers
  - Relevant once symmetry is spontaneously broken
  - Physical state maintains symmetry
  - Restore symmetry in approximate treatment through projection
  - Future implementation to restore $U(1)$ and $SO(3)$ symmetry
- Include three-body forces at least at normal-ordered two-body level
  - Inclusion of three-body forces relevant for accurate results and trends
  - Full treatment already derived in general indices
  - Normal-ordered two-body contribution nearly derived in m-scheme implementation
- Longer-term extensions based on advances in standard CC methods

Backup slides

Comparison of binding energies of ^{16}O

CCD and CCSD are nearly indistinguishable



CCSD results for ^{16}O

Table: Minimum CCSD energies and associated frequencies for ^{16}O with different $N_{\max}$

$N_{\max}$	$\hbar\omega_{\min}$	$E_{\min}$
6	26	-119.211
8	24	-122.776
10	24	-123.400
12	22	-123.502

- CC code is optimized
- Dimensions of J-coupled scheme are significantly reduced relative to m-scheme
- Larger model spaces can be accessed (BCC code limited to $N_{\max} = 8$)
- Convergence can also be studied as a function of $\hbar\omega$