Bogoliubov coupled cluster theory
Or: Many-body methods for open-shell nuclei

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TRIUMF workshop, 17-20 February 2015, Vancouver, BC

Motivation: computing open-shell nuclei

- 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
  - Exclusion of nuclear reaction dynamics and continuum at the moment
  - Multiple methods are necessary
  - Access to other observable properties beyond energy of strong interest
- Ab initio methods have been developed
  - CC, IM-SRG, SCGF, CI/SM
- Three different philosophies
  1. Multireference (MR-CC, MR-IM-SRG)
  2. Effective interaction (from CC, NCSM, IM-SRG)
  3. Symmetry breaking (BCC, Gorkov Green's function methods)
- Require accurate treatment of nuclear forces to reproduce experiment
- Ab initio calculations of nuclei provide feedback on accuracy of potentials

Ab initio techniques for (truly) open-shell nuclei

- Expansion techniques break down for calculations of (truly) open-shell nuclei
  - Extensions beyond doubly-closed subshell nuclei exist via multi-reference methods (e.g., particle-attached equation-of-motion CC)
  - Computationally demanding as more particles are added
  - Not suited to calculate truly open-shell nuclei due to phase transition
- Reference state explicitly breaking symmetry can account for superfluid nature
- Build CC techniques around Bogoliubov vacuum
  - More relevant away from light isotopes
  - 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)
  - L.Z. Stolarczyk and H.J. Monkhorst, Mol. Phys. **108**, 3067 (2010)
- 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

$$c_l^\dagger = \sum_k U_{lk}^* \beta_k^\dagger + V_{lk} \beta_k \qquad c_l = \sum_k U_{lk} \beta_k + V_{lk}^* \beta_k^\dagger$$

- Bogoliubov vacuum $|\Phi\rangle \equiv \mathcal{C} \prod_j \beta_j |0\rangle$
- Natural extension from particle-hole language
- Simplifies some aspects of standard CC theory
- Rewrite Hamiltonian, i.e. normal order with respect to $|\Phi\rangle$
  - Derived including three-body interactions (to include implicit two-body component)

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

Each matrix element can be written as a function of NN, NNN, U, V

Bogoliubov coupled cluster theory

- Complete details can be found at A. Signoracci et al., arXiv:1412:2696
- 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 $\bar{\Omega} = e^{-\mathcal{T}} \Omega e^{\mathcal{T}}$

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

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

CCEI calculations in the *sd* shell

- Production of effective interactions
  - Similar to prior work, now focusing on full interactions in *sd* shell
  - Requires solution of ^{16,17,18}O,^{17,18}F,^{18}Ne with CC methods
  - Projection onto valence space components for shell model calculations
  - More complicated than prior work, but straightforward extension
- Additional truncation
  - Current results for $N_{\max} = 10, E_{3\max} = 10$
  - Calculations underway to match prior bases for publication
  - Expect minimal effect in low-lying spectra
  - Nevertheless, all results are preliminary
- Ongoing work on operators
  - Effective operators in the valence space
  - Implemented one-body component of charge radius operator
  - Induced two-body operator necessary, under investigation
  - Will not show results at the moment
  - Soon can treat B(E2), B(GT), double beta decay, etc. consistently

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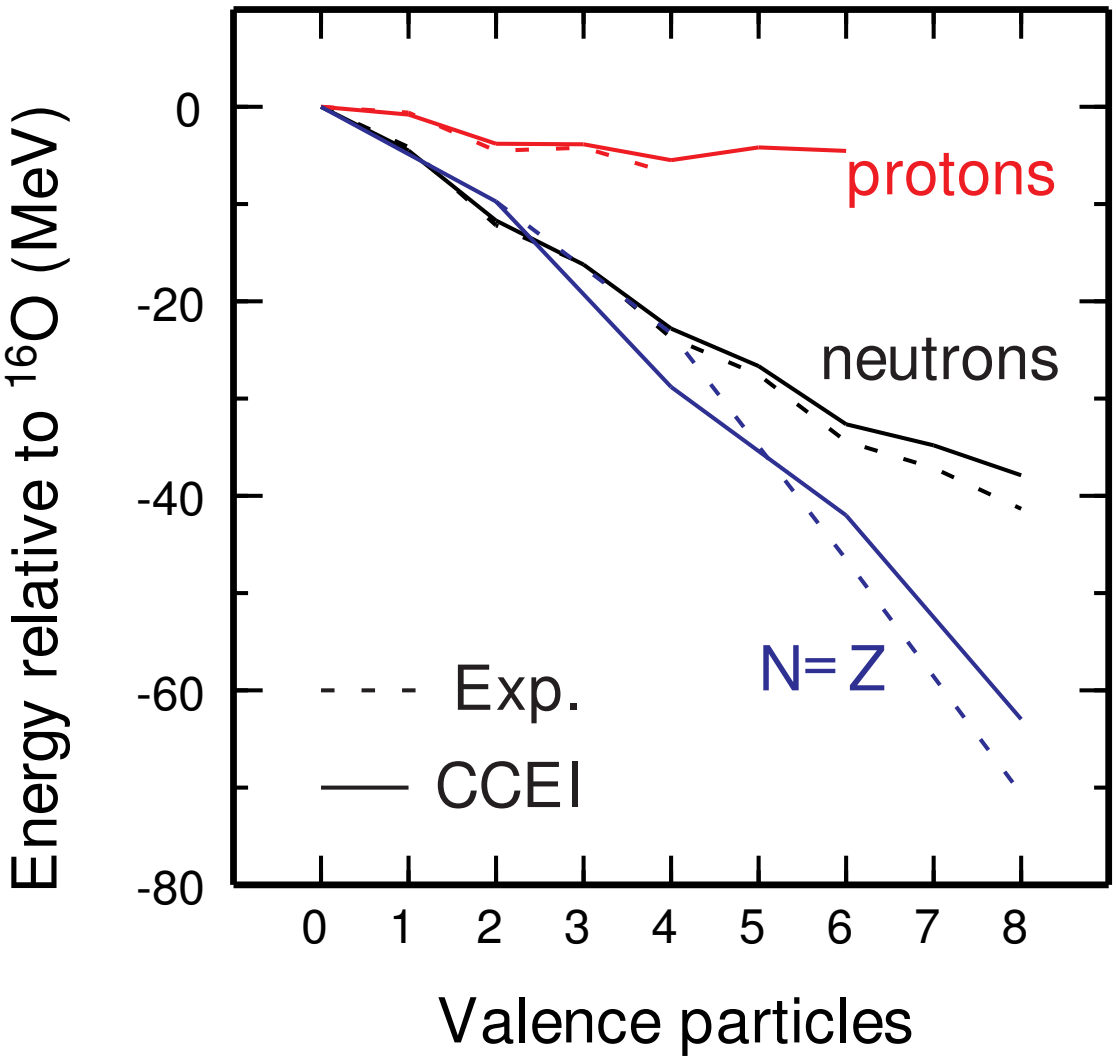
Binding energies in sd shell

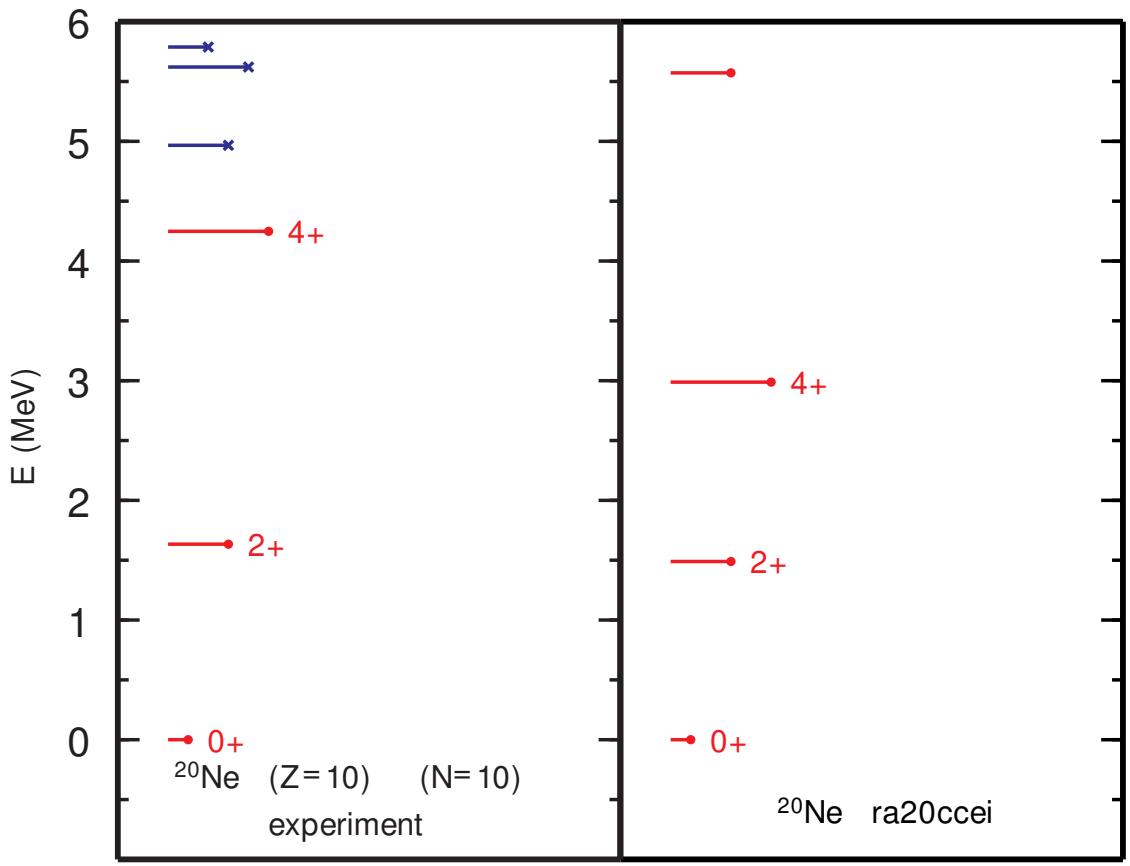
All isotopes can now be computed



Representative spectra

No fine-tuning, essentially no parameters

Deformed system



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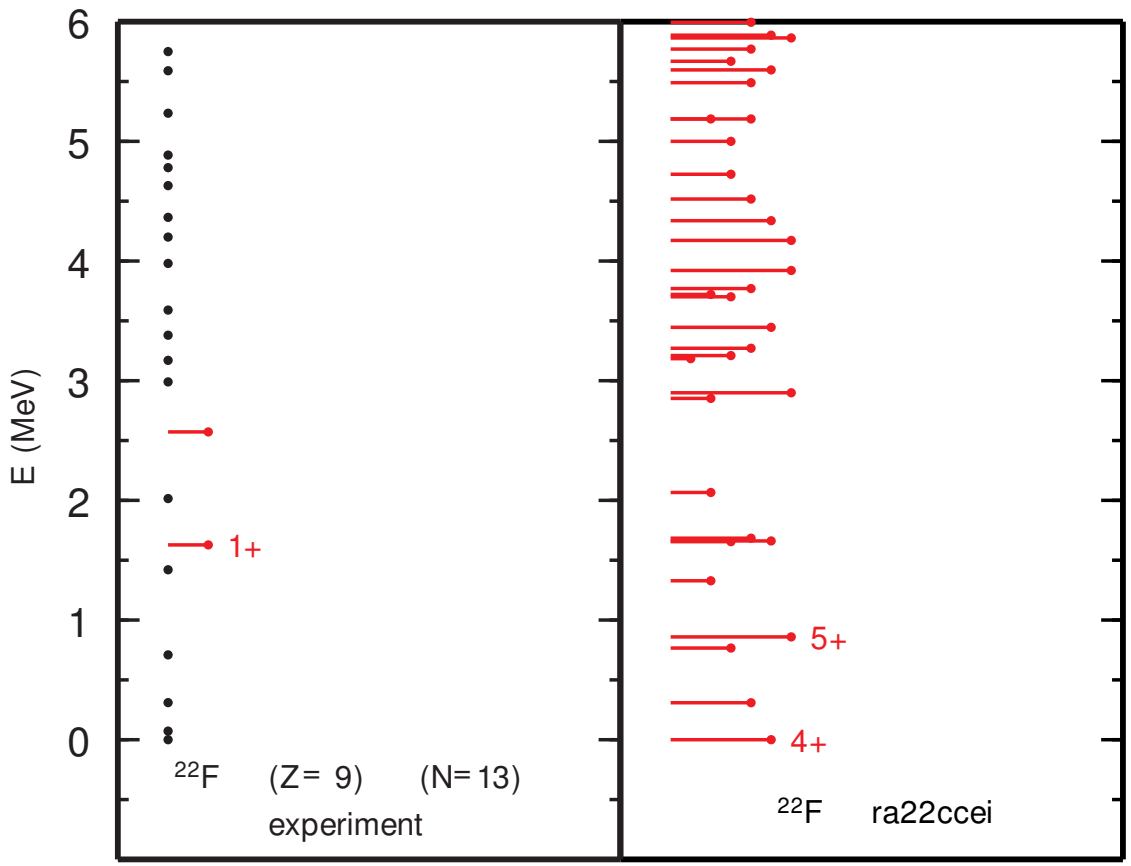
One proton systems



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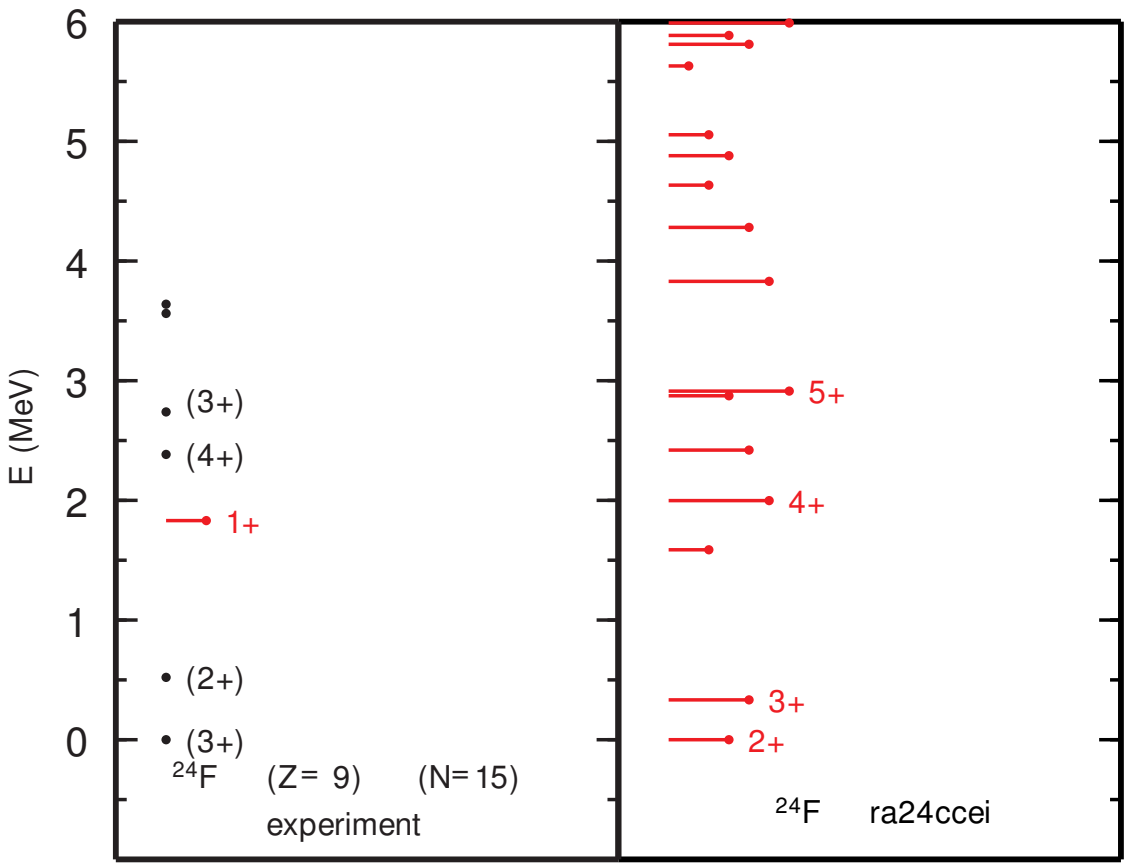

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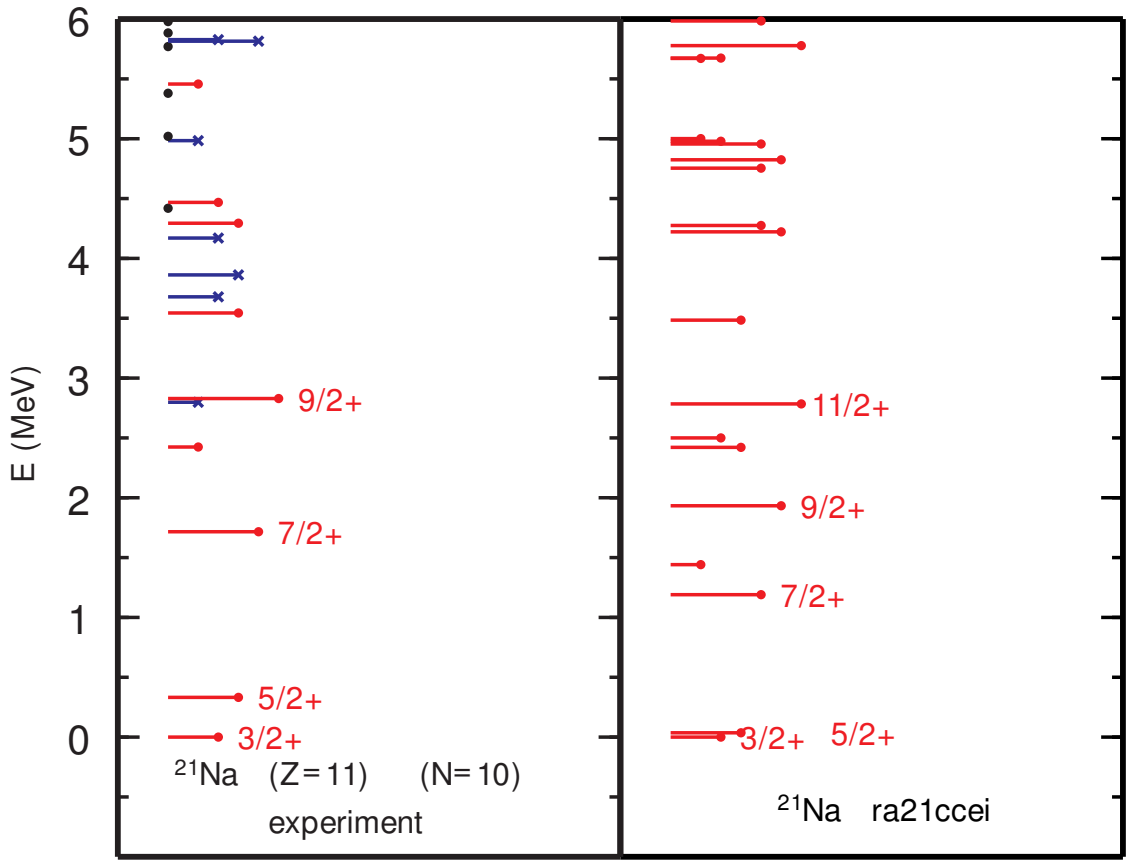
Odd mass nucleus



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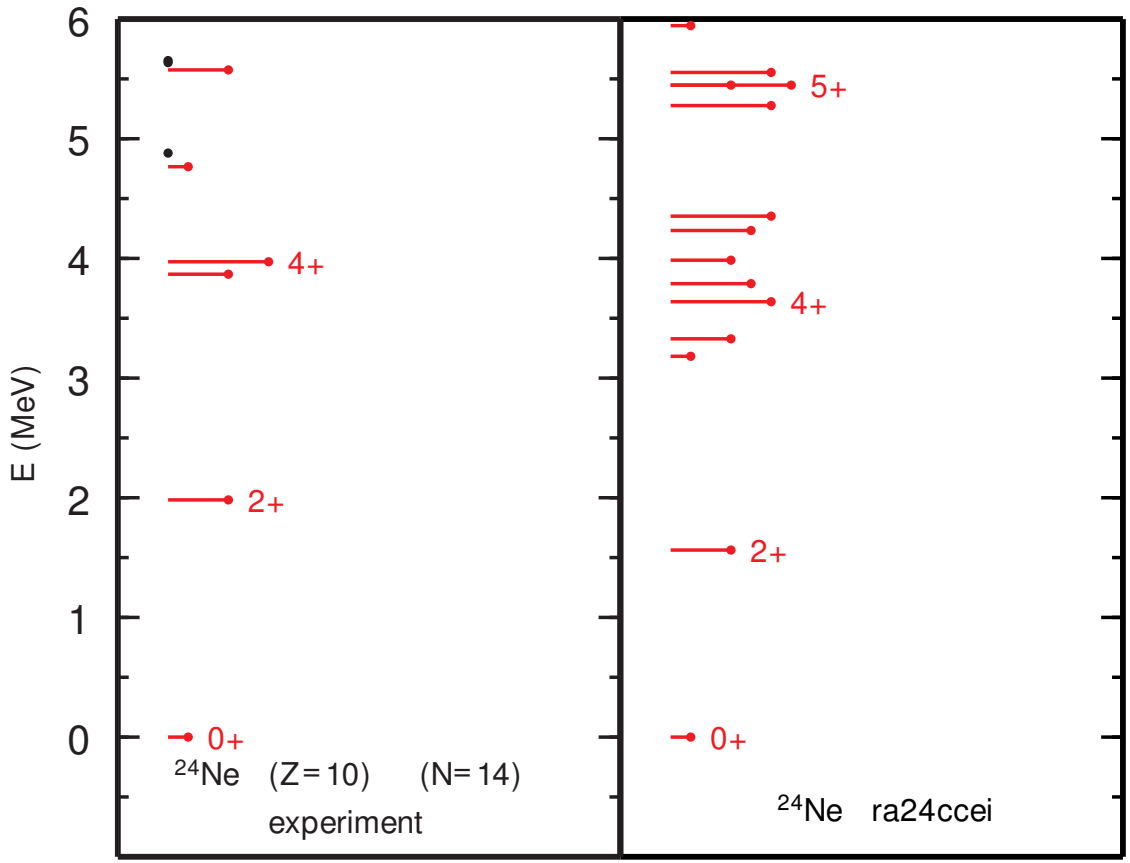
Mirror nuclei



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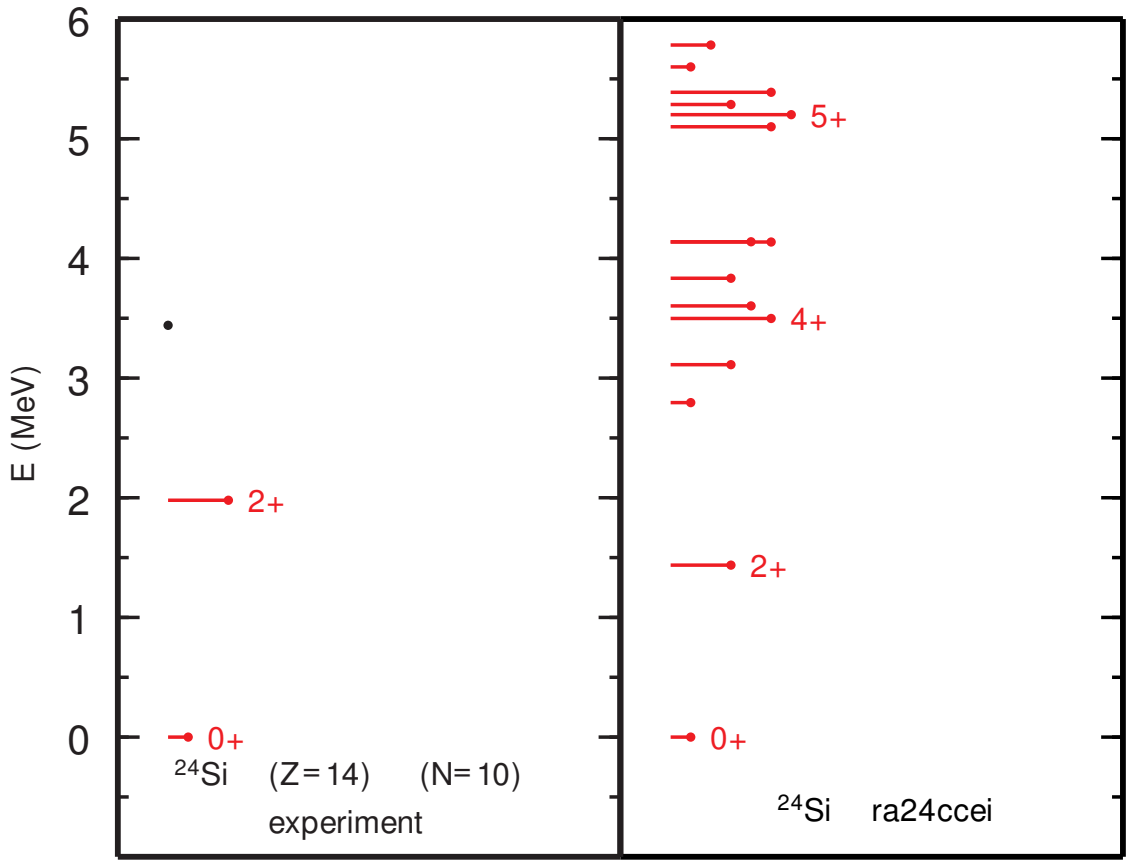

Current status of ab initio BCC theory

- Formalism
  - Derivation of BCCSD complete, evaluated equivalently in multiple ways
  - Includes two- and three-body microscopic forces
  - Can recover standard CCSD in Slater determinant limit
    - Produce more general extended coupled cluster method in straightforward limit
  - BCCSDT derivation straightforward from application of diagrammatic rules
- Implementation
  - Utilize *NN* interactions from chiral potential (+RG)
  - Bogoliubov vacuum from solution of HFB equations
    - *m*-scheme version of HFB code
    - Initialized with diagonal spherical BCS solutions
    - 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 CC calculations
  - Evaluation of one- and two- body operators
    - One-body operator A essential to solve system of equations
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Proof-of-principle calculations: Methodology

- Illustration using BCCD
  - Truncation to $\mathcal{T} = \mathcal{T}_2$
  - Should include most important effects at lowest order
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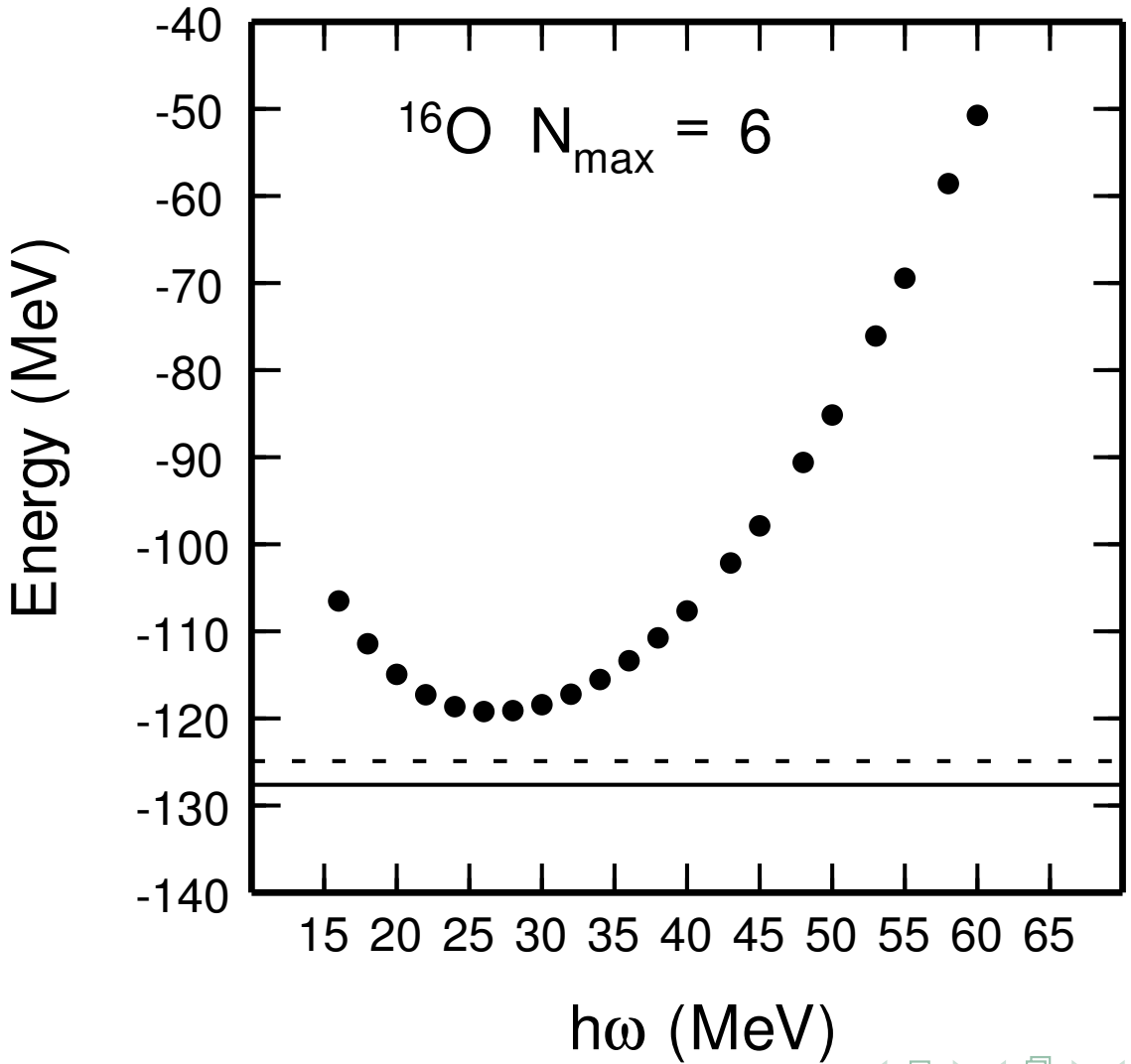
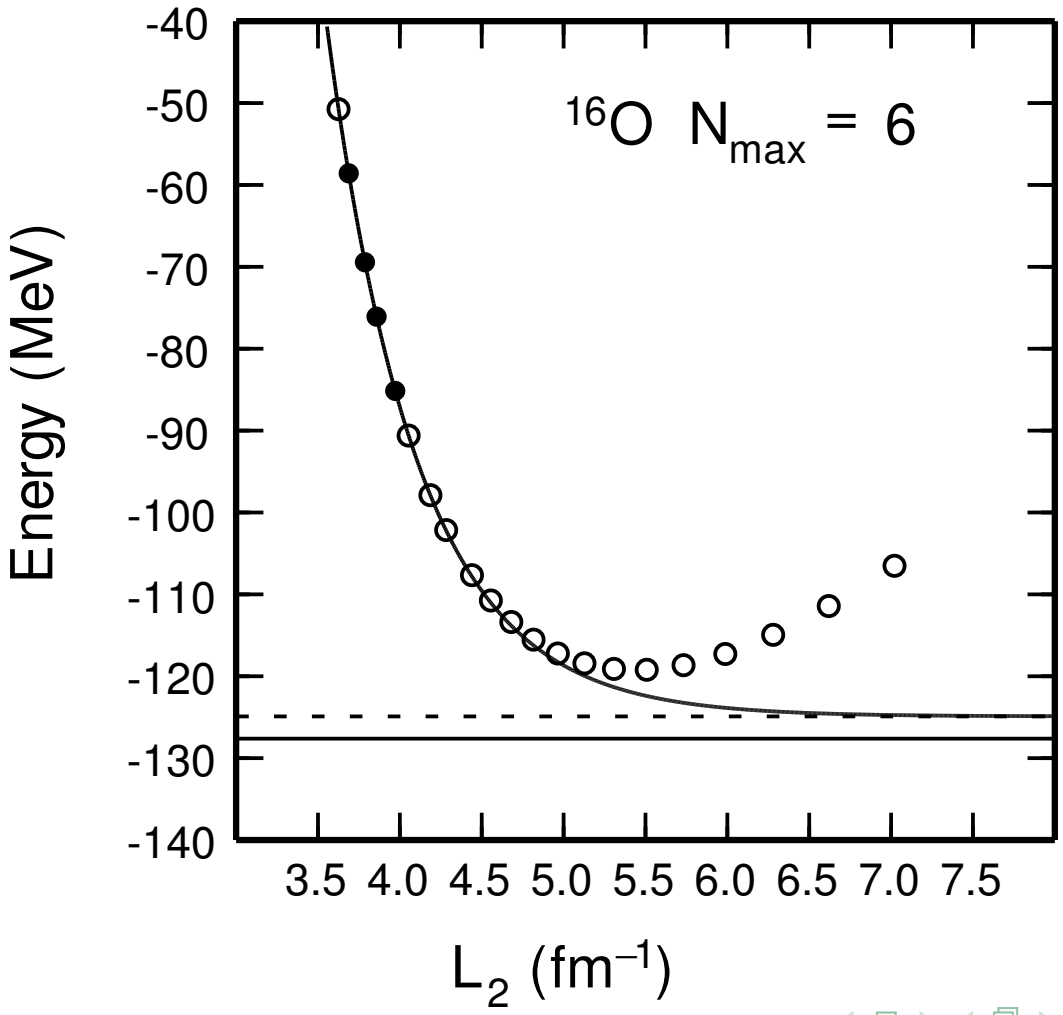
^{16}O: Energies and extrapolations

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



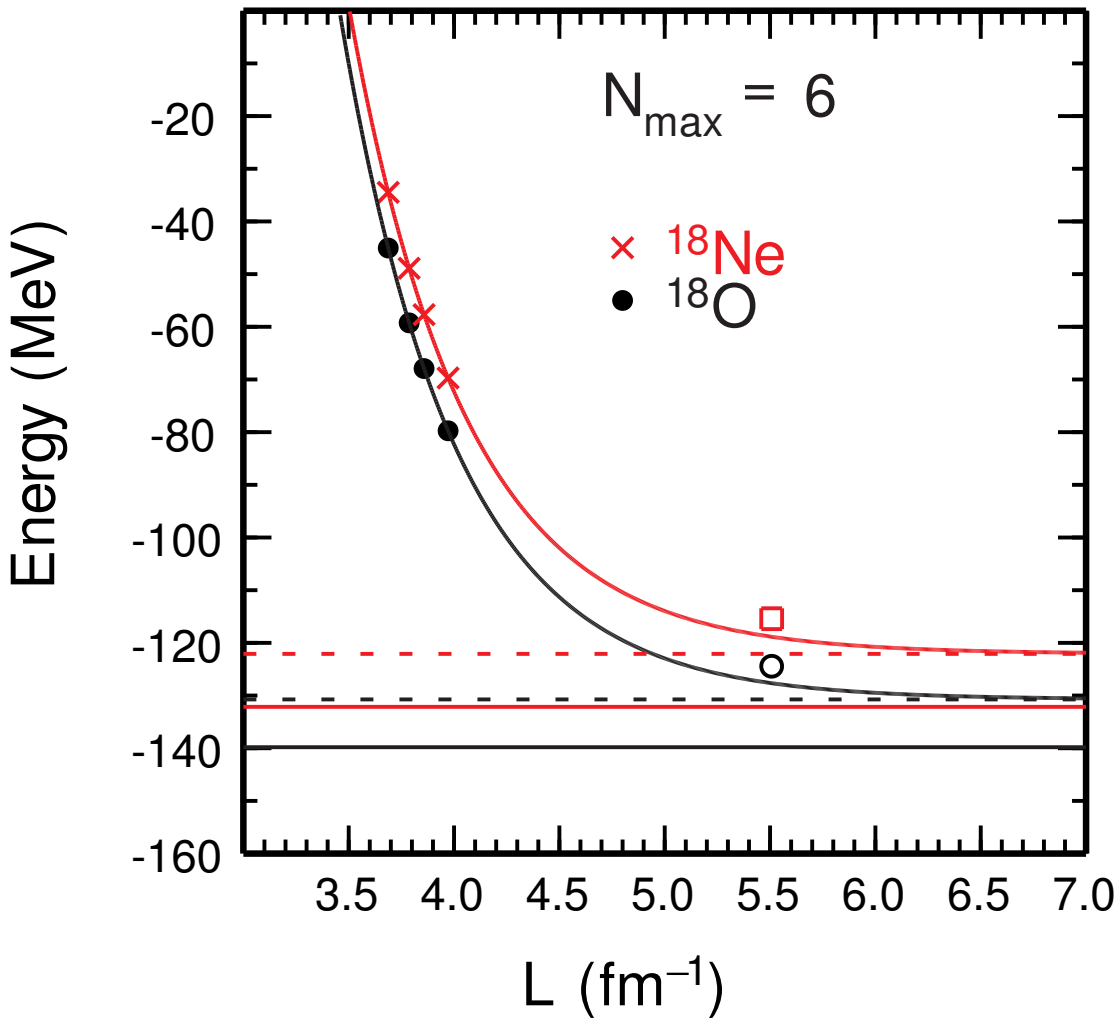
^{16}O: Energies and extrapolations

CCSD energy as a function of effective size of basis L_2
Infrared extrapolation of R.J. Furnstahl et al., J. Phys. G **42** 034032 (2015)
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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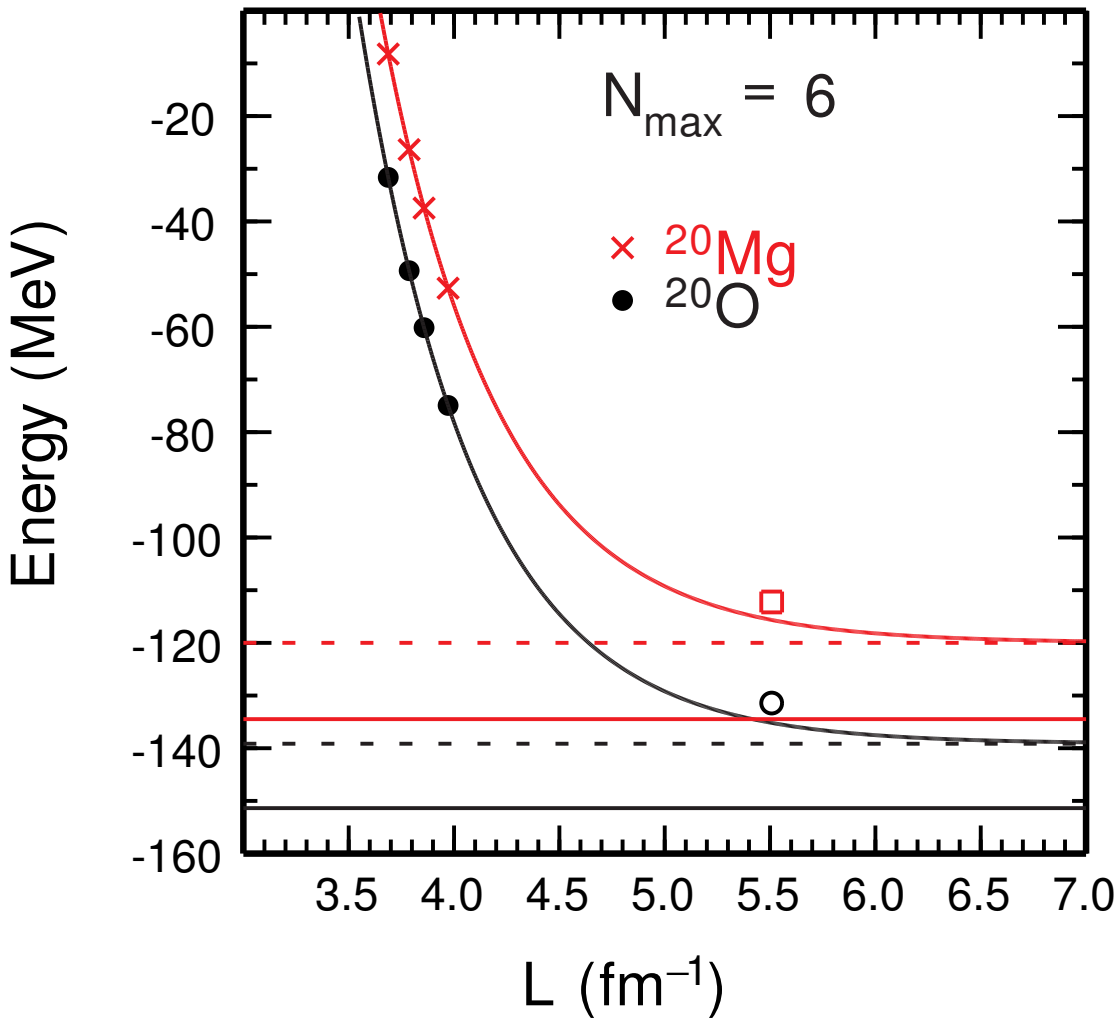

Compiled results of *sd*-shell nuclei

Nucleus	$E^{\mathrm{BCC}}_{N=6}$	$E^{\mathrm{CC}}_{N=6}$	E_∞	$E^{\mathrm{CC}}_{N=12}$	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_∞
- CCSD results
  - For ^{16}O, standard CCSD 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

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
  - Expect symmetry to be restored as more correlations are added
  - 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)

Table: σ_A at N=6

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

Short-term outlook

- Converged results of open-shell nuclei forthcoming
  - Compare CI with CC effective interactions to BCC
  - Benchmark results against in-medium SRG/Gorkov-Green's function results
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  - Compute other observables to provide predictions for upcoming experiments
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    - Significant improvement due to reduction of dimensions
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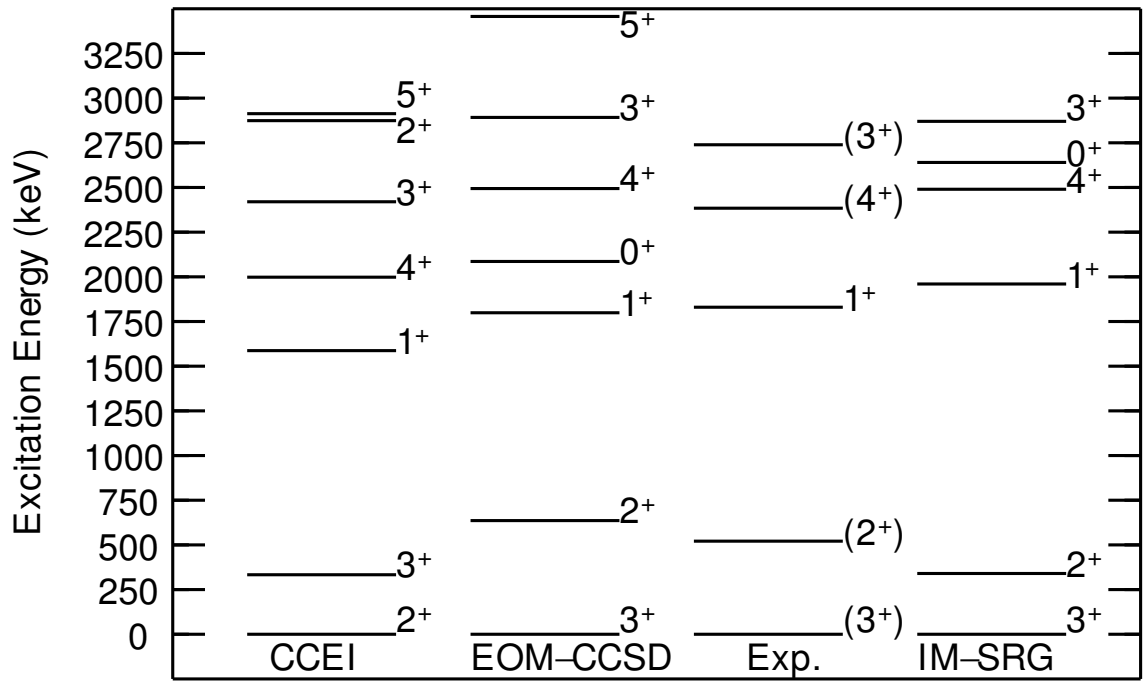
Outlook for BCC theory (including longer-term goals)

- Extend to equation-of-motion BCC
  - Equation-of-motion BCC enables the computation of odd nuclei and excited states
  - One-particle attached (or removed) is sufficient due to explicit treatment of pairing
  - With one-body density matrices, allows for computation of observables, e.g. B(E2)
- 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
  - Verify that explicit three-body component can be neglected
- 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
- Long-term extensions and ideas
  - Advances in standard CC theory typically are relevant to BCC theory as well
  - Standard coupled cluster theory is an active area of research
  - Include continuum when necessary
  - Incorporate nuclear dynamics, e.g. Lorentz Integral Transformation
  - Provide insight on nuclear interactions
  - Charge-exchange/beta-decay with isospin-invariant HFB solution

Backup slides

Comparison of spectra in ^{24}F

Same interaction used ($N_{\max} = 10, E_{3\max=10}$)



^{24}F Level Scheme

Effect of model space? Induced three-body from Okubo-Lee-Suzuki?

Standard coupled cluster (CC) theory

- State of the art computational tool
  - Many-Body Methods in Chemistry and Physics, I. Shavitt and R.J. Bartlett
  - G. Hagen et al., Phys. Rev. C **82**, 034330 (2010)
  - Successfully implemented for ^{24}O, ^{40}Ca, ^{132}Sn ...
- Exponential ansatz $|\Psi\rangle = e^T|\Phi\rangle$, where T is the cluster operator
- Cluster Operator $T = T_1 + T_2 + T_3 + \dots$

$$T_1 = \sum_{ia} t_i^a a^\dagger i$$

$$T_2 = \frac{1}{(2!)^2} \sum_{ijab} t_{ij}^{ab} a^\dagger i b^\dagger j$$

- Physical wavefunction is built through np-nh excitations of Slater determinant $|\Phi\rangle$
- Approximate solution to Schrödinger equation by truncating T
- Typically use HF solution as reference state $|\Phi\rangle$
- Schrödinger equation with similarity-transformed Hamiltonian $\mathcal{H} = e^{-T} H e^T$

$$(H - E)e^T|\Phi\rangle = 0$$
$$(\mathcal{H} - E)|\Phi\rangle = 0$$

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CC formalism

- Baker-Campbell-Hausdorff expansion

$$\mathcal{H} = H + [H, T] + \frac{1}{2!}[[H, T], T] + \frac{1}{3!}[[[H, T], T], T] + \frac{1}{4!}[[[[H, T], T], T], T] + \dots$$

- Truncation to four T operators assuming two-body Hamiltonian
- Final expression of similarity-transformed Hamiltonian

$$\mathcal{H} = H + \Big(HT\Big)_c + \frac{1}{2!}\Big(HTT\Big)_c + \frac{1}{3!}\Big(HTTT\Big)_c + \frac{1}{4!}\Big(HTTTT\Big)_c = (He^T)_c$$

- Energy and amplitude equations

$$(\mathcal{H} - E)|\Phi\rangle = 0$$

1. Energy equation multiply on the left by $\langle\Phi|$
2. Amplitude equations multiply on the left by $\langle\Phi^{ab\cdots}_{ij\dots}|$
   - Need as many amplitude equations as terms in cluster operator T
3. Assume intermediate normalization $\langle\Phi|\Psi\rangle = 1$

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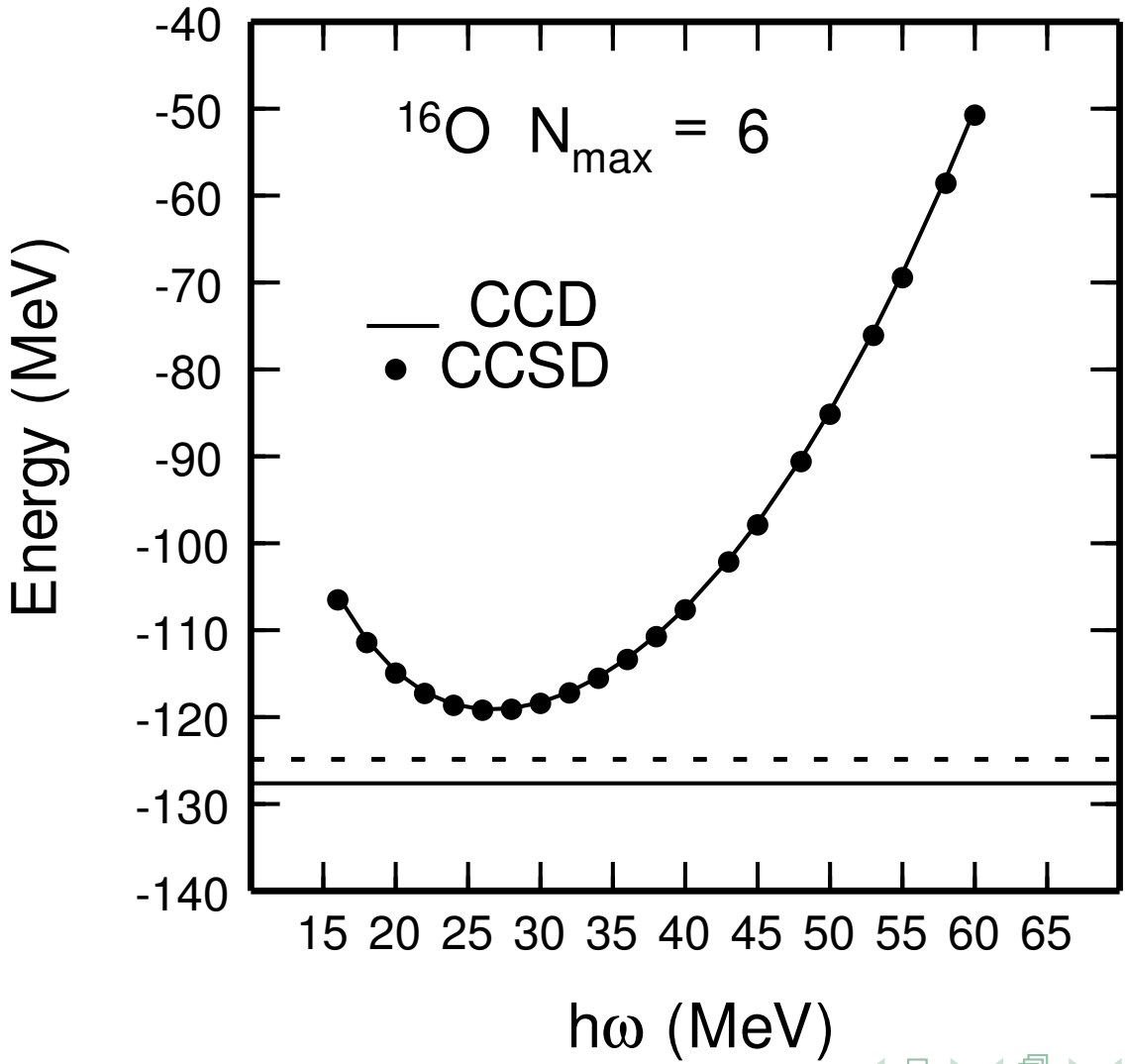
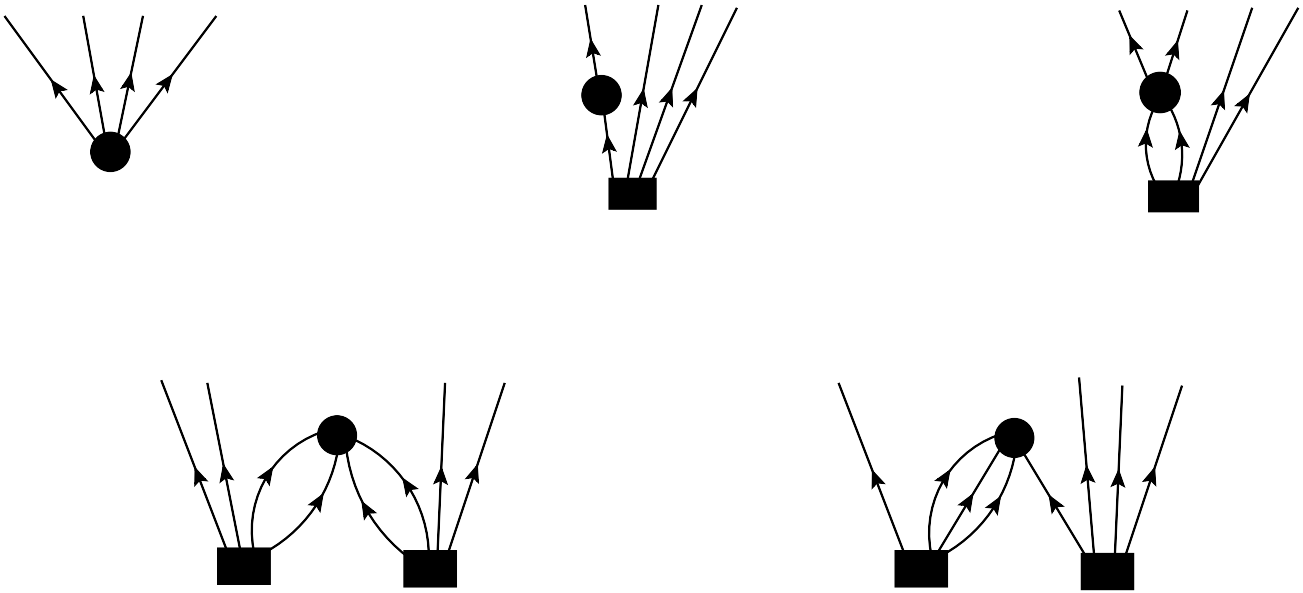
Comparison of binding energies of ^{16}O

CCD and CCSD are nearly indistinguishable

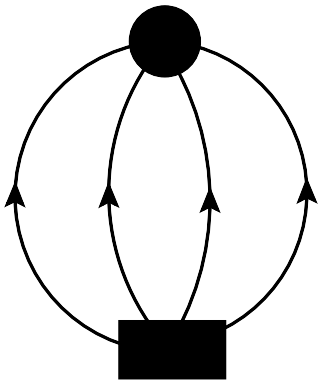


Bogoliubov coupled cluster theory with doubles (BCCD): diagrammatic

Amplitude terms



Energy term



Bogoliubov coupled cluster with doubles (BCCD): algebraic

- Energy equation

$$\Delta\Omega_0^{BCCD} = \langle\Phi|\bar{\Omega}_N|\Phi\rangle_C = \langle\Phi|\Omega_N\mathcal{T}_2|\Phi\rangle$$

- With fully antisymmetrized matrix elements of grand canonical potential
  - $\tilde{\Omega}^{ij}_{k_1\ldots k_i k_{i+1}\ldots k_{i+j}} = (-1)^{\sigma(P)}\Omega^{ij}_{P(k_1\ldots k_i|k_{i+1}\ldots k_{i+j})}$
  - $\sigma(P)$ refers to the signature of the permutation P
  - $P(\ldots|\ldots)$ denotes separation between quasiparticles and quasiholes

$$\Delta\Omega_0^{BCCD} = \frac{1}{(4!)^2}\sum_{\substack{k_1k_2k_3k_4\\k_1'k_2'k_3'k_4'}}\langle\Phi|\tilde{\Omega}^{04}_{k_1k_2k_3k_4}\beta_{k_1}\beta_{k_2}\beta_{k_3}\beta_{k_4}\tilde{\mathbf{t}}_{k_1'k_2'k_3'k_4'}\beta^\dagger_{k_1'}\beta^\dagger_{k_2'}\beta^\dagger_{k_3'}\beta^\dagger_{k_4'}|\Phi\rangle$$

- Full solution

$$\Delta\Omega_0^{BCCD} = \frac{1}{4!}\sum_{k_1k_2k_3k_4}\tilde{\Omega}^{04}_{k_1k_2k_3k_4}\tilde{\mathbf{t}}_{k_1k_2k_3k_4}$$

- Find quasiparticle amplitudes from amplitude equation

$$0 = \langle\Phi^{\alpha\beta\gamma\delta}|\bar{\Omega}_N|\Phi\rangle_C = \langle\Phi^{\alpha\beta\gamma\delta}|\Omega^{40}|\Phi\rangle + \langle\Phi^{\alpha\beta\gamma\delta}|\Omega\mathcal{T}_2|\Phi\rangle_C + \frac{1}{2}\langle\Phi^{\alpha\beta\gamma\delta}|\Omega\mathcal{T}_2^2|\Phi\rangle_C$$

BCCD- amplitude equation

$$
\begin{aligned}
0 = \tilde{\Omega}^{40}_{\alpha\beta\gamma\delta} &+ \sum_{k_1} \Big[\tilde{\Omega}^{11}_{\alpha k_1} \tilde{\mathbf{t}}_{k_1\beta\gamma\delta} + \tilde{\Omega}^{11}_{\beta k_1} \tilde{\mathbf{t}}_{\alpha k_1\gamma\delta} + \tilde{\Omega}^{11}_{\gamma k_1} \tilde{\mathbf{t}}_{\alpha\beta k_1\delta} + \tilde{\Omega}^{11}_{\delta k_1} \tilde{\mathbf{t}}_{\alpha\beta\gamma k_1} \Big] \\
&+ \frac{1}{2} \sum_{k_1 k_2} \Big[\tilde{\Omega}^{22}_{\alpha\beta k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2\gamma\delta} + \tilde{\Omega}^{22}_{\alpha\gamma k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2\delta\beta} + \tilde{\Omega}^{22}_{\alpha\delta k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2\beta\gamma} \\
&\qquad + \tilde{\Omega}^{22}_{\beta\gamma k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2\alpha\delta} + \tilde{\Omega}^{22}_{\beta\delta k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2\gamma\alpha} + \tilde{\Omega}^{22}_{\gamma\delta k_1 k_2} \tilde{\mathbf{t}}_{k_1 k_2\alpha\beta} \Big] \\
&+ \frac{1}{12} \sum_{k_1 k_2 k_3 k_4} \tilde{\Omega}^{04}_{k_1 k_2 k_3 k_4} \Big[2(\tilde{\mathbf{t}}_{\alpha k_1 k_2 k_3} \tilde{\mathbf{t}}_{k_4\beta\gamma\delta} + \tilde{\mathbf{t}}_{\beta k_1 k_2 k_3} \tilde{\mathbf{t}}_{\alpha k_4\gamma\delta} \\
&\qquad + \tilde{\mathbf{t}}_{\gamma k_1 k_2 k_3} \tilde{\mathbf{t}}_{\alpha\beta k_4\delta} + \tilde{\mathbf{t}}_{\delta k_1 k_2 k_3} \tilde{\mathbf{t}}_{\alpha\beta\gamma k_4}) \\
&\qquad + 3(\tilde{\mathbf{t}}_{k_1 k_2\alpha\beta} \tilde{\mathbf{t}}_{k_3 k_4\gamma\delta} + \tilde{\mathbf{t}}_{k_1 k_2\alpha\gamma} \tilde{\mathbf{t}}_{k_3 k_4\delta\beta} + \tilde{\mathbf{t}}_{k_1 k_2\alpha\delta} \tilde{\mathbf{t}}_{k_3 k_4\beta\gamma}) \Big]
\end{aligned}
$$

- Also need constraint equation for average particle number
- Solve system of equations iteratively
- Update Lagrange parameter each iteration