Adapting the ab-initio IMSRG for open-shell atomic systems

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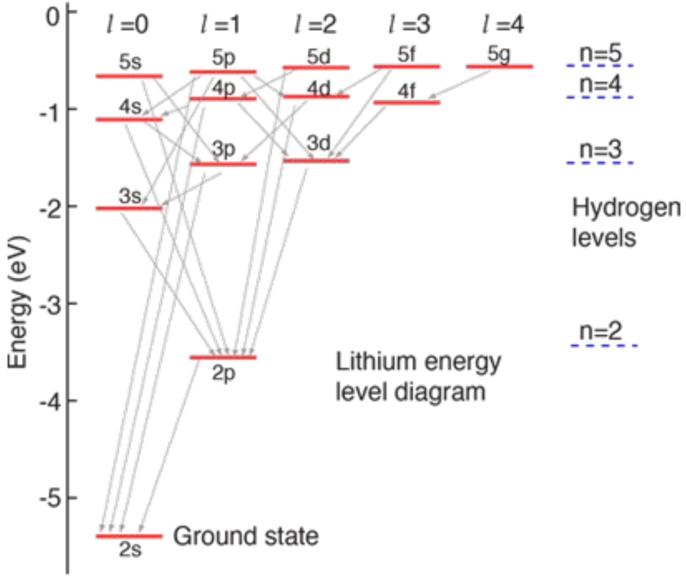
Motivation: Isotope Shift in Atoms

$$H = \sum_{i}^{N} -\frac{\nabla_i^2}{2} - \frac{Z}{r_i} + \sum_{i<j}^{N} \frac{1}{r_{ij}}$$



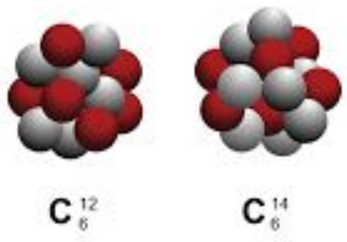
➔ Many-body atomic hamiltonian - assuming **point-like nucleus**

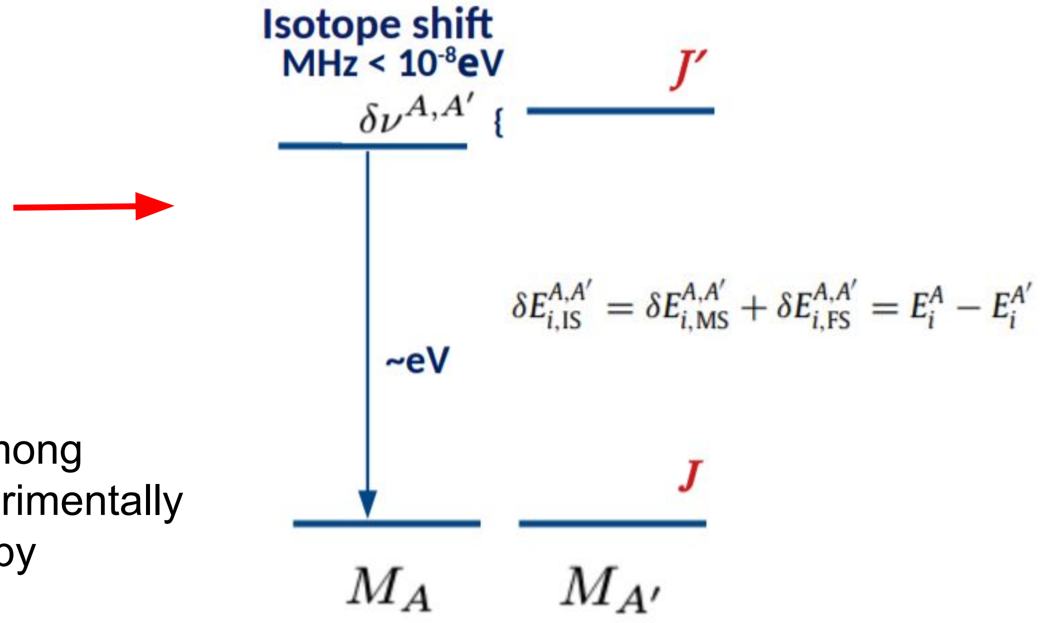
➔ Get spectrum - can be experimentally measured by spectroscopy

Motivation: Isotope Shift in Atoms

$$\frac{1}{r} \longrightarrow \rho_{nuc}(r)$$

➔ Nuclear structure modifies Coulomb potential





➔ Differing ***nuclear structure*** among isotopes ***shifts spectra -*** experimentally measured by laser spectroscopy

Motivation: Isotope Shift in Atoms

Mass Shift:

$$\delta E_{i,\mathrm{MS}}^{A,A'} = \left(\frac{M'-M}{MM'}\right)(K_{i,\mathrm{NMS}} + K_{i,\mathrm{SMS}}) = \left(\frac{M'-M}{MM'}\right) K_{i,\mathrm{MS}}$$

$$\hat{H}_{NMS} = \frac{1}{2M}\sum_{j=1}^{N}\left(\mathbf{p}_j^2 - \frac{\alpha Z}{r_j}\alpha_j \cdot \mathbf{p}_j\right)$$

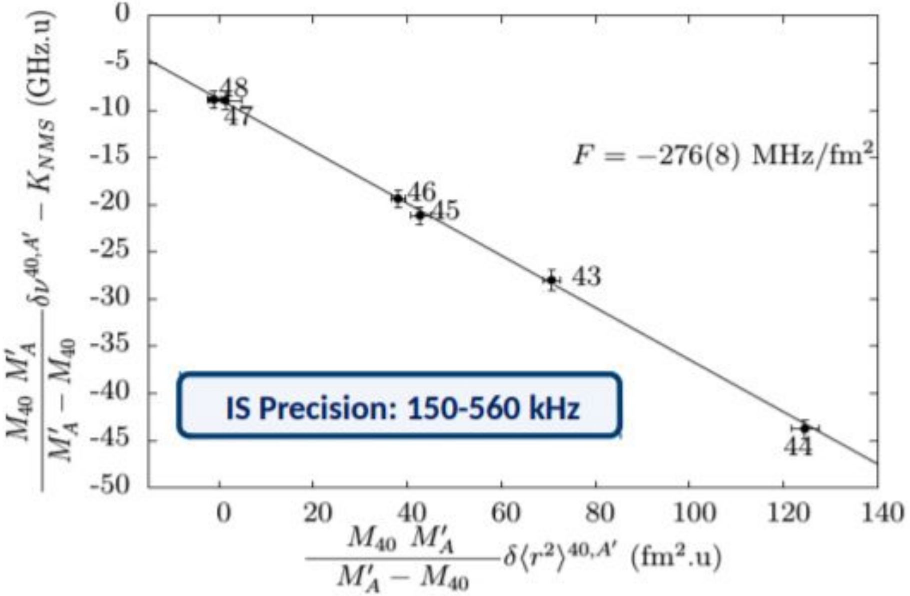
$$\hat{H}_{SMS} = \frac{1}{2M}\sum_{j\neq k}^{N}\left(\mathbf{p}_j \cdot \mathbf{p}_k - \frac{\alpha Z}{r_j}\alpha_j \cdot \mathbf{p}_k\right)$$

Field Shift:

$$\delta E_{i,\mathrm{FS}}^{(1)A,A'} = -\int_{\mathbf{R}^3}\left[V^A(\mathbf{r}) - V^{A'}(\mathbf{r})\right]\rho_i^e(\mathbf{r})d^3\mathbf{r}, \quad \approx \sum_n F_{i,n}\delta\langle r^{n+2}\rangle^{A,A'}$$

$$\delta\nu^{A,A'} = K_{MS}\frac{M_{A'} - M_A}{M_{A'}M_A} + F\delta\langle r^2\rangle^{A,A'}$$

Motivation: Isotope Shift in Atoms



Ca:<r^2>:Garcia Ruiz et al. Nature Phys. 12, 594 (2016)

➔ Non-linearities in "**King plots**" point to new electron-nucleon interactions.

Flambaum et al. Phys Rev A 97, 032510 (2018)

➔ Laser spectroscopy can be used to probe BSM physics

Stadnik et al. Phys Rev Lett 120, 223202 (2018) - Long range neutrino mediated forces

Similarity Renormalization Group (SRG)

Basic Idea - Diagonalize a matrix by performing continuous Unitary transformations on it, using a suitable generator

$$H(s) = U(s)HU^{\dagger}(s) \equiv H^{\mathrm{d}}(s) + H^{\mathrm{od}}(s) \rightarrow H^{\mathrm{d}}(\infty)$$

➔ Unitarity preserves inner products - eigenvalues unchanged

$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = [\eta(s), H(s)]$$

$$\eta_I(s) = \left[H^{\mathrm{d}}(s), H^{\mathrm{od}}(s)\right]$$

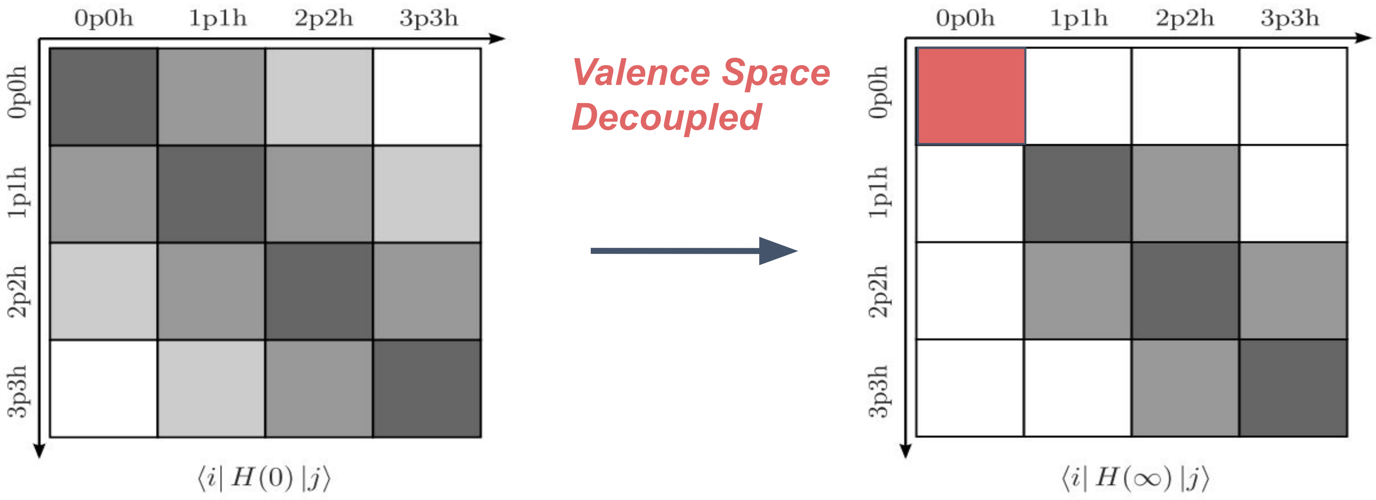
Flow equation for generator - $\eta(s)$

"Wegner Generator"

Valence Space In-Medium SRG

$$H^{\text{od}} = \langle p|H|h\rangle + \langle pp|H|hh\rangle + \cdots + \text{h.c.}$$

➔ Redefine Hamiltonian using particle-hole excitations from Hartree-Fock ground state.

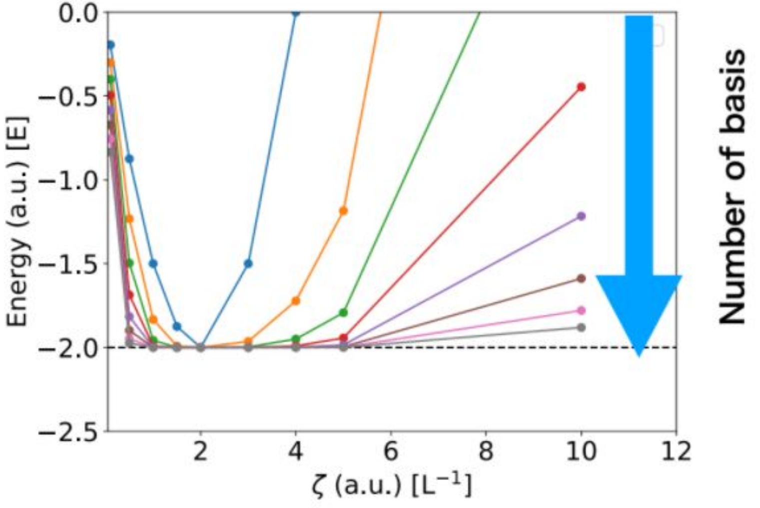


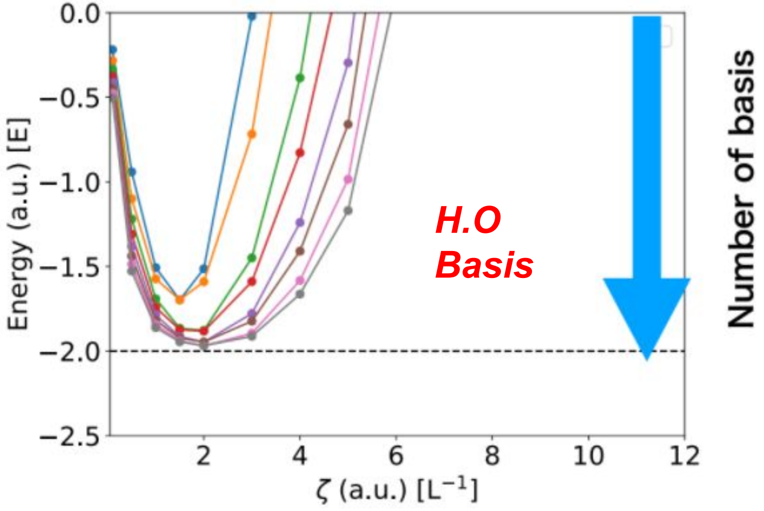
Setup for Atomic Systems

Choice of basis function: ***Laguerre function*** + Spherical Harmonics

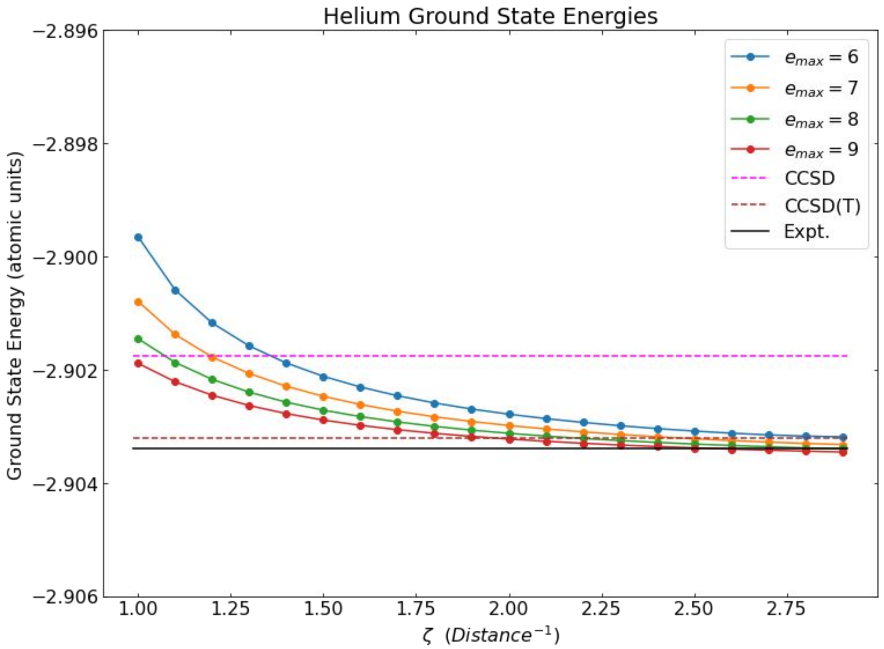
$$R_{nl}(r) = \sqrt{\left(\frac{2\zeta}{a_0}\right)^3 \frac{n!}{(n+2l+2)!}} x^l e^{-x/2} L_n^{2l+2}(x), x = \frac{2\zeta}{a_0} r$$

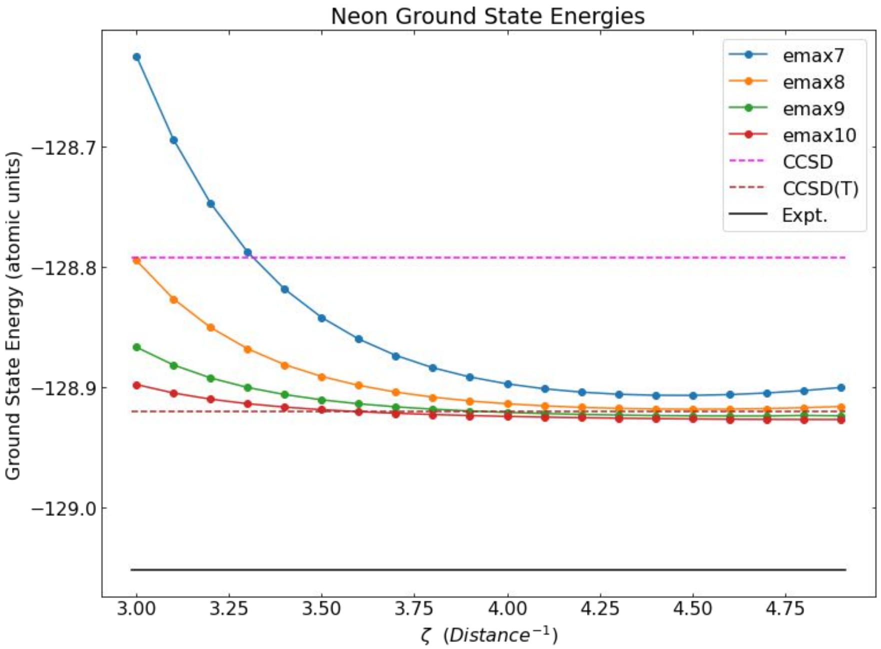
A. E. McCoy and M. A. Caprio, J. Math. Phys. 57, (2016)





Results - Closed shell

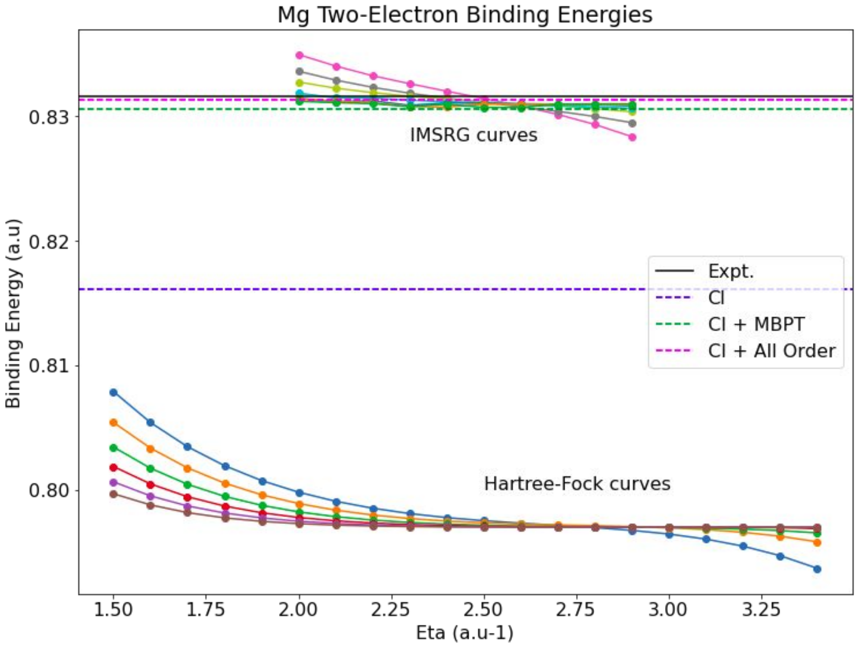


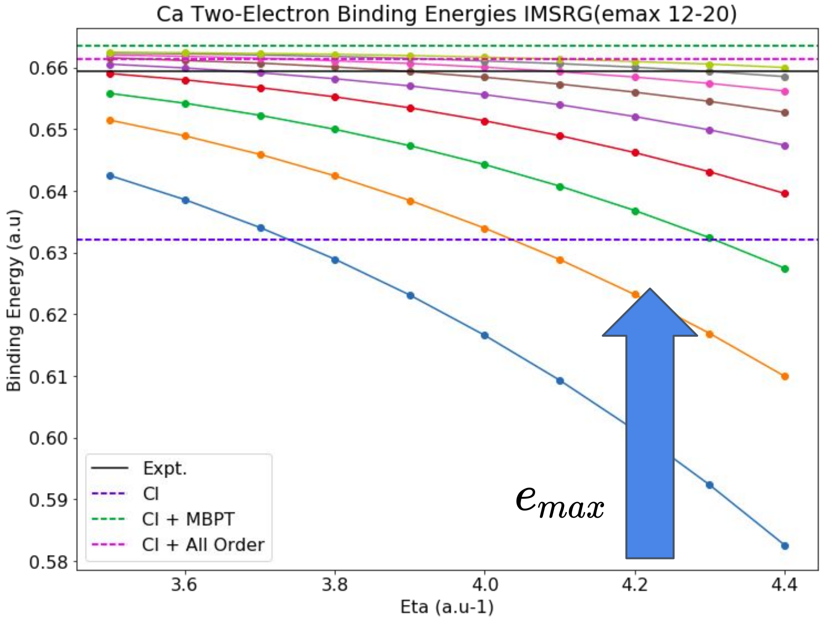


Stopkowicz S, et al. J Chem Phys. 2015

Results - Open shell

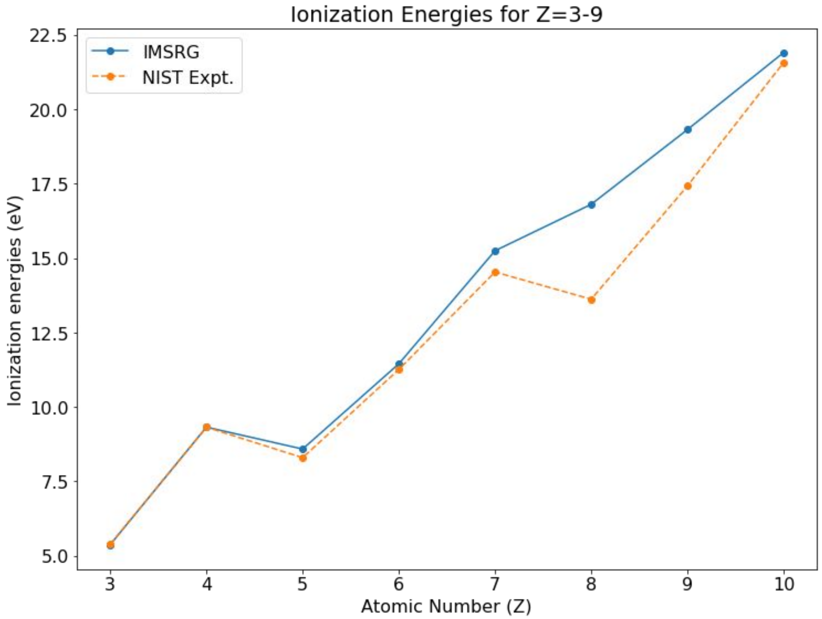
➔ Valence space diagonalization done by k-shell to get excited states

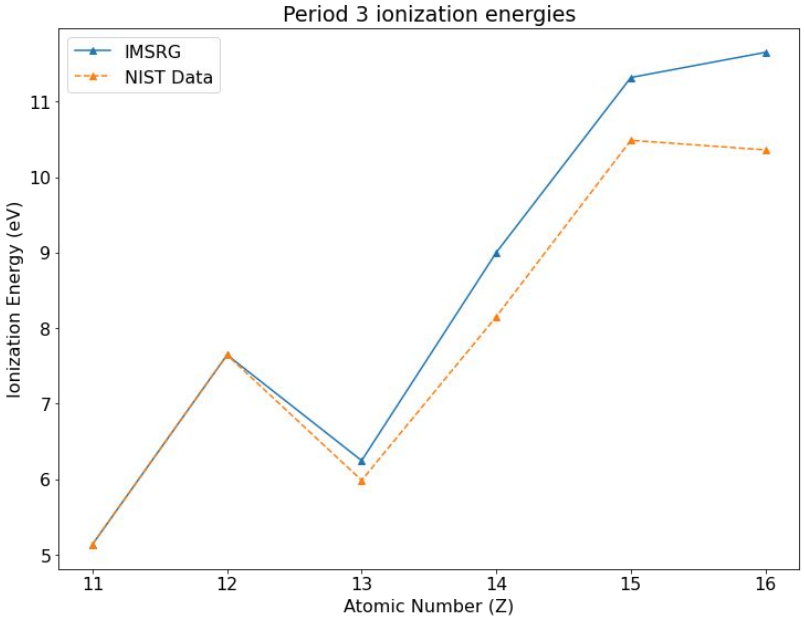




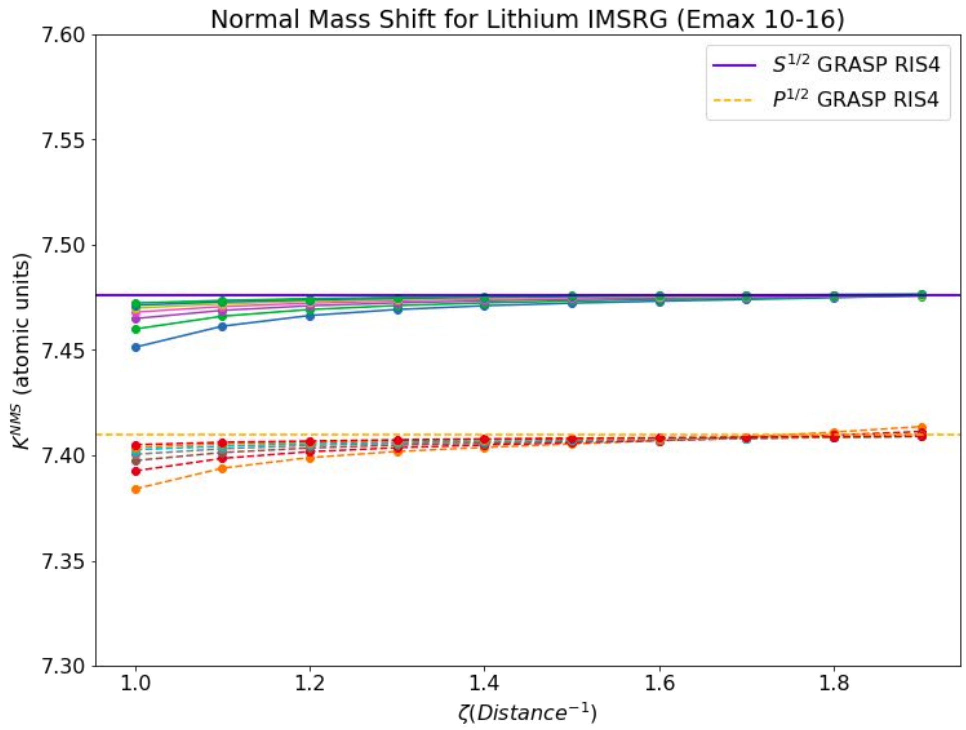
M. S. Safronova et al. Phys. Rev. A 80, 012516 (2009)

Results - Open Shell



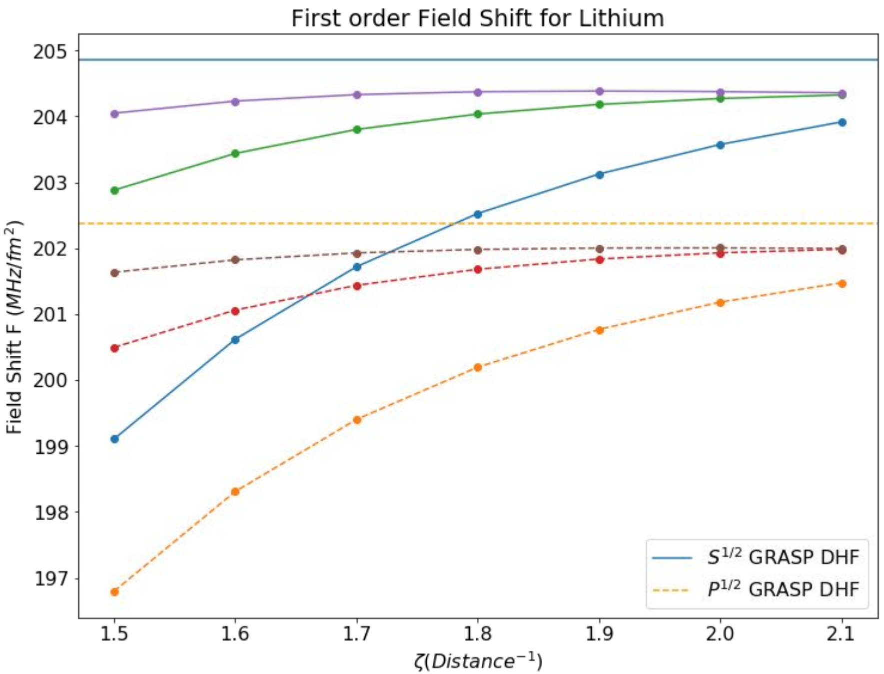


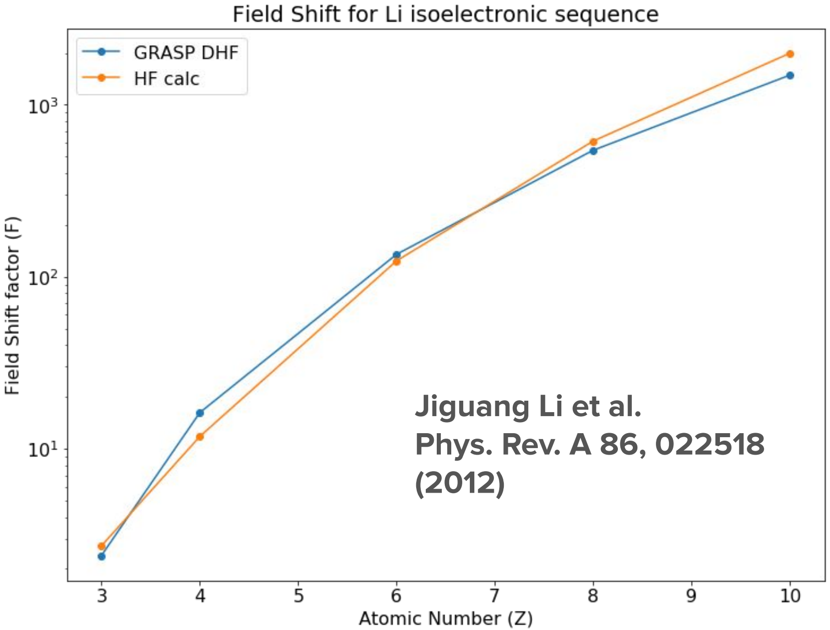
Results - Isotope Shifts



➔ Results comparable to current state of the art Relativistic Isotope Shift program (RIS4)
Ekman et al. (2019)

Results - Isotope Shifts





Jiguang Li et al.
Phys. Rev. A 86, 022518 (2012)

Future Work

➔ Many body relativistic corrections - ***Breit Hamiltonian (Partial progress)***

$$H = H_{el} + H_{rel} + H_D + H_{SSC} + H_{OO} + H_{SO} + H_{SSD}$$

- Spin-Orbit / Orbit-Orbit interactions

➔ Higher order corrections to isotope shifts

➔ Incorporate nuclear moments for hyperfine structure effects.

$$W^{M1}_{F,J} = A_{\mathrm{hf}}\mathbf{I}.\mathbf{J}$$

$$W^{E2}_{F,J} = B_{\mathrm{hf}}\frac{3(\mathbf{I}.\mathbf{J})^2 + \frac{3}{2}(\mathbf{I}.\mathbf{J}) - I(I+1)J(J+1)}{2I(2I-1)J(2J-1)}.$$

Summary

- ➔ Isotope shifts in atomic spectra allow probing of nuclear structure through laser spectroscopy.

- ➔ VS-IMSRG is a robust ab-initio method to diagonalize atomic many-body Hamiltonians, comparable to Coupled Cluster theory, MBPT.

- ➔ Promising results for spectra, isotope shift factors - with potential for further extensions (fine/hyperfine structure).

Thank You!
Merci!

IMSRG equation

$$\hat{H} = E + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{4}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{36}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

$$E = \left(1 - \frac{1}{A}\right)\sum_a \langle a|\,\hat{t}^{[1]}\,|a\rangle n_a + \frac{1}{2}\sum_{ab}\langle ab|\,\frac{1}{A}\hat{t}^{[2]} + \hat{v}^{[2]}\,|ab\rangle n_a n_b + \frac{1}{6}\sum_{abc}\langle abc|\,\hat{v}^{[3]}\,|abc\rangle n_a n_b n_c\,,$$

$$f_{ij} = \left(1 - \frac{1}{A}\right)\langle i|\,\hat{t}^{[1]}\,|j\rangle + \sum_a \langle ia|\,\frac{1}{A}\hat{t}^{[2]} + \hat{v}^{[2]}\,|ja\rangle n_a + \frac{1}{2}\sum_{ab}\langle iab|\,\hat{v}^{[3]}\,|jab\rangle n_a n_b\,,$$

$$\Gamma_{ijkl} = \langle ij|\,\frac{1}{A}\hat{t}^{(2)} + \hat{v}^{[2]}\,|kl\rangle + \sum_a \langle ija|\,\hat{v}^{[3]}\,|kla\rangle n_a\,,$$

$$W_{ijklmn} = \langle ijk|\,\hat{v}^{[3]}\,|lmn\rangle\,.$$