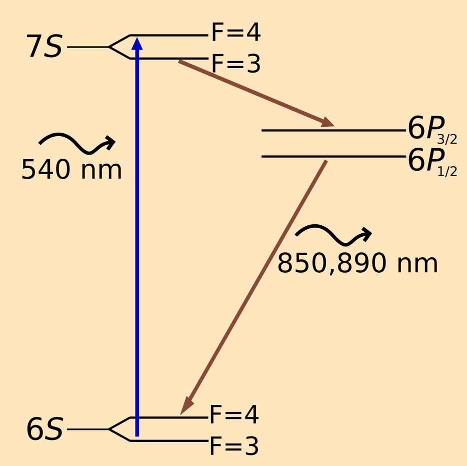
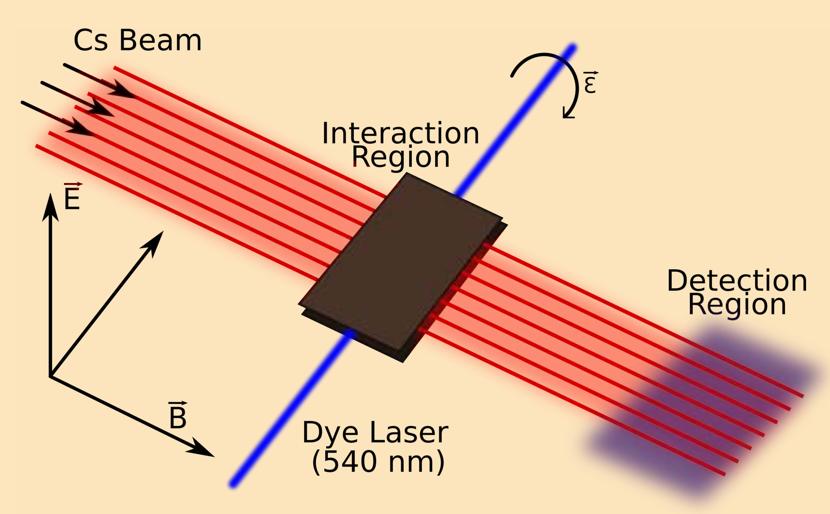
High-precision atomic structure theory: Electric dipole transition amplitudes

Benjamin M. Roberts, Carter J. Fairhall, Jacinda S. M. Ginges, arXiv:2211.11134

Electric dipole (E1) matrix elements

- Leading contribution to atomic transitions
- Determine lifetimes, decay widths
- Required for studies of
  - Atomic parity violation
  - Electric dipole moments
  - Atomic polarisabilities
  - Development of atomic clocks
  - Test atomic theory at the 0.1% level





Atomic Parity Violation

- Forbidden transitions become allowed: weak interaction
- Z-boson exchange between quarks and atomic electrons
- Measure rate: extract nuclear weak charge
- Weak charge: low-energy probe of Standard Model
- Atomic theory is bottle-neck. Strive for 0.1% accuracy

Wood, Bennett, Cho, Masterson, J. Roberts, Tanner, Wieman, Science 275, 1759 ('97)

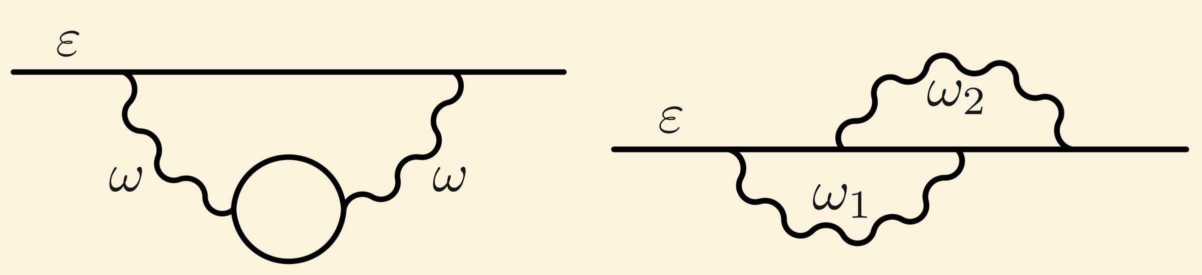
Theory: Dzuba, Flambaum, Ginges, Phys. Rev. D 66, 076013 ('02);
Porsev, Beloy, Derevianko, Phys. Rev. Lett. 102, 181601 ('09);
Dzuba, Berengut, Flambaum, BMR, Phys. Rev. Lett. 109, 203003 ('12)

Many-body atomic method: All-orders Feynman technique

- Accurate method based on Feynman diagram technique
- Dominating diagrams summed exactly to all-orders:
  - Screening of Coulomb interaction - polarisation of core
  - Hole-particle interaction (modification of HF potential)
  - Chaining of correlation potential (Brueckner orbitals)
- Core polarisation (RPA): all-orders in Coulomb interaction
- Highly accurate, highly stable, highly efficient
- No basis/spectrum required: integrate over frequencies
- Integration performed in complex plane: avoid poles
- Feynman Greens' function: evaluated at imaginary energies

Dzuba, Flambaum Sushkov, Phys. Lett. A 140, 493 (1989).

Correlation potential: direct and exchange

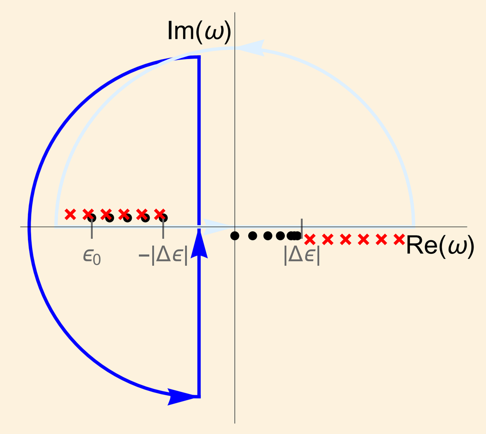


$$\Sigma^{(\mathrm{direct})} = \int \frac{\mathrm{d}\omega}{2\pi} G_{12}(\varepsilon+\omega) Q_{1i} \Pi_{ij}(\omega) Q_{j2}$$

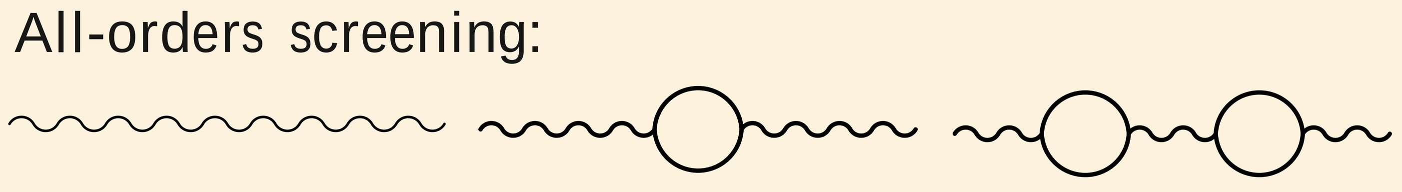
Polarisation operator:

$$\Pi_{12}(\omega) = \int \frac{\mathrm{d}\varepsilon'}{2\pi} G_{12}(\varepsilon') G_{21}(\omega+\varepsilon').$$

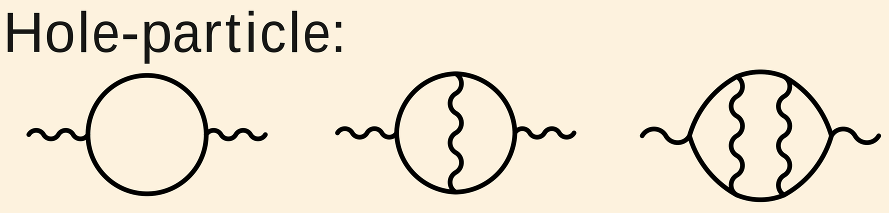
Rotate to complex plane:



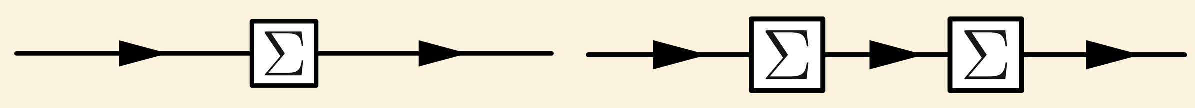
All-orders screening:



Hole-particle:



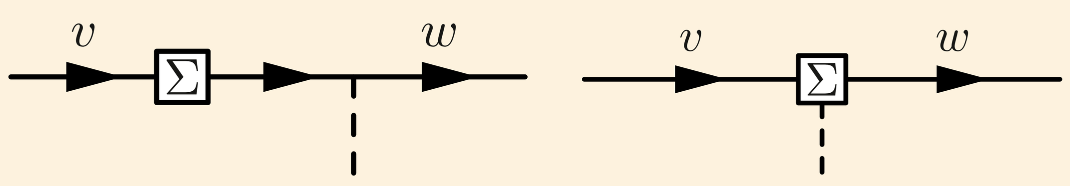
Chaining (Brueckner):



Other corrections:

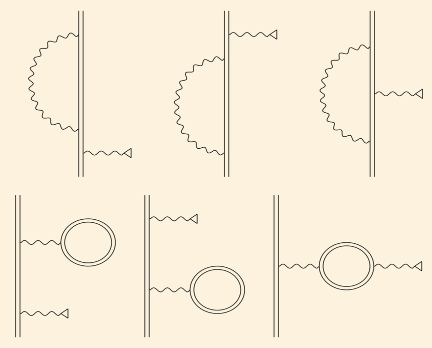
- Structure radiation (external field inside correlations)
- Renormalisation of many-body wavefunction
  Johnson, Idrees, Sapirstein, Phys. Rev. A 35, 3218 ('87);
  Dzuba, Flambaum, Silvestrov, Sushkov, J. Phys. B 20, 1399 ('87)
- Breit (relativistic correction to Coulomb interaction)
  Derevianko, Phys. Rev. Lett. 85, 1618 (2000);
  Dzuba, Harabati, Johnson, Safronova, Phys. Rev. A 63, 044103 (2001)
- Radiative (one-loop) quantum electrodynamics
  Flambaum, Ginges, Phys. Rev. A 72, 052115 (2005)

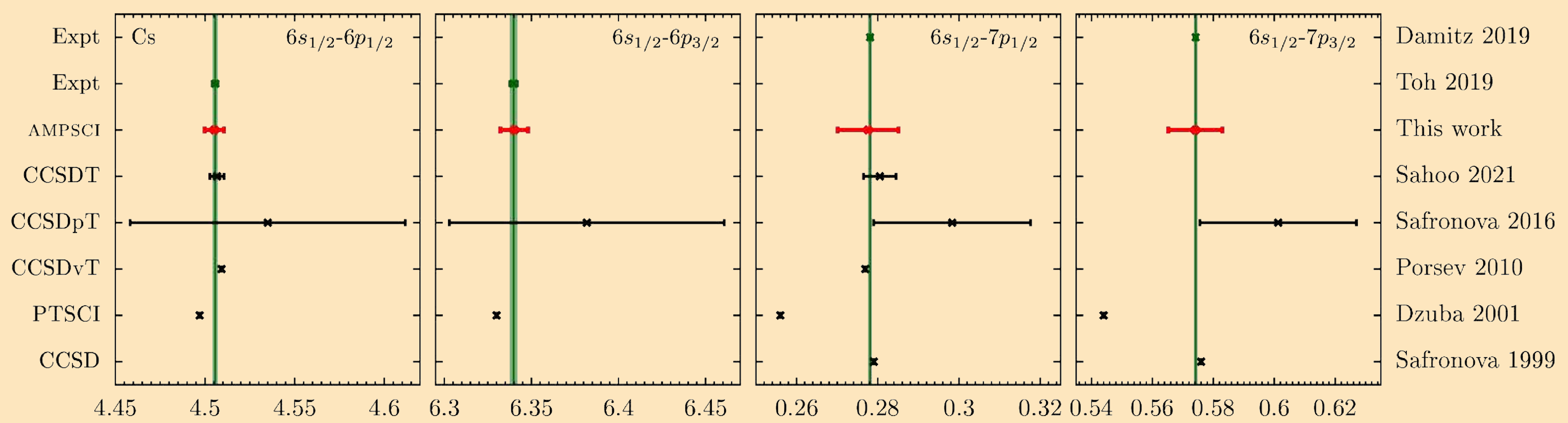
Structure Radiation:

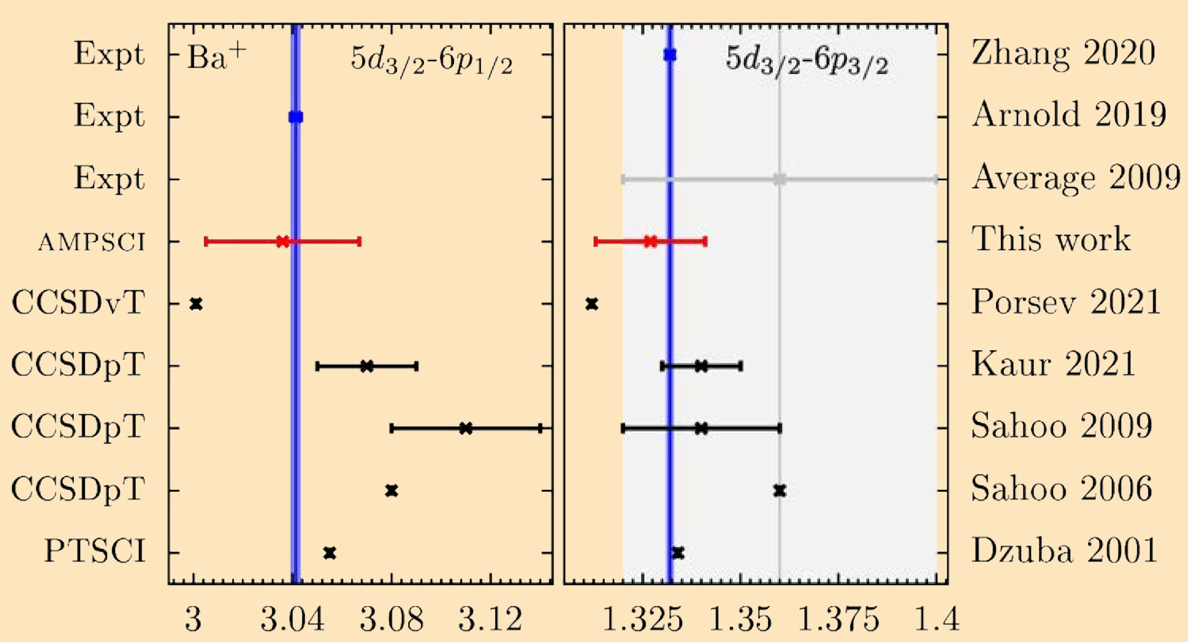


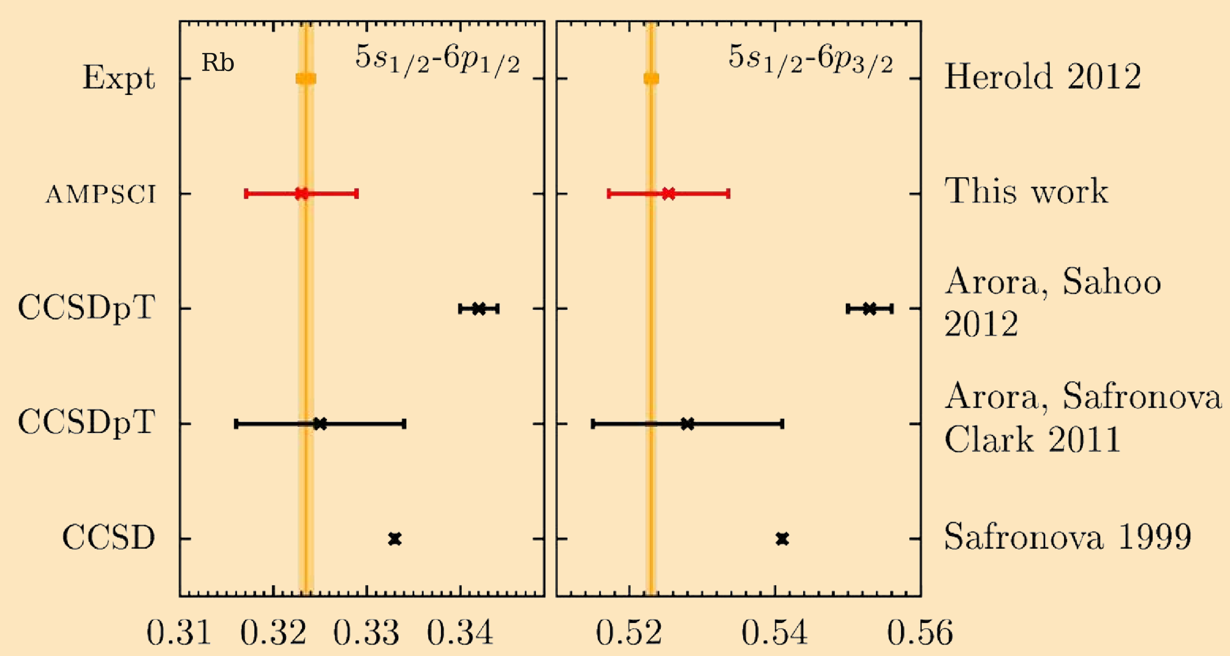
Self-energy:

Vacuum Polarisation:



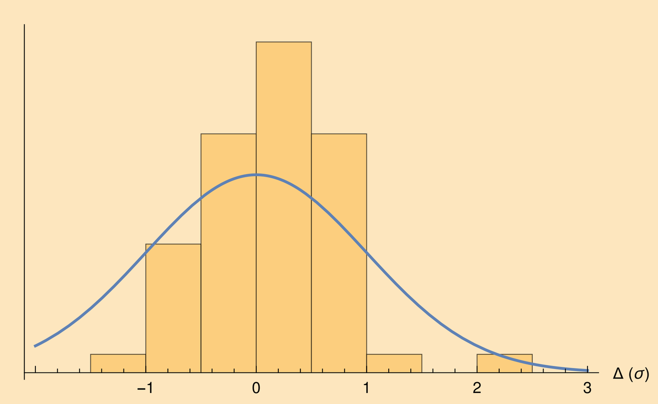






Results: Extraordinary Accuracy

- E1 amplitudes for s,p,d states of heavy atoms
- Alkali metals: K, Rb, Cs, Fr
- Alkali-like ions: Ca^+, Sr^+, Ba^+, Ra^+
- ~50 high-precision experimental E1 to compare
- + Large number of previous theory results
- Statistical analysis: better than expected
- Theory error-bars are robust, overly cautious
- 50% lie within experimental uncertainties: unprecedented theoretical precision
- Provably at level of 0.1% accuracy
- Some other calculations: underestimated errors



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Draft (pre-release) version of code available: **ampsci.dev/**