Lamb shifts and many-body effects in neutral atoms

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Synopsis We study the effect of inclusion of many-body corrections on the self-energy and vacuum polarization shifts in the binding energies in alkali-metal atoms. It is demonstrated that many-body effects must be included for an accurate description of the shifts, particularly for non-s-states.

Atomic many-body calculations in heavy neutral atoms have reached the level of accuracy where in some applications, e.g. atomic parity violation, account of quantum electrodynamic (QED) radiative corrections is important.

We explore the role of many-body effects on the QED radiative shifts (Lamb shifts) in the binding energies in neutral atoms using the radiative potential method [1]. The local radiative potential mimics the effects of QED radiative corrections (the one-loop self-energy and vacuum polarization) on electron energies and wave functions. The radiative potential is expected to give accurate results in many-electron atoms as long as (i) it reproduces "exact" Lamb shifts for high states in hydrogen-like ions and (ii) electron correlations are considered to high accuracy.

The radiative potential may be expressed as

$$\Phi_{\rm rad} = \Phi_{\rm SE} + \Phi_{\rm VP} = \Phi_{\rm mag} + \Phi_{\rm el}^{\rm high} + \Phi_{\rm el}^{\rm low} + \Phi_{\rm VP} \ ,$$

where $\Phi_{\rm mag}$, $\Phi_{\rm el}^{\rm high}$, $\Phi_{\rm el}^{\rm low}$ are magnetic and high- and low-frequency electric parts of the self-energy, and Φ_{VP} is the vacuum polarization potential (dominated by the well-known Uehling potential). See Refs. [1, 2, 3] for explicit expressions. The electric parts of the self-energy, $\Phi_{\rm el}^{\rm high}$ and $\Phi_{\rm el}^{\rm low}$, contain factors found by fitting to self-energy shifts for hydrogen-like s, p, and d waves for $n = 5$ across $10 \leq Z \leq 120$, where Z is the nuclear charge. Accuracy of the fits is $5s \sim 0.1\%$, $5p \sim 1\%$, $5d \sim 1\%$.

Calculations performed in frozen atomic potentials and comparison with the results of rigorous QED [4] for s states demonstrate that the radiative potential is accurate to $\sim 1\%$.

Many-body calculations begin in the relativistic Hartree-Fock (RHF) approximation and the effects of *core relaxation* and *valence-core correlations* are studied. The first effect corresponds to the addition of a new potential found by solving the RHF equation self-consistently with the radiative potential included. This leads to a relaxation correction $\delta\varepsilon^{\rm relax}$,

$$\delta\varepsilon = -\langle\varphi|\Phi_{\rm rad} + \delta V_{\rm HF}^{\rm rad}|\varphi\rangle = \delta\varepsilon^{(1)} + \delta\varepsilon^{\rm relax},$$

where $\delta\varepsilon^{(1)}$ is the first-order shift. The relaxation potential typically has a much larger range than the radiative potential, leading to significant overlap with wave functions with orbital angular momenta $l > 0$ and therefore leading to very sizeable relative corrections compared to first-order results.

The valence-core correlations are accounted for by the addition of a correlation potential in the RHF equation for the valence electron, producing Brueckner orbitals. With both many-body effects included,

$$\delta\varepsilon_{\rm Br} = -\langle\varphi_{\rm Br}|\Phi_{\rm rad} + \delta V_{\rm HF}^{\rm rad}|\varphi_{\rm Br}\rangle = \delta\varepsilon_{\rm Br}^{(1)} + \delta\varepsilon_{\rm Br}^{\rm relax}.$$

Self-energy results [3] for Cs are presented in the table in different approximations. It is seen that for states $l > 0$, account of many-body effects is *crucial* for the correct size and sign of the shifts. The account of many-body corrections is also important for accurate determination of the shifts for s-states. The results are similar for the other alkali-metal atoms.

Table 1. Self-energy corrections to binding energies in Cs in the radiative potential approach. Numbers in square brackets [] denote powers of 10. Units: a.u.

State	$\delta\varepsilon^{(1)}$	$\delta\varepsilon$	$\delta\varepsilon_{\rm Br}$
$6s_{1/2}$	8.128[-5]	8.431[-5]	1.152[-4]
$6p_{1/2}$	1.077[-6]	-3.831[-6]	-5.355[-6]
$6p_{3/2}$	3.183[-6]	-9.203[-7]	-1.093[-6]
$5d_{3/2}$	-6.066[-7]	-1.212[-5]	-2.681[-5]
$5d_{5/2}$	7.174[-7]	-1.115[-5]	-2.350[-5]

References

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