

where “RNMS” stays for the relativistic NMS. The corresponding two-electron correction is

$$H_{\text{RSMS}} = -\frac{1}{2M} \sum_{i \neq j} \frac{\alpha Z}{r_i} \left[\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_i) \mathbf{r}_i}{r_i^2} \right] \cdot \mathbf{p}_j, \quad (4)$$

where “RSMS” denotes the relativistic SMS.

The recoil correction to a given atomic state to first order in m/M is obtained as the expectation value of H_M on the Dirac wave function (here and in what follows, the Dirac wave functions are the eigenvectors of the Dirac-Coulomb-Breit Hamiltonian). In Ref. [33] the Hamiltonian (2) was employed to calculate the $(\alpha Z)^4 m/M$ corrections to the energy levels in He- and Li-like ions to zeroth order in $1/Z$. Later in Refs. [34, 35], this Hamiltonian was used to evaluate the relativistic recoil effect in low- and middle- Z ions and atoms to all orders in $1/Z$.

The recoil correction of the first order in m/M is conveniently expressed in terms of the constant K defined by

$$\Delta E = \langle \psi | H_M | \psi \rangle \equiv K/M, \quad (5)$$

where $|\psi\rangle$ is the eigenvector of the Dirac-Coulomb-Breit Hamiltonian. With this constant, the mass isotope shift for two different isotopes with nuclear masses M_1 and M_2 can be written as $\delta E = K \left(\frac{1}{M_1} - \frac{1}{M_2} \right)$.

The recoil correction which is beyond the Breit approximation (2) is referred to a QED recoil effect. This effect has to be also taken into account, especially for high- Z ions. For H- and Li-like ions the QED recoil corrections have been calculated to all orders in αZ and to zeroth order in $1/Z$ in Refs. [36, 37]. In what follows, we focus on the calculations of the coefficient K to all orders in $1/Z$ for the $2p_j - 2s$ transitions in a wide range of Li-like ions. We investigate relative contributions of the relativistic and QED corrections to the total recoil effect and the influence of the electron correlations on the recoil effect.

B. Method of calculation

Expectation values of the MS operator (2) are very sensitive to the electron correlations. In the present investigation the large-scale configuration-interaction (CI) Dirac-Fock-Sturm (DFS) method was employed to solve the Dirac-Coulomb-Breit equation with high accuracy. This method was developed by Tupitsyn and partially presented in Ref. [38]. It was