On the isotopic shifts in the light two-electron atoms and ions.

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Abstract

The isotopic shifts are determined to high accuracy for a number of light two-electron Li$^+$, Be$^{2+}$, B$^{3+}$ and C$^{4+}$ ions. The field components of these isotopic shifts have been determined with the use of the exact Racah-Rosental-Breit formula.

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The dependence of the total energies of bound states of different isotopes of the same chemical element upon the ‘isotope numbers’ is called the isotopic shift. By the ‘isotope numbers’ we mean the mass of the nucleus and its electric charge density distribution (or proton density distribution). In general, the isotopic shift can be observed in arbitrary, in principle, atomic system which has a central, heavy nucleus with the finite mass, positive electric charge and finite radius. In general, the isotopic shift ∆\(E\) of the bound state level with the total energy \(E\) has the two following components: the first component which depends upon the mass of the nucleus and the second component which mainly depends upon the electric charge density distribution in the atomic nucleus. In turn, the first component is represented as the sum of the normal and specific components. Each of these two components is proportional to the factor \(\frac{m_e}{M}\), where \(m_e\) is the mass of the electron, while \(M\) is the nuclear mass. For few-electron (\(N\)−electron) atoms and ions the exact formula for the isotopic shift \(\Delta E\) takes the form

\[\Delta E = \Delta E_n + \Delta E_s = \frac{m_e}{M} \left( \sum_{i=1}^{N} \frac{p_i^2}{2m_e} \right) + \frac{m_e}{M} \left( \sum_{i(i\neq k)=1}^{N} \frac{p_i \cdot p_k}{2m_e} \right)\]  (1)

where the notation \(\langle \hat{X} \rangle\) designates the expectation value of the operator \(\hat{X}\). For the two-electron (or helium-like) atoms and ions in atomic units \(\hbar = 1, m_e = 1, e = 1\) the last formula is reduced to the form

\[\Delta E = \Delta E_n + \Delta E_s = \frac{1}{M} \langle p_1^2 \rangle + \frac{1}{2M} \langle p_1 \cdot p_2 \rangle\]  (2)

As follows from this formula the expression for the normal and specific components of the isotopic shift are

\[\Delta E_n = \frac{1}{M} \langle p_1^2 \rangle \quad \text{and} \quad \Delta E_s = \frac{1}{2M} \langle p_1 \cdot p_2 \rangle\]  (3)

respectively. As follows from Eq.(3) to determine the normal and specific components of the isotopic shift in two-electron atom/ion one needs to obtain the expectation values of the \(p_1^2\) and \(p_1 \cdot p_2\) operators. Everywhere in this study we assume that the wave functions of the two-electron atom/ion are properly symmetrized upon spin-spatial permutations of the two electrons and, therefore, the corresponding single-electron expectation values are always equal to each other, e.g., \(\langle p_1^2 \rangle = \langle p_2^2 \rangle\).

In actual two-electron atomic systems, i.e. in the systems with the finite nuclear mass \(M\), one can use the condition which follows from the conservation of the total momentum
\[ \mathbf{P}_N = \mathbf{p}_1 + \mathbf{p}_2, \] where \( \mathbf{P}_N \) is the momentum of the nucleus, while \( \mathbf{p}_1 \) and \( \mathbf{p}_2 \) are the electron momenta. From here one finds:

\[ \frac{1}{2} \langle \mathbf{P}_N^2 \rangle = \langle \mathbf{p}_1^2 \rangle + \langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle \] (4)

and, therefore, from Eqs.(2) and (4) we have

\[ \Delta E = \frac{1}{2M} \langle \mathbf{P}_N^2 \rangle \] (5)

i.e. the mass dependent component of the isotopic shift is the expectation value of the kinetic energy of the atomic nucleus with the large (but finite!) mass. In many books and textbooks the formula, Eq.(5), is considered as the original (or fundamental) expression, while Eq.(1) is derived from this formula.

As mentioned above the field component of the isotopic shift explicitly depends upon the nuclear size (radius) \( R \) and proton distribution density in the nucleus. It is clear that this component also depends upon the mass of atomic nucleus \( M \), since the nuclear matter is a saturated matter (in contrast with the Coulomb matter). Therefore, the nuclear radius \( R \) is uniformly related to the number of nucleons \( A \) in the nucleus: \( R = r_0 \cdot A^{\frac{1}{3}} \), where the ‘constant’ radius \( r_0 \approx 1.17 - 1.25 \cdot 10^{-13} \text{ cm} = 1.17 - 1.25 \text{ fm} \) (fermi), where \( 1 \text{ fm} = 1 \cdot 10^{-13} \text{ cm} \). Briefly, this means that the field component of the total isotopic shift is also a function of the nuclear mass \( M \), since \( A \approx \frac{\cal M}{m_p} \), where \( m_p \) is the proton mass. The more accurate formula for the nuclear mass as the function of \( A, Z(=N_p) \), where \( Z \) is the electric charge of the nucleus (= number of protons \( N_p \)) and \( N_n \) (number of neutrons) is given by the Weizäcker formula. This formula is discussed in the Appendix.

Let us present here the well known formula obtained by Racah, Rosental and Breit for the field shift (see, e.g., [1] and references therein)

\[ E_{fs}^f = \frac{4\pi a_0^2}{Q} \cdot \frac{b + 1}{\Gamma(2b + 1)}^2 \cdot B(b) \cdot \left( \frac{2QR}{a_0} \right)^{2b} \cdot \frac{\delta R}{R} \cdot \langle \delta(\mathbf{r}_eN) \rangle \] (6)

where \( Q \) is the nuclear charge, \( R \) is the nuclear radius and \( b = \sqrt{1 - \alpha^2Q^2} \), where \( \alpha = \frac{e^2}{hc} \approx \frac{1}{137} \) is the dimensionless constant which is the small parameter in QED. In Eq.(6) the notation \( \Gamma(x) \) stands for the Euler’s gamma-function, while the factor \( B(b) \) is directly related to the proton density distribution in the atomic nucleus. By assuming the uniform distribution of the proton density over the volume of the nucleus one finds the following expression for the factor \( B(b) \)

\[ B(b) = \frac{3}{(2b + 1)(2b + 3)} \] (7)
For light nuclei with $Q \leq 6$ we have $b \approx 1$ and $B \approx \frac{1}{3}$. The formula, Eq.(6), was used in many theoretical papers for numerical evaluations of the field component of the isotopic shift, or field shift for short. In some works, however, this formula was written with a number of ‘obvious simplifications’. Many of such ‘simplifications’ are based on the fact that for light nuclei the numerical value of the factor $b$ is close to unity. Furthermore, in some papers the factor $b$ was mistakenly called and considered as the Lorentz factor, while the actual Lorentz factor $\gamma$ is its inverse value $\gamma = \frac{1}{b} = \frac{1}{\sqrt{1-\alpha^2 Q^2}}$. Such a factor $\gamma$ always exceeds unity.

In this study we evaluate the isotopic shift for a number of the ground $1^1S(L=0)$–states in the light two-electron ions by using the exact (not approximate!) formula, Eq.(6). Such evaluations allow one to evaluate the numerical errors which arise from the use of approximate expressions. Our main interest in this study is related with the field component of the isotopic shift. As follows from Eq.(6) to evaluate the field component of the field shift one needs to determine to very high accuracy the expectation value of the electron-nuclear delta-function (or the $\langle \delta(r_{eN}) \rangle$) value. In this study for each light element/atom all isotopic shifts are determined in respect to the model (or idealized) isotope which has the infinitely heavy nucleus with zero spatial radius (zero charged radius). In this case the ratio $\frac{4R}{r_e}$ in Eq.(6) equals unity, and this equation can be re-written to the form (in atomic units)

$$E_{M}^{fs} = 4^{b+1} \pi Q^{2b-1} \cdot \alpha^{4b} \cdot \frac{3(b+1)}{\Gamma(2b+1)(2b+1)(2b+3)} \cdot \left(\frac{R}{r_e}\right)^{2b} \cdot \langle \delta(r_{eN}) \rangle$$

where $r_e = \alpha^2 a_0 \approx 2.817940 \text{ fm}$ ($1 \text{ fm} = 1c \cdot 10^{-13} \text{ cm}$) is the classical radius of the electron. For light atomic nuclei the dimensionless factor $\frac{R}{r_e}$ in the last formula is close to unity. Also, in our calculations we have used the following numerical values for the physical constants: $\alpha = 7.297352569 \cdot 10^{-3}$ and $a_0 = 5.291772109 \cdot 10^{-9} \text{ cm}$. The formula, Eq.(8), has been used in all calculations performed for this study. As follows from Eq.(8) to determine the field component of the isotopic shift one needs to know the expectation value of the electron-nuclear delta-function $\delta(r_{eN})$ and numerical value of the nuclear radius $R$. The expectation value of $\delta(r_{eN})$ can be found from the results of highly accurate atomic computations, while the nuclear radius must be taken from nuclear experiments (see, e.g., [6]).

In this study we consider a few light two-electron (or He-like) ions: Li$^+$, Be$^{2+}$, B$^{3+}$ and C$^{4+}$. The total energies and some other properties (or expectation values) of the corresponding model ions (with the infinite nuclear mass and zero spatial radii) can be found in Tables I - IV. The convergence of the results upon the total number of basis function $N$
used in calculations is also shown in Tables I - IV. For these Tables we have computed the expectation values of the following operators: $\delta(r_{eN}), \nu_{eN}, p_1^2, p_1 \cdot p_2$ and $p_{2N}^2$. The notation $\nu_{eN}$ designates the electron-nuclear cusp value which is defined by the following equation

$$
\nu_{eN} = \frac{\langle \delta(r_{eN}) \frac{\partial}{\partial r_{eN}} \rangle}{\langle \delta(r_{eN}) \rangle}
$$

Formally, it is an averaged velocity of the electron at the nucleus. In the general case, this expectation value gives the relative velocity of the two particles ($i$ and $j$) at the $(ij)$-collision point. For pure Coulomb systems, e.g., for the atom with the nuclear charge $Q$, such a velocity is known from the corresponding classical problem. In particular, for the atom with the nuclear charge $Q$, the electron-nuclear cusp $\nu_{eN}$ must be equal (in atomic units)

$$
\nu_{eN} = -Qe^2 \frac{m_e M_N}{m_e + M_N} = -Q
$$

since $M_N = \infty$.

The coincidence of the computed $\nu_{eN}$ value with the nuclear charge $Q$ (or $-Q$) indicates the quality of the variational (atomic) wave functions around the nucleus and overall accuracy of the computed expectation value of the electron-nuclear delta-function. In all calculations performed for this study we have used our exponential variational expansion in relative coordinates described in detail in our earlier papers, see, e.g., [2], [3]. Here we do not want to repeat these descriptions of our variational expansion. Note also that in our calculations we have determined many dozens of different expectation values, including singular expectation values. However, in Tables I - IV only a few expectation values are presented. All these values are needed for numerical evaluation of the isotopic shifts.

Table V contains the numerical values of the field components of isotopic shifts (in $a.u.$) determined with the use of the formula Eq.(8). In this Table we also present the numerical values of the following factors from that formula: $R$ (the actual nuclear radius), $b, X = 4^{b+1} \pi Q^{2b-1} \cdot \alpha^{4b} \cdot \frac{3(b+1)}{(2b+1)(2b+2)(2b+3)}$ and $Y = \left( \frac{R}{r_e} \right)^{2b}$. The expectation values of the electron-nuclear delta-functions were taken from Tables I - IV. To evaluate the Euler’s gamma-function $\Gamma(x)$ we have used the approximate 7-term formula derived by Lanczos [7]. The overall accuracy of this formula is $\approx 1 \cdot 10^{-10} - 2 \cdot 10^{-10}$.

Appendix I.

The formula which provides the uniform relation between the nuclear mass $M$ and total number of nucleons $A$, nuclear charge $Z$ (= number of protons $N_p$) and number of neutrons $N_n$ of a nucleus is
$N_n$ in the nucleus was derived in 1937 by Bethe, Weizäcker and others. Now, this formula is
know as the Weizäcker formula [8], or Bethe-Weizäcker formula. This five-term formula for
the nuclear binding energy $E_b$ was produced 75 years ago and since then its general structure
has never been changed. First, note that the mass formula for an arbitrary nucleus is written
in the form

$$M = m_p [Z + N \left( \frac{m_n}{m_p} \right) - \frac{E_b}{m_p c^2}]$$  \hspace{1cm} (11)

where $M$ is the nuclear mass of the nucleus with $A$ nucleons, $Z$ protons and $N$ neutrons
$A = Z + N$). Also in this formula $E_b$ is the binding energy of the nucleus, $c$ is the speed of
light in vacuum, while $m_p$ and $m_n$ are the masses of the proton and neutron, respectively.
The factors $m_p c^2 = 938.272910$ MeV and $m_n c^2 = 939.565378$ MeV. The advantage of
the formula, Eq.(11), is obvious, since it contains only dimensionless ratios and two integer
numbers ($Z$ and $N$). For instance, if we chose in Eq.(11) $m_p = 1836.152701 m_e$, then $M$
will be given in $m_e$ (or in atomic units if $m_e = 1$). This is very convenient for highly accurate
computations of different few-electron ions.

The parameter $E_b$ in Eq.(11) is called the binding energy of the nucleus. The explicit
expression for the nuclear binding energy $E_b$ is written as the following sum (the Weizäcker
formula):

$$E_b = a_V A - a_S A^{\frac{3}{2}} - a_C \frac{Z^2}{A^{\frac{3}{2}}} - a_A \frac{(N - Z)^2}{A} + \delta(A, Z)$$  \hspace{1cm} (12)

where the five terms in the right-hand side of this equation are called the volume term,
surface term, Coulomb term, asymmetry term and pairing term, respectively. The pairing
term $\delta(A, Z)$ equals zero, if $A$ is odd. If $A$ is even and both $Z$ and $N$ are even, then
$\delta(A, Z) = \frac{a_p}{\sqrt{A}}$. The Weizäcker formula is relatively accurate for regular nuclei (i.e. for nuclei
which are not far from the stability region). In reality, such an accuracy directly depends
upon the numerical values of parameters $a_V, a_S, a_C, a_A$ and $a_p$ in Eq.(12). In our calculations
we have used the following values of these parameters: $a_V = 15.8$ MeV, $a_S = 18.3$ MeV,
$a_C = 0.714$ MeV, $a_A = 23.2$ MeV and $a_p = 12.0$ MeV. The Weizäcker formula with these
coefficients is sufficiently accurate for all light nuclei which are located in the stability region.

Appendix II.

In general, the bound state in any few-electron atom arises in the result of proper balance
between kinetic energy $T_e$ of atomic electrons, electron-nuclear (Coulomb) attraction $U_{en}$ and
electron-electron (Coulomb) repulsion $U_{ee}$. The total energy $E$ of this bound state is written as the following sum:

$$E = T_e + U_{ne} + U_{ee} = \frac{1}{2} (U_{ne} + U_{ee})$$  \hspace{1cm} (13)

where in the right-hand side we have used the virial theorem for the Coulomb potential (see, e.g., [9]) $T_e = -\frac{1}{2} (U_{ne} + U_{ee})$. To solve the problem we need the explicit expression for the correlation energy $U_{ee}$ in terms of the electron-nuclear attraction energy $U_{ne}$. Such an analytical relation can be found in a few restricted cases, e.g., in the Thomas-Fermi method one finds: $U_{ee} = -\frac{1}{7} U_{ne}$ and $E = \frac{3}{7} U_{ne}$. For highly accurate method the situation is significantly more complicated, but qualitatively the actual relations between $T_e, U_{ne}$ and $U_{ee}$ are similar to the relations obeyed in the Thomas-Fermi model.

First, note that the Schrödinger equation for an arbitrary non-relativistic $N$–electron atom/ion takes the form

$$\left[ \frac{\hbar^2}{2m_e} \sum_{i=1}^{N} \mathbf{p}_i^2 - Qe^2 \sum_{i=1}^{N} \frac{1}{r_i} + e^2 \sum_{i>j=1}^{N} \frac{1}{r_{ij}} \right] \Psi = E \Psi$$ \hspace{1cm} (14)

where $Q$ is the electric charge of the nucleus and the mass of the central nucleus is assumed to be finite. Here we shall not assume that $N = Q$. In Eq. (14) the terms in the first sum ($\sim \mathbf{p}_i^2$) represent the kinetic energies of electrons, while other terms correspond to the electron-nuclear Coulomb attraction and/or electron-electron Coulomb repulsion. From this equation one finds the following relation for the expectation values (in atomic units):

$$\left[ \frac{N}{2} \langle \mathbf{p}_e^2 \rangle - Q N \langle \frac{1}{r_{en}} \rangle + \frac{N(N-1)}{2} \langle \frac{1}{r_{ee}} \rangle \right] = E$$ \hspace{1cm} (15)

where the subscript $e$ means the electron, while the subscript $n$ stands for the nucleus.

Let us assume that we know the highly accurate solution of the Schrödinger equation, i.e. the wave function $\Psi$ in Eq. (14) is known. In this case the following condition must be obeyed for these three expectation values:

$$\langle \mathbf{p}_e^2 \rangle = Q \langle \frac{1}{r_{en}} \rangle - \frac{(N-1)}{2} \langle \frac{1}{r_{ee}} \rangle$$ \hspace{1cm} (16)

which is known as the virial theorem (see, e.g., [9]). Now, after a few steps of simple transformations one finds the following formula for the total energy $E$ (in atomic units)

$$E = -\frac{1}{2} N \cdot Q \cdot \langle \frac{1}{r_{en}} \rangle + \frac{1}{4} N(N-1) \cdot \langle \frac{1}{r_{ee}} \rangle$$

$$= -\frac{1}{2} N \cdot Q \cdot f_1(N, Q) + \frac{1}{4} N(N-1) \cdot f_2(N, Q)$$ \hspace{1cm} (17)
where \( f_1(N, Q) \) and \( f_2(N, Q) \) are the functions of the number of electrons \( N \) and electric charge of the nucleus \( Q \). For neutral atoms we have \( Q = N \), while for positively charged ions \( Q > N \). For instance for the two-electron \( C^{4+} \) ion (i.e. for \( N = 2 \) and \( Q = 6 \)) we found that \( \langle \frac{1}{r_{\text{en}}} \rangle \approx 5.687615325399107305988929 \text{ a.u.} \) and \( \langle \frac{1}{r_{\text{ee}}} \rangle \approx 3.438890700992227050791016158 \text{ a.u.} \) (results from calculations with 3700 basis functions). By using these expectation values one finds the total energy \( E \) from Table IV. In the general case, \( \langle \frac{1}{r_{\text{ee}}} \rangle = \lambda(N, Q)\langle \frac{1}{r_{\text{en}}} \rangle \), where the parameter \( \lambda < 1 \). The factor \( \lambda(N, Q) \) can be approximated to very high accuracy with the use of highly accurate results obtained for different \( N \) and \( Q \).

The formula, Eq.(17), is also applied in the case of \( N = 1 \) (hydrogen-like atoms and ions). In this case the electron-electron repulsion is not defined, but it is multiplied by a factor which equals zero. As follows from Eq.(17), if we can determine the two unknown functions \( f_1(N, Q) \) and \( f_2(N, Q) \) in Eq.(17), then we can predict the total energy of an arbitrary \( N \)-electron atom/ion to very high accuracy. It can be done, e.g., by using the results of highly accurate computations of different few-electron atoms and ions (with different \( Q \) and \( N \)). If we know the results of highly accurate computations for a large number of light atoms/ions, then we can reconstruct the two functions \( f_1(N, Q) \) and \( f_2(N, Q) \) in Eq.(17) to very high accuracy. This procedure works well for mixtures of light elements at different temperatures and allows one to predict the properties of high-temperature plasmas which consists of such elements.

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TABLE I: The total energies $E$ and expectation values of the electron-nuclear delta-function $\delta_{eN}$, electron-nuclear cusp $\nu_{eN}$ and some other operators for the two-electron lithium ion Li$^+$ (in atomic units). $K$ is the total number of basis functions used.

| $K$  | $E$(Li$^+$) | $\langle \delta_{eN} \rangle$ | $\nu_{eN}$ |
|------|------------|-------------------------------|-----------|
| 3500 | -7.279913  | 412669 305964 91708          | 6.8520 094343 431 | -3.0000 00000 158 |
| 3700 | -7.279913  | 412669 305964 91743          | 6.8520 094343 456 | -3.0000 00000 125 |
| 3840 | -7.279913  | 412669 305964 91766          | 6.8520 094343 460 | -2.9999 99999 918 |
| 4000 | -7.279913  | 412669 305964 91785          | 6.8520 094343 462 | -2.9999 99999 901 |

| $K$  | $\frac{1}{2}\langle p_1^2 \rangle$ | $\langle p_1 \cdot p_2 \rangle$ | $\frac{1}{2}\langle p_N^2 \rangle$ |
|------|---------------------------------|---------------------------------|---------------------------------|
| 3500 | 3.63995 670633 465298 240       | 0.288975 786393 989535 661      | 7.56888 919906 329532 141       |
| 3700 | 3.63995 670633 465298 241       | 0.288975 786393 989535 661      | 7.56888 919906 329532 143       |
| 3840 | 3.63995 670633 465298 241       | 0.288975 786393 989535 662      | 7.56888 919906 329532 144       |
| 4000 | 3.63995 670633 465298 242       | 0.288975 786393 989535 662      | 7.56888 919906 329532 145       |

TABLE II: The total energies $E$ and expectation values of the electron-nuclear delta-function $\delta_{eN}$, electron-nuclear cusp $\nu_{eN}$ and some other operators for the two-electron berillium ion Be$^{2+}$ (in atomic units). $K$ is the total number of basis functions used.

| $K$  | $E$(Be$^{2+}$) | $\langle \delta_{eN} \rangle$ | $\nu_{eN}$ |
|------|----------------|-------------------------------|-----------|
| 3500 | -13.6556623842 358670 20757 | 17.1981 72544 645 | -3.9999 99999 962 |
| 3700 | -13.6556623842 358670 20767 | 17.1981 72544 640 | -3.9999 99999 921 |
| 3840 | -13.6556623842 358670 20772 | 17.1981 72544 638 | -4.0000 00000 125 |
| 4000 | -13.6556623842 358670 20777 | 17.1981 72544 635 | -4.0000 00000 148 |

| $K$  | $\frac{1}{2}\langle p_1^2 \rangle$ | $\langle p_1 \cdot p_2 \rangle$ | $\frac{1}{2}\langle p_N^2 \rangle$ |
|------|---------------------------------|---------------------------------|---------------------------------|
| 3500 | 6.82778 311921 179335 084       | 0.420520 303439 441862 011     | 14.07608 654186 302856 368      |
| 3700 | 6.82778 311921 179335 086       | 0.420520 303439 441862 010     | 14.07608 654186 302856 369      |
| 3840 | 6.82778 311921 179335 089       | 0.420520 303439 441862 009     | 14.07608 654186 302856 370      |
| 4000 | 6.82778 311921 179335 091       | 0.420520 303439 441862 009     | 14.07608 654186 302856 371      |
TABLE III: The total energies $E$ and expectation values of the electron-nuclear delta-function $\delta_{eN}$, electron-nuclear cusp $\nu_{eN}$ and some other operators for the two-electron boron ion B$^{3+}$ (in atomic units). $K$ is the total number of basis functions used.

| $K$ | $E$(B$^{3+}$) | $\langle\delta_{eN}\rangle$ | $\nu_{eN}$ |
|-----|---------------|----------------|-----------|
| 3500 | -22.03097 1580242 781541 65339 | 34.758 743660 955 | -5.0000 0000 319 |
| 3700 | -22.03097 1580242 781541 65376 | 34.758 743660 965 | -5.0000 0000 235 |
| 3840 | -22.03097 1580242 781541 65394 | 34.758 743660 947 | -5.0000 0000 107 |
| 4000 | -22.03097 1580242 781541 65418 | 34.758 743660 935 | -5.0000 0000 119 |

| $K$ | $\frac{1}{2}\langle p_{1}^{2}\rangle$ | $\langle p_{1} \cdot p_{2}\rangle$ | $\frac{1}{2}\langle p_{N}^{2}\rangle$ |
|-----|----------------|----------------|----------------|
| 3500 | 11.01548 579012 139077 100 | 0.552752 631642 101467 789 | 22.58372 421188 488300 979 |
| 3700 | 11.01548 579012 139077 089 | 0.552752 631642 101467 734 | 22.58372 421188 488300 952 |
| 3840 | 11.01548 579012 139077 086 | 0.552752 631642 101467 715 | 22.58372 421188 488300 942 |
| 4000 | 11.01548 579012 139077 083 | 0.552752 631642 101467 701 | 22.58372 421188 488300 938 |
TABLE IV: The total energies $E$ and expectation values of the electron-nuclear delta-function $\delta_{eN}$, electron-nuclear cusp $\nu_{eN}$ and some other operators for the two-electron carbon ion C$^{4+}$ (in atomic units). $K$ is the total number of basis functions used.

| $K$       | $E$(C$^{4+}$) | $\langle \delta_{eN} \rangle$ | $\nu_{eN}$ |
|-----------|---------------|-------------------------------|------------|
| 3500  -32.40624 660189 853031 05527 | 61.443 578056 445 | -5.9999 99999 765 |
| 3700  -32.40624 660189 853031 05535 | 61.443 578056 514 | -5.9999 99999 871 |
| 3840  -32.40624 660189 853031 05539 | 61.443 578056 537 | -6.0000 00000 048 |
| 4000  -32.40624 660189 853031 05542 | 61.443 578056 543 | -6.0000 00000 037 |

| $K$       | $\frac{1}{2} \langle p_1^2 \rangle$ | $\langle p_1 \cdot p_2 \rangle$ | $\frac{1}{2} \langle p_2^2 \rangle$ |
|-----------|----------------------------------|-------------------------------|----------------------------------|
| 3500 16.20312 330094 926515 523 | 0.685334 822135 598924 527 | 33.09158 142403 412923 500 |
| 3700 16.20312 330094 926515 524 | 0.685334 822135 598924 535 | 33.09158 142403 412923 502 |
| 3840 16.20312 330094 926515 525 | 0.685334 822135 598924 536 | 33.09158 142403 412923 502 |
| 4000 16.20312 330094 926515 525 | 0.685334 822135 598924 537 | 33.09158 142403 412923 503 |

TABLE V: The nuclear radius $R$ (fm), parameter $b$, factors $X$ and $Y$ (see the main text) and field components of the total isotopic shift $\Delta E^{fs}$ (all values are in atomic units) for each isotope.

| isotope | $Q$ | $R$       | $b$            | $X$       | $Y$       | $\Delta E^{fs}$ |
|---------|-----|-----------|----------------|-----------|-----------|-----------------|
| $^6$Li  | 3   | 2.5385    | 0.99976034018621 | 4.297056149289-10$^{-8}$ | 0.81154478 2.389469390-10$^{-7}$ |
| $^7$Li  | 3   | 2.4312    | 0.99976034018621 | 4.297056149289-10$^{-8}$ | 0.74440369 2.191782729-10$^{-7}$ |
| $^9$Be  | 4   | 2.5180    | 0.99957389838248 | 5.749782211793-10$^{-8}$ | 0.79852685 7.896292299-10$^{-7}$ |
| $^{10}$B | 5   | 2.4278    | 0.99933413638122 | 7.219245621776-10$^{-8}$ | 0.74241787 1.862996331-10$^{-6}$ |
| $^{11}$B | 5   | 2.4059    | 0.99933413638122 | 7.219245621776-10$^{-8}$ | 0.72909310 1.829527229-10$^{-6}$ |
| $^{12}$C | 6   | 2.4073    | 0.99904101579314 | 8.7092766851788-10$^{-8}$ | 0.76867983 4.113429628-10$^{-6}$ |
| $^{13}$C | 6   | 2.4614    | 0.99904101579314 | 8.7092766851788-10$^{-8}$ | 0.76315629 4.083871553-10$^{-6}$ |
| $^{14}$C | 6   | 2.5037    | 0.99904101579314 | 8.7092766851788-10$^{-8}$ | 0.78958608 4.225305034-10$^{-6}$ |