

# On the breakdown of the Dirac kinetic energy operator for estimating normal mass shifts

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**Abstract.** The Dirac kinetic energy form of the normal mass shift is widely used in relativistic atomic structure calculations. In the present paper, we illustrate the progressive breakdown of this operator with the increase of the nuclear charge along the lithium isoelectronic series.

## 1 Introduction

The isotope shifts (IS), which consist of the field shift and the mass shift, always play a key role in extracting nuclear properties such as nuclear mean-square charge radii [1–5]. The mass shift, however, generally gives rise to large uncertainties in the IS due to its sensitivity to electron correlation. As a result, the determination of the mass shift always attracts one's attention.

The mass shift is made up of two parts, as suggested at first by Hughes and Eckart in 1930 [6], that are the so-called normal mass shift (NMS) and specific mass shift (SMS). If the nucleus is treated as a nonrelativistic parti-

cle, the mass-shift Hamiltonian can be written as [6, 7]

$$H_{\text{MS}} = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2M} + \sum_{i \neq j}^N \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{2M}, \quad (1)$$

where  $\mathbf{p}_i$  is the electron momentum and  $M$  is the nuclear mass. The one- and two-body operators correspond to the NMS and SMS contributions, respectively.

In the nonrelativistic framework, two approaches based on perturbation theory have been proposed to evaluate the NMS. The first one uses the infinite mass approximation as the zero-order Hamiltonian [8]

$$H_{\infty}^{\text{NR}} = \sum_{i=1}^N \left( \frac{\mathbf{p}_i^2}{2m_e} - \frac{Ze^2}{(4\pi\epsilon_0)r_i} \right) + \sum_{i < j}^N \frac{e^2}{(4\pi\epsilon_0)r_{ij}} \quad (2)$$

with the electron mass  $m_e$ , and treats both the NMS and SMS terms as a first-order energy correction,

$$E_M^{(1)} - E_{\infty} = \langle \Phi_{\infty} | \frac{1}{2M} \sum_{i,j}^N \mathbf{p}_i \cdot \mathbf{p}_j | \Phi_{\infty} \rangle. \quad (3)$$

The second approach adopts the finite mass Hamiltonian excluding the SMS term,

$$H_M^B \equiv H_\infty^{\text{NR}} + \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2M} \quad (4)$$

as the zero-order Hamiltonian and uses its eigenfunctions as zero-order wave functions to estimate the two-body SMS contribution. In this approach, the NMS is treated rigorously at all orders since the eigenfunctions and eigenvalues of  $H_M^B$  are merely related to the solutions of the infinite mass Hamiltonian  $H_\infty$  through the simple scaling transformation [6, 8]

$$E_M^B = \frac{\mu}{m_e} E_\infty \quad \text{and} \quad \Phi^B(\mathbf{r}) = \Phi_\infty\left(\frac{\mu}{m_e} \mathbf{r}\right), \quad (5)$$

where  $\mu = \frac{m_e M}{m_e + M}$  is the reduced mass.

Unfortunately, the scaling law (5) becomes invalid in the relativistic scheme [9], even if restricting the relativistic corrections to the spin-orbit interaction [7, 10, 11]. Consequently, only the first method mentioned above remains possible. The relativistic Hamiltonian of the atomic system in the infinite nuclear mass approximation is [12],

$$H_\infty^{\text{R}} = \sum_{i=1}^N [T_i - V(r_i)] + \sum_{i<j}^N V(i, j), \quad (6)$$

where

$$T_i = c \boldsymbol{\alpha}_i \cdot \mathbf{p}_i + (\beta_i - 1) m_e c^2 \quad (7)$$

is the Dirac kinetic energy operator and  $V(i, j)$  is the electron-electron interaction in the low-frequency limit, which contains the Coulomb interaction  $\frac{1}{r_{ij}}$  and the Breit interaction  $-\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{2r_{ij}} - \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_{ij})(\boldsymbol{\alpha}_j \cdot \mathbf{r}_{ij})}{2r_{ij}^3}$ . The mass shift operators have the same form as Eq. (1) if the nucleus is treated as a nonrelativistic particle and the retardation

and magnetic effects due to the motion of the nucleus are omitted [7, 13–15].

In the relativistic framework however, the mass shift operators are built from the relativistic momentum

$$\mathbf{p}^2 = \frac{T^2}{c^2} + 2m_e T, \quad (8)$$

leading to the NMS Hamiltonian

$$H_{\text{NMS}} = \frac{1}{2M} \sum_{i=1}^N \left[ \frac{(T_i)^2}{c^2} + 2m_e T_i \right], \quad (9)$$

as derived by Parpia *et al.* [16].

Neglecting the first term in square brackets, the NMS operator can be approximated as

$$H_{\text{NMS}} \approx \mathcal{H}_{\text{NMS}} = \frac{m_e}{M} \sum_{i=1}^N T_i. \quad (10)$$

This approximated NMS operator has been widely used in the relativistic atomic structure calculations [12, 17–19].

Although, as pointed out by Parpia *et al.* [16], the operator (10) reproduces the nonrelativistic expression of the NMS operator (first term of Eq. (1)) when treating the electrons as nonrelativistic particles ( $T \approx \frac{1}{2} m_e v^2$ ), its adequacy in the relativistic framework has never been investigated to the knowledge of the authors.

In this paper, we calculate the NMS factors through the expectation values of  $H_{\text{NMS}}$  and  $\mathcal{H}_{\text{NMS}}$ , ie.  $K \equiv M \langle H \rangle$  and  $\mathcal{K} \equiv M \langle \mathcal{H} \rangle$ , for the ground  $1s^2 2s^2 S_{1/2}$  and the excited  $1s^2 2p^2 P_{1/2,3/2}^o$  states, and for the three transitions between these levels, along the lithium isoelectronic sequence. We assess the reliability of the approximation (10) by monitoring the relative error

$$\epsilon = \frac{\langle H \rangle - \langle \mathcal{H} \rangle}{\langle H \rangle} = \frac{K - \mathcal{K}}{K} \quad (11)$$

along the sequence.

## 2 Computational Method

For a many-electron atomic system, the main uncertainty of physical quantities arises from electron correlation effects. In this work, the multiconfiguration Dirac-Hartree-Fock (MCDHF) method is used to yield the atomic state wave functions (ASF). Based on the MCDHF method, the ASF is represented by a linear combination of configuration state functions (CSFs) with same parity  $P$ , total angular momentum  $J$  and its component along  $z$ -direction  $M_J$  as

$$\Psi_{\infty}(PJM_J) = \sum_{i=1}^{n_c} c_i \Phi(\gamma_i PJM_J), \quad (12)$$

where  $\{c_i\}$  are the mixing coefficients and  $\{\gamma_i\}$  is the set of quantum numbers needed for specifying the  $i^{\text{th}}$  CSF. The subscript  $\infty$  indicates that the ASFs are eigenstates corresponding to the infinite nuclear mass Hamiltonian (6). Applying the variational principle, the ASF is obtained through minimizing the energy of the level(s) considered. This is achieved either by optimizing the mixing coefficients along with the single-electron orbital wave functions in the self-consistence field (SCF) calculations, or by solving the relativistic configuration interaction (RCI) problem to determine the mixing coefficients, in a given orbital basis set.

Electron correlation effects are systematically captured using the active space (AS) approach. With the AS method the configuration space is expanded by means of single (S) and double (D) excitations from the (multi)reference space. Triple (T) excitations are discarded due to their tiny contributions, as found in [20]. The active set is enlarged layer by layer, which makes it possible to monitor

the convergence of the physical quantities concerned. For each layer, labelled by  $n = 2, 3, 4, \dots, 9$ , respectively, it contains orbitals of different orbital angular momenta up to  $l = 6$  (ie. up to  $ni_{11/2,13/2}$  for  $n \geq 7$ ). In the SCF calculations, the occupied orbitals of the reference space are treated as spectroscopic and the others from the active set are treated as correlation orbitals. The orbitals of the added correlation layer are optimized while the previous ones are kept frozen. The Breit interaction is taken into account in the subsequent RCI processes.

Since electron correlation effects become weaker towards the high- $Z$  end of the sequence, the number of correlation layers is gradually decreased. For instance, the  $\text{Mo}^{39+}$  active set is reduced by three correlation layers comparatively with the one adopted for  $\text{C}^{3+}$ . Additionally, the reduction of the correlation orbitals number also avoids the convergence problems arising from the interaction of bound states with the negative energy continuum [21]. All calculations are performed using the latest GRASP2K package [22,23] in which a new code has been implemented to evaluate the relativistic mass shift [15,24].

To investigate the quality of our correlation models, we report the electronic NMS factors  $K$  and  $\mathcal{K}$  of Li-like C and Mo for the three levels considered, as functions of the active sets, in Table 1 and Table 2, respectively. All results are nicely converged, demonstrating that the orbital sets are almost saturated for the property we are interested in.

### 3 Results and Discussion

In Table 3 we present the electronic  $K$  and  $\mathcal{K}$  factors for the three lowest levels along the Li-like isoelectronic sequence within  $6 \leq Z \leq 60$ . It is found that the relative error  $\epsilon$ , as defined by (11)<sup>1</sup>, grows rapidly from 0.22% to 22% for the three levels. This observation is not really surprising due to the relativistic origin of the neglected term  $H - \mathcal{H} = \sum_{i=1}^N (T_i^2/2Mc^2)$  in the approximation (10).

The transition NMS factors  $\Delta\tilde{K}(\equiv \Delta K/h)$  and  $\Delta\tilde{\mathcal{K}}(\equiv \Delta\mathcal{K}/h)$ , together with the corresponding relative errors,

$$\Delta\epsilon = \frac{\Delta\tilde{K} - \Delta\tilde{\mathcal{K}}}{\Delta\tilde{K}} \quad (13)$$

are presented in Table 4 for the two transitions  $2s - 2p_{1/2}$  and  $2s - 2p_{3/2}$  and the transition within the fine structure  $2p_{1/2} - 2p_{3/2}$ . As can be seen from this table, the two factors are in good agreement with each other at the beginning of the isoelectronic sequence but become strikingly different as the atomic number  $Z$  increases. For the Li-like Nd transition  $2s - 2p_{1/2}$ , the omitted term constitutes a crucial contribution to the NMS of about 90 %. For the  $2s - 2p_{3/2}$  transition, the contribution, albeit smaller than for the other component, still reaches 54 %. Additionally, we compare these values with the transition NMS factor calculated using the scaling law (5) and the ab initio transition energies. These results, marked as  $\Delta\tilde{K}^{sc}$ , are presented in the same table. One observes from Table 4 that

<sup>1</sup> Note that defining  $\tilde{\epsilon} \equiv \frac{\langle H \rangle - \langle \mathcal{H} \rangle}{\langle \mathcal{H} \rangle}$  instead of  $\epsilon$ , we found  $\tilde{\epsilon} = (1/2m_e c^2) \frac{\langle \sum_i T_i^2 \rangle}{\langle \sum_i T_i \rangle}$ . Can it be interpreted “physically” for explaining the  $Z$ -dependence of the error associated with the use of the Dirac kinetic energy operator for estimating NMS?

the scaling transformation gives reliable estimations to the NMS for low- $Z$  ions where relativistic effects are negligible, but remarkably deviates from both the  $\Delta\tilde{K}$  and the approximated  $\Delta\tilde{\mathcal{K}}$  values for heavier systems, even though the calculated relativistic transition energies are used. The breakdown of the scaling law is this way illustrated.

### 4 Conclusion

Taking the Li-like ions as examples, we show that the approximated normal mass shift operator  $\frac{m_e}{M} \sum_{i=1}^N T_i$ , widely used in the literature (see for instance [12]), becomes invalid for relativistic atomic systems. It is indeed found that this approximated NMS operator, based on the Dirac kinetic energy operator, systematically underestimates the normal mass shifts not only for the levels but also for the transitions, since the relativistic contribution arising from the  $\sum_{i=1}^N (T_i^2/2Mc^2)$  term is neglected. We stress that this missing part that originates from relativity cannot be omitted for heavy elements.

For reliable relativistic atomic structure calculations, we strongly recommend the use of the entire normal mass shift operator

$$\frac{1}{2M} \sum_{i=1}^N \left[ \frac{(T_i)^2}{c^2} + 2m_e T_i \right]$$

that is strictly equivalent to  $\sum_{i=1}^N \frac{\mathbf{p}_i^2}{2M}$  [16]. In any case, one should keep in mind that, for getting more accurate normal mass shifts, this operator should also be refined by using the more complete operator

$$H_{\text{NMS}} = \frac{1}{2M} \sum_{i=1}^N \left\{ \mathbf{p}_i^2 - \frac{\alpha Z}{r_i} \left[ \boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i \cdot \mathbf{r}_i) \cdot \mathbf{r}_i}{r_i^2} \right] \cdot \mathbf{p}_i \right\} \quad (14)$$

for taking the retardation and magnetic effects due to the nuclear motion [7,13,15] into account. The latter indeed can give rise to observable shifts for transition energies [3, 14,25] in highly charged ions.

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**Table 1.** Electronic normal mass shift factors,  $K$  and  $\mathcal{K}$  (in  $[E_h m_e]$ ), for the ground state  $1s^2 2s$  ( $J = 1/2$ ) and the first two excited states  $1s^2 2p$  ( $J = 1/2, 3/2$ ) of Li-like C. Absolute errors  $\Delta = K - \mathcal{K}$ .

Model	$1s^2 2s$ ( $J = 1/2$ )			$1s^2 2p$ ( $J = 1/2$ )			$1s^2 2p$ ( $J = 3/2$ )		
	$K$	$\mathcal{K}$	$\Delta$	$K$	$\mathcal{K}$	$\Delta$	$K$	$\mathcal{K}$	$\Delta$
DF	34.852	34.774	0.0785	34.552	34.476	0.0754	34.550	34.474	0.0754
2SD	34.870	34.791	0.0786	34.562	34.487	0.0754	34.561	34.485	0.0754
3SD	34.883	34.804	0.0786	34.581	34.506	0.0755	34.580	34.504	0.0755
4SD	34.887	34.808	0.0787	34.583	34.508	0.0755	34.582	34.506	0.0755
5SD	34.889	34.810	0.0787	34.588	34.513	0.0755	34.587	34.511	0.0755
6SD	34.890	34.812	0.0787	34.590	34.515	0.0755	34.589	34.513	0.0755
7SD	34.891	34.812	0.0787	34.591	34.516	0.0755	34.590	34.514	0.0755
8iSD	34.893	34.815	0.0787	34.594	34.518	0.0755	34.592	34.517	0.0755
9iSD	34.893	34.815	0.0787	34.594	34.519	0.0755	34.593	34.517	0.0755

**Table 2.** Electronic normal mass shift factors,  $K$  and  $\mathcal{K}$  (in  $[E_h m_e]$ ), for the ground state  $1s^2 2s$  ( $J = 1/2$ ) and the first two excited states  $1s^2 2p$  ( $J = 1/2, 3/2$ ) of Li-like Mo. Absolute errors  $\Delta = K - \mathcal{K}$ .

Model	$1s^2 2s$ ( $J = 1/2$ )			$1s^2 2p$ ( $J = 1/2$ )			$1s^2 2p$ ( $J = 3/2$ )		
	$K$	$\mathcal{K}$	$\Delta$	$K$	$\mathcal{K}$	$\Delta$	$K$	$\mathcal{K}$	$\Delta$
DF	2353.57	2092.51	261.06	2334.07	2088.88	245.19	2318.18	2073.78	244.39
2SD	2353.18	2092.16	261.02	2330.20	2085.70	244.50	2314.71	2070.93	243.78
3SD	2349.82	2089.43	260.38	2329.99	2085.45	244.54	2314.65	2070.85	243.80
4SD	2349.82	2089.44	260.38	2329.80	2085.33	244.47	2314.48	2070.74	243.74
5SD	2349.60	2089.31	260.29	2329.71	2085.27	244.44	2314.43	2070.71	243.71
6SD	2349.63	2089.30	260.33	2329.72	2085.26	244.46	2314.45	2070.72	243.73

**Table 3.** Electronic normal mass shift factors,  $K$  and  $\mathcal{K}$  (in  $[E_h m_e]$ ), for the ground state  $1s^2 2s$  ( $J = 1/2$ ) and the first two excited states  $1s^2 2p$  ( $J = 1/2, 3/2$ ) along the Li-like isoelectronic sequence ( $6 \leq Z \leq 60$ ). Absolute errors,  $\Delta = K - \mathcal{K}$ , with the corresponding relative errors ( $\epsilon$ ).

Ions	$1s^2 2s$ ( $J = 1/2$ )			$1s^2 2p$ ( $J = 1/2$ )			$1s^2 2p$ ( $J = 3/2$ )		
	$K$	$\mathcal{K}$	$\Delta(\epsilon)$	$K$	$\mathcal{K}$	$\Delta(\epsilon)$	$K$	$\mathcal{K}$	$\Delta(\epsilon)$
C <sup>3+</sup>	34.893	34.815	0.0787 (0.23%)	34.594	34.519	0.0755 (0.22%)	34.593	34.517	0.0755 (0.22%)
O <sup>5+</sup>	64.629	64.369	0.260 (0.40%)	64.174	63.926	0.248 (0.39%)	64.166	63.918	0.248 (0.39%)
Ne <sup>7+</sup>	103.70	103.05	0.65 (0.63%)	103.08	102.46	0.62 (0.60%)	103.05	102.43	0.620 (0.60%)
Si <sup>11+</sup>	210.71	208.11	2.61 (1.24%)	209.67	207.20	2.47 (1.18%)	209.56	207.09	2.47 (1.18%)
Ar <sup>15+</sup>	358.16	350.82	7.34 (2.05%)	356.52	349.59	6.93 (1.94%)	356.16	349.24	6.92 (1.94%)
Ti <sup>19+</sup>	549.16	532.35	16.81 (3.06%)	546.62	530.78	15.84 (2.90%)	545.73	529.90	15.83 (2.90%)
Fe <sup>23+</sup>	787.86	754.20	33.66 (4.27%)	783.94	752.24	31.70 (4.04%)	782.09	750.43	31.67 (4.05%)
Zn <sup>27+</sup>	1079.60	1018.25	61.35 (5.68%)	1073.60	1015.87	57.73 (5.38%)	1070.14	1012.49	57.65 (5.39%)
Kr <sup>33+</sup>	1631.88	1498.66	133.22 (8.16%)	1620.76	1495.53	125.22 (7.73%)	1613.05	1488.09	124.96 (7.75%)
Mo <sup>39+</sup>	2349.63	2089.30	260.33 (11.08%)	2329.72	2085.26	244.46 (10.49%)	2314.45	2070.72	243.73 (10.53%)
Xe <sup>51+</sup>	4468.43	3657.10	811.33 (18.16%)	4411.15	3650.64	760.50 (17.24%)	4362.91	3606.41	756.49 (17.34%)
Nd <sup>57+</sup>	6013.99	4673.21	1340.78(22.29%)	5920.60	4665.06	1255.54(21.21%)	5840.96	4593.83	1247.13(21.35%)



**Table 4.** Electronic normal mass shift factors,  $\Delta\tilde{K}$  and  $\Delta\tilde{\mathcal{K}}$  (in [GHz u]) for the transitions  $2p_{1/2}-2s$ ,  $2p_{3/2}-2s$  and  $2p_{3/2}-2p_{1/2}$  along the Li-like isoelectronic sequence ( $6 \leq Z \leq 60$ ). Absolute errors ( $\Delta\tilde{K} - \Delta\tilde{\mathcal{K}}$ ), with the corresponding relative errors  $\Delta\epsilon$  in parentheses. Scaling law NMS factors ( $\Delta\tilde{K}^{sc}$ ), using ab initio transition energies.

Ions	$2p_{1/2} - 2s$			$2p_{3/2} - 2s$			$2p_{3/2} - 2p_{1/2}$		
	$\Delta\tilde{K}$	$\Delta\tilde{\mathcal{K}}$	$\Delta\tilde{K} - \Delta\tilde{\mathcal{K}}$	$\Delta\tilde{K}$	$\Delta\tilde{\mathcal{K}}$	$\Delta\tilde{K} - \Delta\tilde{\mathcal{K}}$	$\Delta\tilde{K}$	$\Delta\tilde{\mathcal{K}}$	$\Delta\tilde{K} - \Delta\tilde{\mathcal{K}}$
C <sup>3+</sup>	1080	1069	12 (1%)	1086	1074	12 (1%)	5	5	0 (0%)
$\Delta\tilde{K}^{sc}$	1061			1063			2		
O <sup>5+</sup>	1645	1601	44 (3%)	1672	1628	44 (3%)	27	27	0 (0%)
$\Delta\tilde{K}^{sc}$	1586			1595			9		
Ne <sup>7+</sup>	2257	2139	118 (5%)	2340	2222	118 (5%)	83	83	0 (0%)
$\Delta\tilde{K}^{sc}$	2110			2137			27		
Si <sup>11+</sup>	3761	3253	508 (13%)	4168	3659	509 (12%)	407	406	2 (0%)
$\Delta\tilde{K}^{sc}$	3166			3300			134		
Ar <sup>15+</sup>	5907	4426	1481 (25%)	7205	5714	1491 (21%)	1298	1289	10 (1%)
$\Delta\tilde{K}^{sc}$	4246			4666			420		
Ti <sup>19+</sup>	9151	5677	3474 (38%)	12348	8837	3511 (28%)	3197	3160	37 (1%)
$\Delta\tilde{K}^{sc}$	5338			6380			1041		
Fe <sup>23+</sup>	14143	7065	7078 (50%)	20803	13614	7189 (35%)	6660	6549	111 (2%)
$\Delta\tilde{K}^{sc}$	6480			8631			2151		
Zn <sup>27+</sup>	21676	8603	13073 (60%)	34148	20790	13358 (39%)	12472	12187	285 (2%)
$\Delta\tilde{K}^{sc}$	7669			11653			3985		
Kr <sup>33+</sup>	40140	11272	28868 (72%)	67947	38132	29816 (44%)	27807	26860	948 (3%)
$\Delta\tilde{K}^{sc}$	9562			18270			8708		
Mo <sup>39+</sup>	71850	14567	57283 (80%)	126978	67063	59915 (47%)	55128	52496	2632 (5%)
$\Delta\tilde{K}^{sc}$	11617			28472			16854		
Xe <sup>51+</sup>	206767	23304	183464 (89%)	380900	182962	197939(52%)	174133	159658	14475 (8%)
$\Delta\tilde{K}^{sc}$	16370			66139			49769		
Nd <sup>57+</sup>	337092	29414	307677 (91%)	624549	286535	338013(54%)	287457	257121	30336 (11%)
$\Delta\tilde{K}^{sc}$	19202			97998			78796		