The effects of electron correlation and the Breit interaction on one- and two-electron one-photon transitions in double K hole states of He-like ions (10 ≤ Z ≤ 47)

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The x-ray energies and transition rates associated with single and double electron radiative transitions from the double K hole state 2p2s to the 1s2s and 1s2p configurations of 11 He-like ions (10 ≤ Z ≤ 47) are evaluated using the fully relativistic multi-configuration Dirac-Fock method. An appropriate electron correlation model is constructed with the aid of the active space method, which allows the electron correlation effects to be studied efficiently. The contributions of electron correlation and the Breit interaction to the transition properties are analyzed in detail. It is found that the two-electron one-photon (TEOP) transition is correlation sensitive. The Breit interaction and electron correlation both contribute significantly to the radiative transition properties of the double K hole state of He-like ions. Good agreement between the present calculation and previous work is achieved. The calculated data will be helpful to future investigations on double K hole decay processes of He-like ions.

I. INTRODUCTION

The energy level structures and radiative decay processes of inner-shell hole states are an important issue in atomic physics [1-6]. An inner-shell hole occurs when the inner shell orbital of an atom or ion is unoccupied, while the outer shell orbital is occupied by electrons. Inner-shell hole states have been observed in high-energy ion-atom collisions [7-9], synchrotron radiation [10], laser-produced plasmas [11], ion beam-foil spectroscopy [12], Tokamak [13], and solar flares [14]. They can also be produced by electron excitation or the ionization of the inner shells of atoms or ions [15], as well as in inner-shell photoionization or photoexcitation processes with high-energy photons [16]. These exotic atoms are extremely unstable and mainly decay through non-radiative Auger processes [17-19] and radiative processes. The former processes are usually more efficient than the latter. With the development of X-ray spectroscopy, weak signal detection technology has helped scientists to understand such processes from the photon perspective.

It is also possible to create an ion with an empty innermost shell, forming a double K shell hole state [20]. Generally, the radiative de-excitation of an atom with an initially empty K shell may take place either through the more probable one-electron one-photon (OEP) transition or through the competing weak two-electron one-photon (TEOP) transition. The initially double K hole state 2p2s in He-like ions can decay either through an OEP transition to a single excited state 1s2s, where a 2p electron transitioning to 1s with a spectator 2s electron, or through a TEOP transition, in which both electrons in the 2s and 2p orbitals transition to 1s orbitals simultaneously, producing the ground state 1s2 due to electron correlation effects. The TEOP process was first predicted theoretically by Heisenberg in 1925 [21] and was observed by Wöfling and co-workers in ion-atom collision experiments between Ni-Ni, Ni-Fe, Fe-Ni and Fe-Fe in 1975 [22]. Since then, TEOP transitions have been widely studied both theoretically and experimentally [23-33].

The TEOP process is forbidden in the independent particle approximation of an atom. Investigations of this process are helpful for explaining electron correlation effects, relativistic effects and quantum electro-dynamics (QED) effects on the energy level structure and radiative transitions of these exotic atoms. Insights into the electron coupling of complex atom systems are also helpful. For astrophysical and laboratory plasmas, some important diagnostics information regarding the composition, temperature and density has also been provided by these basic atomic physics processes [23-24].

There have been many works related to the energy levels and transition properties of inner-shell hole states in the past several decades [25-35], but only a few studies have focused on He-like ions [25-28]. The He-like ion is a two-electron system with a simple structure and an electron correlation effect and is a good candidate with which to study the TEOP process. Kadelkar and Natarajan calculated the transition properties and branching ratios between OEP and TEOP transitions in He-like ions with 2s2p configurations using the multi-configuration Dirac-Fock (MCDF) method [30] and found that the contribution from the TEOP transition is considerable for low-Z ions. The influence of the configuration interaction on single-electron allowed E1 transitions is negligible. They also calculated both OEP and TEOP transition rates from 2s2p and 2p2 of He-like Ni, including electric dipole transitions (E1) and magnetic quadrupole transitions (M2) [31] and found that higher order corrections are more important for Δn = 0 than for Δn = 1 transitions of He-like Ni. After that, Natarajan conducted research on the orthogonality of the basis. The biorpheg-
binary and common basis sets give almost the same transition rates for light and medium heavy elements while the differences are substantial for heavy elements [31]. The contributions from correlation and higher-order corrections, consisting of Breit and QED effects, to the energies and transition rates were analyzed. Experimentally, transitions from 2s2-1s2p in He-like Si have been observed in laser-produced plasma experiments at the TRIDENT facility by Elton et al. 32. Tawara and Richard et al. have observed Ar K X-rays under 60 keV/u Ar16+/Ar collisions from the KSU EBIS [33].

Previous theoretical and experimental investigations of OEOP and TEOP transitions have mostly focused on the low-Z atoms, with only a few works focusing on high-Z ions [36, 37]. The present work provides an MCDF calculation of OEOP and TEOP transitions from double K hole 2s2p configurations in 11 selected He-like ions (10 ≤ Z ≤ 47). The electron correlation effects are accounted for by choosing appropriate electron correlation models using the active space method. The Breit interaction and QED effects are included perturbatively in relativistic configuration interaction (RCI) calculations. The finite nuclear size effects are described by a two-parameter Fermi distribution model. The purpose of the present calculations is to explore how the effects of electron correlation and the Breit interaction on the transition energies and rates of OEOP and TEOP transitions vary with increasing Z. The results will be helpful to future theoretical and experimental work on the radiative decay processes of double K hole states. The calculations were performed using the Grasp2K code [38].

II. THEORETICAL METHOD

The multi-configuration Dirac-Fock (MCDF) method has been widely used to investigate relativistic, electron correlation, Breit interaction, and quantum electrodynamics (QED) effects on the structure and transitions of complex atoms or ions based on relativistic atomic theory [39–41]. The method was expounded in Grant’s monograph [42] and implemented in the Grasp family code [38, 43–46]. Here, only a brief introduction to the MCDF method is provided.

In the MCDF method, the atomic state wave function (ASFs) Ψ(PJMj) for a given state with certain parity P, total angular momentum J, and its z component Mj is represented by a linear combination of configuration state functions (CSFs) Φ(γiPJMj) with the same P, J, Mj, which can be expressed as:

\[ \Psi(PJM_j) = \sum_{i=1}^{N_c} c_i \Phi(\gamma_iPJM_j). \]  

where \( N_c \) is the number of CSFs and \( \gamma_i \) denotes all the other quantum numbers necessary to define the configuration, \( c_i \) is the mixing coefficient. The CSFs are linear combinations of the Slater determinants of the many-particle system consisting of single electron orbital wave functions. The extended optimal level (EOL) mode is used in the self-consistent field (SCF) calculation to optimize the radial wave functions. The mixing coefficients \( c_i \) of CSFs are determined variationally by optimizing the energy expectation value of the Dirac-Coulomb Hamiltonian, which is defined as in the following equation:

\[ H_{DC} = \sum_{i=1}^{N} [\alpha_i \cdot p_i + (\beta_i - 1)c^2 + V_i^N] + \sum_{i>j}^{N} 1/r_{ij}, \]  

(2)

The RCI calculations are done by including higher-order interactions in the Hamiltonian. The transverse photon interaction plays a dominant role in the calculations, especially for high-Z ions, which can be expressed as follows:

\[ H_{\text{trans}} = \sum_{i,j}^{N} [\alpha_i \cdot p_i \cos(\omega_{ij})/r_{ij} + (\alpha_i \cdot \nabla_j)(\alpha_j \cdot \nabla_j)] (3) \cos(\omega_{ij}) - 1/\omega^2_{ij} r_{ij} \]

(3)

The Breit interaction is the low-frequency limit of eq. 3. QED effects including vacuum polarization and self-energy are also taken into account in the present calculation perturbatively.

III. ELECTRON CORRELATION MODEL AND CALCULATION STRATEGY

The electron correlation effects are taken into account by choosing an appropriate electron correlation model. The correlation model used in the present calculation is similar to the model used by Kadrekar and Nataraajan [28]. The major electron correlation effects can be captured by including the CSFs, which were formed by allowing single and double (SD) excitations from the interested reference configurations to some virtual orbital space. The configuration space was extended by increasing the active orbital set layer by layer to study the correlation contributions. Generally, the zero-order Dirac-Fock (DF) wave functions were first generated from the reference configurations of He-like ions in EOL mode for the initial and final states. In the EOL method, the radial wave functions and the mixing coefficients are determined by optimizing the energy functional, which is the weighted sum of the selected eigenstates. For a double K hole state, the minimum basis (MB) was generated by considering limited expansion and allowing SD substitutions of electrons from the reference configurations. Since this procedure results in better optimized wave functions than the DF functions, all the examinations of the correlation effects here are carried out with respect to the MB. Then, the active space was expanded to the first layer, i.e. \( n = 3, l = 2 \) (\{n3l2\}) virtual orbitals and all the newly added orbital functions were optimized while the
1s, 2s and 2p orbitals were kept fixed from the MB. These steps were repeated, increasing the virtual orbitals to ensure that the eigenenergy and wave function converged. To ensure the stability of the numeric data and reduce the calculation time, only the newly added layer was optimized at each step and the previous calculated orbits were all kept frozen. As the virtual orbitals increased, the number of CSFs increased rapidly. In order to keep the calculation manageable, the principle quantum number of the virtual orbitals was limited to \( n = 6 \).

IV. RESULTS AND DISCUSSION

The energy levels and transition properties of the He-like Ne, Si, Ar, Ca, Fe, Ni, Cu, Zn, Kr, Nb, and Ag ions were calculated using MCDF with the active space method. The energy levels (in eV) of the double excited configuration 2s2p and the single excited configuration 1s2s of He-like Ne and Ag ions are presented in Table I to show the convergence. Since the correlation model of MB provides better optimized wave functions than the DF functions, all our investigations on the correlation effects and higher-order corrections were carried out with respect to the MB. It can be speculated from the table that with an increase in the active space, the eigenenergies tend to converge for both low-Z and high-Z ions. The energy \( E \) of 2s2p relative to the ground state \( ^1S_0 \) 1s\(^2 \) of He-like Ne was provided with available theoretical results. Excellent agreement of the relative errors (\( \leq 0.1\% \)) between the present calculation and previous work that also used the MCDF method was achieved. Therefore the present calculation was restricted to the \( \{n6l3\} \) correlation models.

The transition energies in eV of the OEO transitions from the 2s2p configuration to the 1s2s configuration of He-like ions (10 \( \leq Z \leq 47 \)) are presented in Table II. The results for \( Z \leq 26 \) He-like ions agree well with the available experimental data and other theoretical calculation results. The average relative error of the current calculation compared to the experimental observation is about 0.01%-0.09\%. Results for the ions with \( Z \geq 28 \) were also calculated for the present work. To the best of the authors’ knowledge, corresponding experimental and theoretical data was otherwise unavailable. Therefore, it will now be helpful to future experimental and theoretical investigations.

In the calculation of transition properties in relativistic atomic theory, the Babushkin (B) and Coulomb (C) gauges are often used, which correspond to the length and velocity gauges in non-relativistic quantum mechanics, respectively. These are equivalent when exact wave functions are used, but they usually give rather different results when approximate wave functions are used. The consistency of the transition rates from different gauges therefore indicates the accuracy of the wave function to some extent. The ratio of the transition rates from the Babushkin and Coulomb gauges has often been adopted as a criterium for ensuring the accuracy of the wave function and the calculation results. In our calculations, the ratio of the transition rates from different correlation models tended towards 1.00 with increased active space. This indicates that the wave function used in the present calculation is good and that the most important correlation effects were included in the present work.

The transition rate of the OEO transition from 2s2p to 1s2s of He-like ions (10 \( \leq Z \leq 47 \)) are presented in Table III. For brevity, only the transition rates in the Babushkin gauge are given in the table. The current calculated transition rates are in good agreement with the result calculated by Kadrekar and Natarajan using the MCDF method [29] and by Goryaev et al. using the Z-expansion method [17]. The Z-expansion method is based on perturbation theory and a hydrogen-like basis, while MCDF includes electron correlation effectively. Four allowed transitions and two dipole forbidden transitions are listed in the table. For transitions from the same initial state \(^3P_1\) to different final states \(^1S_0\) and \(^3S_1\), the ratio of the two transition rates is approximately 10^{-3} when \( Z=10 \), while the ratio increases to 10^{-1} when \( Z=47 \). This indicates that the intensity of these dipole forbidden transitions increases sharply with increasing Z, which provides a candidate for the observation of E1 forbidden transitions in high-Z ions. For high temperature plasmas, some important diagnostics information is provided by these transitions.

The transition energies and rates of TEOP transitions from the initial 2s2p configuration to the final 1s^2 configuration are listed in Table IV. The ratio of the transition rates in the Babushkin and Coulomb gauges is about 1.2-1.5. The TEOP transition energy is approximately twice the corresponding OEO transition energy, as expected. In general, good agreement between the present rate and the length gauge rate of Kadrekar et al. [29] can be obtained.

The electron correlation effect on the OEO and TEOP transition energies and rates is shown in Fig. 1. The correlation contributions to the transition energy from \( \{n6l3\} \) are with respect to the MB. The correlation contribution to the transition energies from the \(^1P_1\) upper level decrease smoothly, while increasing with Z for the others. The correlation effect contributes to the dipole allowed transition energy by 0.2 eV to 1.0 eV, while it is 0.2 eV to 1.5 eV for dipole forbidden transitions. However, for the TEOP transition, the contribution to the transition energy is 0.2 eV to 1.5 eV.

The percentage correlation contribution to the OEO and TEOP transition energies from \( \{n6l3\} \) with respect to the MB are given in Figs. 1(a) and (b). The contribution from the electron correlation to the transition energy increases with increasing Z for TEOP transitions and the \(^3P_1\)-\(^1S_0\) OEO transition while the others decrease.

The percentage contribution of electron correlation to the transition rates in the Babushkin gauge of OEO and TEOP transitions from \( \{n6l3\} \) with respect to the MB are shown in Figs. 1(c) and (d). The correlation contri-
\begin{table}[h]
\centering
\small
\begin{tabular}{lcccccc}
\hline
\multicolumn{7}{c}{He-like Ne} \\
Active sets & \multicolumn{2}{c}{2s2p} & \multicolumn{4}{c}{1s2s} \\
\hline
DF & $3P_0$ & $1P_1$ & $3P_2$ & $3P_1$ & $3S_1$ & $1S_0$ \\
MB & -645.71 & -629.80 & -645.30 & -645.58 & -1653.06 & -1643.25 \\
n3l2 & -645.68 & -630.16 & -645.26 & -645.55 & -1653.00 & -1642.07 \\
n4l3 & -645.72 & -630.36 & -645.31 & -645.59 & -1653.01 & -1642.16 \\
n5l3 & -645.74 & -630.74 & -645.38 & -645.62 & -1653.03 & -1642.23 \\
n6l3 & -645.80 & -630.92 & -645.39 & -645.67 & -1653.03 & -1642.26 \\
E & 1911.70 & 1926.58 & 1912.11 & 1911.83 & 904.47 & 915.24 \\
Ref & 1911.48 & 1926.13 & 1911.89 & 1911.60 & 904.41 & 914.82 \\
NIST & 1912.26 & 1926.63 & 1912.83 & 1911.97 & 905.08 & 915.34 \\
\hline
\multicolumn{7}{c}{He-like Ag} \\
Active sets & \multicolumn{2}{c}{2s2p} & \multicolumn{4}{c}{1s2s} \\
\hline
DF & $3P_0$ & $1P_1$ & $3P_2$ & $3P_1$ & $3S_1$ & $1S_0$ \\
MB & -15437.72 & -15146.58 & -15203.39 & -15417.21 & -38550.42 & -38489.71 \\
n3l2 & -15437.46 & -15146.22 & -15203.17 & -15416.90 & -38550.33 & -38487.92 \\
n4l3 & -15437.66 & -15146.84 & -15203.36 & -15417.21 & -38550.38 & -38488.33 \\
n5l3 & -15437.70 & -15147.04 & -15203.41 & -15417.29 & -38550.39 & -38488.42 \\
n6l3 & -15437.72 & -15147.42 & -15203.48 & -15417.35 & -38550.41 & -38488.51 \\
\hline
\end{tabular}
\caption{Energies (in eV) of the initial and final states of He-like Ne and Ag ions in various active space sets. The notation DF denotes the Dirac-Fock calculation, MB the minimum basis, \{nafb\} the active set consisting of all orbitals from \(n=a\) to \(l=b\), and \(E\) the energy relative to the ground state \(3S_0\) 1s\(^2\). For details see Sec. [III].}
\end{table}

The contribution to the transition rate of OEOP processes becomes smaller while that to TEOP transitions becomes larger with increasing \(Z\). However, for the low-Z elements, especially \(15 \leq Z \leq 25\), anomalies in the contribution to the E1 forbidden transition rate were observed. This might be caused by the fact that the Coulomb interaction between the nucleus and electrons competes with the electron-electron interaction for low-Z elements. For high-Z ions, the Coulomb interactions between the nucleus and electrons are dominant and the correlation contribution becomes smaller.

Fig. 2 shows the contribution from the Breit interaction to the transition energies and rates of OEOP and TEOP transitions. It is seen in Fig. 2(a) and (b) that the Breit interaction decreases the \(1P_1\)-\(1S_0\) and \(3P_1\)-\(1S_0\) transition energies for both OEOP and TEOP transitions, while it slightly increases the transition energy of the transition to the \(3S_1\) state in OEOP transitions. This is due to the Breit interaction reducing the binding energy of each state of the 2s2p configuration and also that of the \(1S_0\) state of the 1s2s configuration but slightly increasing the binding energy of the \(3S_1\) state of the 1s2s configuration, which makes the transition energy of \(1P_1\)-\(1S_0\) and \(3P_1\)-\(1S_0\) smaller and the energies of the other transitions to the \(3S_1\) state slightly increase. It is found that the contribution from the electron correlation is larger than that from the Breit interaction for low-Z elements, while the latter becomes significant for high-Z ions.

In Fig. 2(c) and (d), the contributions of the Breit interaction to the transition rates in the length gauge of the OEOP and TEOP transitions is given. Unlike the correlation contribution, the Breit interaction reduces the rates of \(1P_1\)-\(1S_0\) and \(3P_1\)-\(1S_0\), and slightly increases the transition rates of other transitions to the \(3S_1\) state in OEOP processes. For TEOP transitions, the Breit interaction increases the transition rate of \(1P_1\)-\(1S_0\) and \(3P_1\)-\(1S_0\) with increasing \(Z\). It can be seen from the figures that the Breit interaction contributions to the \(1P_1\)-\(3S_1\) and \(3P_1\)-\(1S_0\) OEOP transition rates are about 3.2% and 2.8% at \(Z = 10\), respectively. These decrease with increasing \(Z\), reaching approximately 0.1% at \(Z = 47\) for both transitions. However, for the TEOP transition, the Breit interaction contribution to the transition rate is about 0.5%-5.5% and 0.1%-4% for the \(3P_1\)-\(1S_0\) and \(1P_1\)-\(1S_0\) transitions, respectively. Since TEOP is a multielectron process, the electron correlation effect plays an essential role in this transition, and the Breit interaction becomes more and more significant with increasing \(Z\), as can be inferred from Fig. 1(d) and 2(d).

The mixing of the CSFs leads to the feasibility of a TEOP transition that is strictly forbidden according to the selection rules. The main component of the 2s2p \(1P_1\) and \(3P_1\) states of the CSFs change from 67% for Ne to 98% for Ag, which indicates a change of the coupling scheme from \(LSJ\) to \(jj\) with a change in the nucleus and the interactions in these ions. The mixing from 1s2p \(1P_1\)
TABLE II. Transition energies (in eV) of one-electron radiative transitions from 2s2p configuration in He-like ions. "*" denotes the spin-forbidden transition.

| Z  | ^3P_1-^1S_0 | ^3P_0-^3S_1 | ^3P_1-^3S_1 | ^3P_2-^3S_1 | ^1P_1-^3S_0 | ^1P_1-^3S_1^* |
|----|--------------|--------------|--------------|--------------|--------------|----------------|
| 10 | 996.38       | 1007.09      | 1007.22      | 1007.50      | 1011.14      | 1021.97        |
|    | Ref^a        | Expt.        |              |              |              | 1007.86^b     |
|    | 996.79       | 1007.07      | 1007.20      | 1007.48      | 1011.32      | 1021.73        |
| 14 | 1968.59      | 1983.91      | 1984.41      | 1985.54      | 1990.22      | 2006.04        |
|    | Ref^a        | Expt.        |              |              |              | 1985.8^c      |
|    | 1968.97      | 1983.88      | 1984.39      | 1985.52      | 1990.39      | 2005.80        |
| 18 | 3272.06      | 3291.73      | 3293.05      | 3296.28      | 3301.40      | 3322.40        |
|    | Theory^b     |              |              |              |              | 3296.2        |
|    | 3272.44      | 3291.69      | 3293.02      | 3296.26      | 3301.56      | 3322.15        |
| 20 | 4049.48      | 4070.68      | 4072.63      | 4077.67      | 4082.73      | 4106.39        |
|    | Theory^b     |              |              |              |              | 4077.6        |
|    | 4049.34      | 4070.64      | 4072.60      | 4077.66      | 4082.89      | 4106.15        |
| 26 | 6886.05      | 6913.88      | 6918.15      | 6933.78      | 6937.35      | 6969.45        |
|    | Ref^a        | Expt.        |              |              |              | 6937.4        |
|    | 6886.41      | 6913.32      | 6918.10      | 6933.77      | 6937.52      | 6969.20        |
| 28 | 8002.38      | 8031.47      | 8037.45      | 8059.10      | 8061.75      | 8096.83        |
|    | 8059.28      | 8022.86      | 8035.88      | 8057.45      | 8065.88      | 8093.48        |
| 30 | 9205.07      | 9235.93      | 9243.22      | 9272.57      | 9274.13      | 9312.28        |
| 36 | 13338.82     | 13375.35     | 13386.87     | 13452.79     | 13450.21     | 13498.25       |
| 41 | 17399.28     | 17441.38     | 17456.47     | 17573.86     | 17567.01     | 17624.2        |
| 47 | 23036.86     | 23086.18     | 23105.36     | 23319.99     | 23307.07     | 23376.57       |

^a Reference[29].
^b Reference[47].
^c Reference[48].
^d Reference[49].
^e Reference[14].

and ^3P_1 is tiny (less than 1%), even though it contributes the main parts for the TEOP transitions. Because the 2p - 1s resonance transition is strong, the TEOP transition matrix elements become non-zero because of this tiny mixing. Besides the mixing of the 1s2p with the excited states 2s2p, there is also a small mixing from 2s2p, 2p2 contributing to the ground state 1s^2 ^1S_0. Therefore, the 2p - 2s and 2s - 2p transition matrix elements could also contribute to the TEOP transition by mixing.

V. CONCLUSION

The energy levels, transition energies and transition rates for one- and two-electron radiative transitions from double K hole 2s2p to 1s2s and 1s^2 configurations of He-like ions were calculated using MCDF method. A reasonable electron correlation model was constructed to study the electron correlation effects based on the active space. Breit interaction and QED effects were taken into account efficiently. The transition energies and rates were found to be in good agreement with those in previous work. It is emphasized in the present work that the TEOP transition is essentially caused by electron correlation effects. It is also found that the electron correlation effect and Breit interaction contribution to the transition energies of both OEOP and TEOP transitions decrease with increasing Z. Competition between the nucleus-electron Coulomb interaction and electron correlation was clearly found for lower Z ions. The former dominates in high Z ions. The calculated data will be helpful for future investigations on OEOP and TEOP transitions of He-like ions.

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TABLE III. Transition rates (in sec\(^{-1}\)) of the one-electron radiative transitions from the 2s2p configuration in He-like ions, with \(^{\star}\) denoting the spin-forbidden transition.

| Z  | \(^3\)P\(_1\)\(^-(\)S\(_0\)\(^{\star}\) | \(^3\)P\(_1\)\(^-(\)S\(_1\) | \(^3\)P\(_1\)\(^-(\)P\(_1\) | \(^3\)P\(_1\)\(^-(\)P\(_3\) | \(^1\)P\(_1\)\(^-(\)S\(_0\) | \(^1\)P\(_1\)\(^-(\)S\(_1\)\(^{\star}\) |
|----|-----------------|----------------|----------------|----------------|----------------|----------------|
| 10 | 1.042(9)        | 5.607(12)      | 5.621(12)      | 5.650(12)      | 5.661(12)      | 8.316(8)       |
|    | Ref\(^a\)       |                |                |                |                |                |
|    | Theory\(^b\)   | 1.17(9)        | 5.79(12)       | 5.80(12)       | 5.80(12)       | 6.02(12)       | 1.22(9)        |
| 14 | 3.090(10)       | 2.243(13)      | 2.239(13)      | 2.236(13)      | 2.237(13)      | 2.736(10)      |
|    | Ref\(^a\)       | 3.375(10)      | 2.268(13)      | 2.262(13)      | 2.259(13)      | 2.318(13)      | 2.938(10)      |
|    | Ref\(^b\)       | 3.19(10)       | 2.29(13)       | 2.28(13)       | 2.29(13)       | 2.35(13)       | 3.31(11)       |
| 18 | 3.611(11)       | 6.240(13)      | 6.179(13)      | 6.198(13)      | 6.178(13)      | 3.318(11)      |
|    | Ref\(^a\)       | 3.818(11)      | 6.283(13)      | 6.238(13)      | 6.246(13)      | 6.346(13)      | 3.465(11)      |
|    | Theory\(^b\)   | 3.63(11)       | 6.36(13)       | 6.33(13)       | 6.38(13)       | 6.47(13)       | 3.75(11)       |
| 20 | 9.8669(11)      | 9.568(13)      | 9.432(13)      | 9.489(13)      | 9.419(13)      | 9.153(11)      |
|    | Ref\(^a\)       | 1.034(12)      | 9.628(13)      | 9.509(13)      | 9.554(13)      | 9.646(13)      | 9.472(11)      |
|    | Theory\(^b\)   | 9.86(11)       | 9.76(13)       | 9.67(13)       | 9.81(13)       | 9.87(13)       | 1.01(12)       |
| 26 | 1.067(13)       | 2.768(14)      | 2.655(14)      | 2.730(14)      | 2.636(14)      | 1.005(13)      |
|    | Ref\(^a\)       | 1.100(13)      | 2.780(14)      | 2.666(14)      | 2.744(14)      | 2.683(14)      | 1.025(13)      |
|    | Theory\(^b\)   | 1.06(13)       | 2.84(14)       | 2.74(14)       | 2.87(14)       | 2.79(14)       | 1.08(13)       |
| 28 | 1.992(13)       | 3.738(14)      | 3.576(14)      | 3.676(14)      | 3.496(14)      | 1.881(13)      |
| 29 | 2.652(13)       | 4.304(14)      | 4.029(14)      | 4.232(14)      | 3.990(14)      | 2.505(13)      |
| 30 | 3.472(13)       | 4.936(14)      | 4.578(14)      | 4.847(14)      | 4.529(14)      | 3.283(13)      |
| 36 | 1.318(14)       | 1.031(15)      | 8.977(14)      | 1.005(15)      | 8.817(14)      | 1.245(14)      |
| 41 | 3.013(14)       | 1.744(15)      | 1.440(15)      | 1.686(15)      | 1.405(15)      | 2.884(14)      |
| 47 | 6.548(14)       | 3.029(15)      | 2.371(15)      | 2.897(15)      | 2.283(15)      | 6.141(14)      |

\(^a\) Reference [28].
\(^b\) Reference [47].
TABLE IV. Transition energies (in eV) and rates (in sec$^{-1}$) in the length gauge of two-electron one-photon transitions from 2s2p to 1s$^2$ in He-like ions. The numbers in the parentheses represent powers of ten.

| Z | $^3\text{P}^1$-$^1\text{S}_0$ Energy | Rate | $^3\text{P}^1$-$^3\text{S}_0$ Energy | Rate |
|---|---|---|---|---|
| 10 | 1926.00 | 6.030(9) | 1911.25 | 1.648(6) |
| 14 | 3844.42 | 1.232(10) | 3822.79 | 1.955(7) |
| 18 | 6425.41 | 2.077(10) | 6396.07 | 1.307(8) |
| 20 | 7966.43 | 2.587(10) | 7932.67 | 2.860(8) |
| 24 | 13604.75 | 4.346(10) | 13553.46 | 1.828(9) |
| 26 | 15827.11 | 5.001(10) | 15767.73 | 2.955(9) |
| 28 | 17003.44 | 5.338(10) | 16939.45 | 3.676(9) |
| 30 | 18223.52 | 5.682(10) | 18154.46 | 4.512(9) |
| 36 | 26475.88 | 7.897(10) | 26364.50 | 1.220(10) |
| 41 | 34603.61 | 1.002(11) | 34435.88 | 2.232(10) |
| 47 | 45918.80 | 1.313(11) | 45647.60 | 3.917(10) |

* Reference [24]

b Reference [4]

* The observed experimental transition energy is about 6.39keV.

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[24] V. Decaux, P. Beiersdorfer, S. M. Kahn, and V. L. Jacobs, Astrophys. J 482, 1076 (1997).
[25] L. Natarajan and A. Natarajan, Phys. Rev. A 75, 062502 (2007).
[26] L. Natarajan, Phys. Rev. A 88, 052522 (2013).
[27] L. Natarajan, Phys. Rev. A 93, 032516 (2016).
[28] C. D. Lin, W. R. Johnson, and A. Dalgarno, Phys. Rev. A 15, 154 (1977).
[29] R. Kadrekar and L. Natarajan, Phys. Rev. A 84, 062506 (2011).
[30] L. Natarajan and R. Kadrekar, Phys. Rev. A 88, 012501 (2013).
[31] L. Natarajan, Phys. Rev. A 90, 032509 (2014).
[32] R. Elton, J. Cobble, H. Griem, D. Montgomery, R. Mancini, V. Jacobs, and E. Behar, J. Quant. Spectrosc. Radiat. Transfer 65, 185 (2000).
[33] E. Trabert, B. C. Fawcett, and J. D. Silver, J. Phys. B: At. Mol. Phys. 15, 3587 (1982).
[34] H. W. S¨ affer, R. W. Dunford, E. P. Kanter, S. Cheng, L. J. Curtis, A. E. Livingston, and P. H. Mokler, Phys. Rev. A 59, 245 (1999).
[35] H. Tawara and P. Richard, Can. J. Phys. 80, 1579 (2002).
[36] R. Kadrekar and L. Natarajan, J. Phys. B: At., Mol. Opt. Phys. 43, 155001 (2010).
[37] J. Li, P. Jnsson, C. Dong, and G. Gaigalas, J. Phys. B: At., Mol. Opt. Phys. 43, 035005 (2010).
[38] P. Jnsson, X. He, C. F. Fischer, and I. P. Grant, Comput. Phys. Commun. 177, 597 (2007).
[39] X. B. Ding, F. Koike, I. Murakami, D. Kato, H. A. Sakaue, C. Z. Dong, N. Nakamura, A. Komatsu, and J. Sakoda, J. Phys. B: At. Mol. Opt. Phys. 44, 145004 (2011).
[40] X. Ding, R. Sun, F. Koike, D. Kato, I. Murakami, H. A. Sakaue, and C. Dong, Eur. Phys. J. D 71, 73 (2017).
[41] K. M. Aggarwal and F. P. Keenan, At. Data Nucl. Data Tables 111-112, 187 (2016).
[42] I. P. Grant, Relativistic Quantum Theory of Atoms and Molecules, Theory and Computation (Springer, New York, 2007).
[43] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. 21, 207 (1980).
[44] J. P. Desclaux, Comput. Phys. Commun. 35, C (1984).
[45] K. G. Dyall, I. P. Grant, C. T. Johnson, F. A. Parpia, and E. P. Plummer, Comput. Phys. Commun. 55, 425 (1989).
[46] F. A. Parpia, C. F. Fischer, and I. P. Grant, Comput. Phys. Commun. 94, 249 (1996).
[47] F. Goryaev, L. Vainshtein, and A. Urnov, At. Data Nucl. Data Tables 113, 117 (2017).
[48] J. P. Mosnier, R. Barchewitz, M. Cukier, R. Dei-Cas, C. Senemaud, and J. Bruneau, J. Phys. B: At. Mol. Phys. 19, 2531 (1986).
[49] T. Nandi, The Astrophysical Journal Letters 673, L103 (2008).
FIG. 1. The electron correlation effect on the transition energies and rates for OEOP and TEOP transitions in He-like ions. 
(a) The percentage correlation contribution to the OEOP transition energies of $2s^2p - 1s^2$. (b) The percentage contribution to the TEOP transition energies of $2s^2p - 1s^2$. (c) The percentage contribution to the OEOP transition rate in the length gauge of $2s^2p - 1s^2$. (d) The percentage contribution to the TEOP transition rate in the length gauge of $2s^2p - 1s^2$. 
FIG. 2. The Breit interaction effect on the transition energies and rates for OEO and TEO transitions in He-like ions. (a) The percentage Breit contribution to the OEO transition energies of $2s^2p - 1s^2s$. (b) The percentage Breit contribution to the TEO transition energies of $2s^2p - 1s^2s$. (c) The Breit contribution to the OEO transition rates in the length gauge of $2s^2p - 1s^2s$. (d) The Breit contribution to the TEO transition rates in the length gauge of $2s^2p - 1s^2s$. 