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Energy-crossings and their effects on the spectra of the neon-like ions*

Dong Chen-Zhong(董晨钟)[a)b)†], Xie Lu-You(颉录有)[a)], Wan Jian-Jie(万建杰)[a)], and Jiang Jun(蒋 军)[a)]

[a)] *College of Physics and Electronics Engineering, Northwest Normal University, Lanzhou 730070, China*

[b)] *National Laboratory of Heavy-Ion Accelerator of Lanzhou, Lanzhou 730000, China*

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Excitation energies, transition wavelengths and probabilities of the $2p^6$, $2p^5\,3l$, $2s\,2p^6\,3l\,(l=0,1,2)$ states along the Ne-like isoelectronic sequence from $Z=21-92$ have been calculated by using the multi-configuration Dirac-Fock (MCDF) package GRASP92 and a newly developed radiative transition program REOS99. In the calculations, the correlation and relaxation effects are included systematically. Based on the calculations, all possible energy crossings among the level groups with the same parity and total angular momentum have been presented. It is found that there are strong configuration interactions in some particular Z regions with energy-crossings, which can cause a dramatic change of the related transition probabilities.

Keywords: MCDF method, energy crossing, configuration interaction, transition probabilities
PACC: 3120B, 3130, 3270F

1. Introduction

The energy structures and spectra of neon-like ions have been a subject of interesting investigations in theory, experiment and application. During the past years, many significative investigations have been carried out.[1−12] In theory, the neon-like ions are a multielectron system with a closed shell structure. It is a very good example to understand the contributions from relativistic, electron correlation, relaxation and quantum electrodynamic (QED) effects in accurate study of energy structures and transition properties. Systematic studying of neon-like ions has become a candidate for testing various aspects of atomic structure theory. For example, the Z-expansion method, model potential method, configuration-interaction method, multiconfiguration Hartree–Fock (MCHF) method, multiconfiguration Dirac–Fock (MCDF) method, and relativistic many-body perturbation theory (MBPT) have been used to produce a great deal of energies and transition probabilities data for many neon-like ions in these years.[1−8] In experiment, the neon-like charge state is relatively stable. It is often the dominant ionization state over a wide range of plasma temperature. The neon-like ions of middle- and high-Z are often present in a variety of high-temperature plasma sources, such as tokamak, laser-produced plasmas, gas-puff Z-pinch, solar atmosphere, EBIT and so on. As a result, the spectra of neon-like ions are the most easily observed lines.[9−12] In application, the properties of neon-like ions suggest their use for diagnostic purposes. In tokamak, for example, the neon-like ions are employed to study the transport and confinement of high-Z impurity ions. Also, the spectra from the neon-like systems may provide diagnostic information on plasma electron temperature, electron density, charge-state abundance, and ion temperatures. In addition, it is also very important for understanding the energy levels and the excitation mechanisms of x-ray laser.[10]

In the present work, systematic calculations on the 37 low-lying energy levels of the $2s^2\,2p^5\,3l$, $2s\,2p^6\,3l\,(l=0,1,2)$ and $2s^2\,2p^6$ configurations and the E1 transition probabilities among those levels were

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†E-mail: dongcz@nwnu.edu.cn

carried out for the neon-like ions in the range of $Z = 21 - 92$. In our calculations, the effects of relativistic, relaxation and correlation have been considered by using the MCDF package GRASP92[13] and a newly developed radiative transition program REOS99.[14] In order to describe the accuracy of the present calculations, some data of the excited energies and E1 transition probabilities are chosen for low-, middle- and high-Z respectively as comparison with the available experiments and calculations. From the calculations, a systematic study on Z-dependence of the energies and transition probabilities along the whole sequence is carried out. Of course, in this paper, much attention is paid on the energy crossings and their effects on transition probabilities.

2. Theoretical method and computational procedure

In this study, wavefunctions have been generated by the widely used atomic structure package GRASP92[13] on the basis of the MCDF method, in which an atomic state is approximated by a linear combination of configuration state functions (CSFs) with the same symmetry

$$|\psi_\alpha (PJM)\rangle = \sum_{r=1}^{n_c} c_r(\alpha)\,|\gamma_r PJM\rangle, \qquad (1)$$

where n_c is the number of CSF and $c_r(\alpha)$ denotes the representation of the atomic state in this basis. In a standard calculation, the CSF are the antisymmetrized products of a common set of orthonormal orbitals which are optimized on the basis of the Dirac–Coulomb Hamiltonian. Further relativistic contributions to the representation $c_r(\alpha)$ of the atomic states due to (transverse) Breit interactions were added by diagonalizing the Dirac–Coulomb–Breit Hamiltonian matrix. The dominant quantum electrodynamic (QED) contributions to the transition energies have also been included in the computations as a perturbation.

To calculate the excited energies corresponding to the $2p^6$, $2p^5\,3l$, $2s\,2p^6\,3l\,(l = 0,1,2)$ configurations and the transition wavelengths and probabilities among these levels, we used the GRASP92 program package developed by Grant and co-workers.[13] A set of subshell wavefunctions for the ground configuration $1s^2\,2s^2\,2p^6$, and that for 36 excited configurations $2l^{-1}\,3l'\,(l = 0,1; l' = 0,1,2)$ (representing that for the $2l$ core-subshell electrons excited to the $3l'$ subshell) were optimized through self-consistent field (SCF) calculations in the (extended) optimal level model of the GRASP92 package.[13] In order to consider systematically the influence of electron correlations in the calculations, the configuration interaction from virtual excitations of electrons from the spectroscopically occupied shells into the unoccupied (sub–) shells are taken into account by using the active space method. In the present computations, all virtual single (S) and double (D) excitations from the 2s, 2p, and $3l$ shells into the (unoccupied) $3l$ shells as well as $4l$ shells are included. It is shown that the effects of those electron correlations are very important for the accuracy of calculations of the transition wavelengths and probabilities in neon-like ions, especially for the low-Z ions.[1]

3. Comparison with available results

In the present work, the energies of the 37 low-lying levels of the $2s^2\,2p^5\,3l$, $2s\,2p^6\,3l\,(l = 0,1,2)$ and $2s^2\,2p^6$ configurations and the E1 transition probabilities among those levels have been calculated for the neon-like ions in the range of $Z = 21 - 92$. In order to illustrate the accuracy of the present calculations, a comparison with available results is given in Table 1 and Table 2, respectively for excited energies and transition probabilities of three selected ions with Z=36, 60 and 92.

In Table 1, the present calculated and the available experimental and theoretical excited energies for seven levels with $J^P = 1^-$ are listed. It can be seen from the table that the present results are in close agreement with the experimental measurements and the other theoretical calculations, and the discrepancy among these results is generally less than 0.3%.

In Table 2, the calculated E1 transition probabilities from the excited states $2l3l'$ with $J^P = 1^-$ to the ground state $2p^6\,{}^1S_0$ are given for the three selected ions. Also some previous theoretical values are listed as comparison. It is found that the present calculations are very close to the results of the MBPT calculations by Safronova *et al*[2] both in low Z, middle Z, and high Z ions. But there are also some very big differences between the present MCDF results and the MBPT calculations of Ivanova *et al*[3] for some transitions in some ions, such as the transitions $2p_{1/2}^{-1}3s_{1/2}(1) - 2p^6\,{}^1S_0$ in Z=60 and $2p_{3/2}^{-1}3d_{3/2}(1) - 2p^6\,{}^1S_0$ in Z=92. We hope these big differences among the different calculations can be tested by experiment in the future.

Table 1. The excited energies (a.u.) of the states $2l^{-1}3l'$ with $J^P = 1^-$ relative to the ground state in ions Kr^{26+}, Nd^{50+} and U^{82+}.

Upper levels	$2p_{3/2}^{-1}3s_{1/2}$	$2p_{1/2}^{-1}3s_{1/2}$	$2p_{3/2}^{-1}3d_{3/2}$	$2p_{3/2}^{-1}3d_{5/2}$	$2p_{1/2}^{-1}3d_{3/2}$	$2s_{1/2}^{-1}3p_{1/2}$	$2s_{1/2}^{-1}3p_{3/2}$
LS sign	$(2p3s\,^3P_1)$	$(2p3s\,^1P_1)$	$(2p3d\,^3P_1)$	$(2p3d\,^3D_1)$	$(2p3d\,^1P_1)$	$(2s3p\,^3P_1)$	$(2s3p\,^1P_1)$
Kr^{26+}							
This work	60.6858	62.6474	65.4389	66.2286	68.0269	71.4827	72.0404
Ref.[2]	60.7146	62.6818	65.4554	66.2256	68.0282		
Ref.[4]	60.7186	62.6860	65.4551	66.2337	68.0330		
Exp [4]	60.7200	62.6860	65.4720	66.2450	68.0660		
Nd^{50+}							
This work	195.1855	214.6993	209.0095	211.5133	229.3980	232.3448	237.6920
Ref.[2]	195.2675	214.8141	208.9688	211.5009	229.3971	231.9030	237.2592
Ref.[4]	195.2755	214.8249	208.9978	211.4833	229.4005		
Exp [4]	195.2910	214.8610		211.500			
U^{82+}							
This work	472.5659	615.7452	528.9562	539.5601	673.4370	651.4699	692.0713
Ref.[2]	472.9120	616.2311	528.6030	539.2600	673.1913	649.1720	689.7912
Ref.[4]	473.0437	616.2809	528.8182	539.3926	673.3128		

Table 2. E1 transition probabilities (s^{-1}) from the excited states $2l^{-1}\,3l'$ with $J^P = 1^-$ to the ground state in ions Kr^{26+}, Nd^{50+} and U^{82+} ($a[b] = a \times 10^b$).

Upper levels	$2p_{3/2}^{-1}3s_{1/2}$	$2p_{1/2}^{-1}3s_{1/2}$	$2p_{3/2}^{-1}3d_{3/2}$	$2p_{3/2}^{-1}3d_{5/2}$	$2p_{1/2}^{-1}3d_{3/2}$	$2s_{1/2}^{-1}3p_{1/2}$	$2s_{1/2}^{-1}3p_{3/2}$
LS sign	$(2p3s\,^3P_1)$	$(2p3s\,^1P_1)$	$(2p3d\,^3P_1)$	$(2p3d\,^3D_1)$	$(2p3d\,^1P_1)$	$(2s3p\,^3P_1)$	$(2s3p\,^1P_1)$
Kr^{26+}							
This work	5.31[12]	3.57[12]	2.72[11]	7.06[13]	9.16[13]	4.90[12]	1.68[13]
Ref.[2]	5.34[12]	3.58[12]	2.56[11]	7.15[13]	8.98[13]	4.93[12]	1.66[13]
Ref.[8]	5.38[12]	3.91[12]	1.79[11]	6.55[13]	1.03[14]		
Nd^{50+}							
This work	5.66[13]	3.73[12]	8.35[12]	1.09[15]	7.71[14]	5.65[13]	1.82[14]
Ref.[2]	5.65[13]	3.96[12]	8.62[12]	1.09[15]	7.67[14]	5.40[13]	1.82[14]
Ref.[8]	5.5[13]	9.9[13]	2.4[12]	1.1[15]	8.0[14]	4.9[13]	1.8[14]
U^{82+}							
This work	4.70[14]	1.16[14]	4.10[14]	6.98[15]	4.56[15]	1.28[15]	9.62[14]
Ref.[2]	4.70[14]	1.20[14]	4.07[14]	6.89[15]	4.42[15]	1.27[15]	9.77[14]
Ref.[8]	4.7[14]	1.0[14]	4.0[13]	7.2[15]	4.6[15]	1.2[15]	9.5[14]

4. Energy-crossings and wavefunction mixing

Based on the MCDF calculations of the excited energies for the neon-like ions in the range of Z=21–92, the Z-dependence of the energy levels is studied systematically. It is found that there are seven pairs of levels with the same parity and J which cross each other in some particular Z regions. The details of such crossings are given in Table 3. As we can see from the table, the situations of crossings in the $J^P = 1^-$ and $J^P = 2^-$ level groups are in agreement with the previous theories[2,3,5] and experiments,[9] but the other three crossings from the level groups with $J^P = 0^+$, $J^P = 1^+$ and $J^P = 0^-$ have not been studied before, and expected to be tested in the future.

Table 3. Energy-crossings along the neon-like sequence.

J^P	Crossing levels	Z-regions	Previous work
0^+	$2p_{1/2}^{-1}\,3p_{1/2}(0)$, $2p_{3/2}^{-1}\,3p_{3/2}(0)$	$Z\sim 23$	
1^+	$2s_{1/2}^{-1}\,3s_{1/2}(1)$, $2p_{1/2}^{-1}\,3p_{3/2}(1)$	$Z\sim 73$	
0^-	$2p_{3/2}^{-1}\,3d_{3/2}(0)$, $2p_{1/2}^{-1}\,3s_{1/2}(0)$	$Z\sim 51$	
1^-	$2p_{3/2}^{-1}\,3d_{3/2}(1)$, $2p_{1/2}^{-1}\,3s_{1/2}(1)$	$Z\sim 51$	Ref.[9]
	$2p_{3/2}^{-1}\,3d_{5/2}(1)$, $2p_{1/2}^{-1}\,3s_{1/2}(1)$	$Z\sim 55$	Ref.[2,3,9]
	$2s_{1/2}^{-1}\,3p_{1/2}(1)$, $2p_{1/2}^{-1}\,3d_{3/2}(1)$	$Z\sim 70$	Ref.[2]
2^-	$2p_{3/2}^{-1}\,3d_{3/2}(2)$, $2p_{3/2}^{-1}\,3d_{5/2}(2)$	$Z\sim 37$	Ref.[2,5]

Usually, such level crossings can cause very strong configuration interactions among the crossing levels, and finally result in a serious mixing of the corresponding wavefunctions. As an example, here the three main wavefunction components of the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ level as a function of Z are shown in Fig.1. It can be seen from the figure that in the main wavefunction components, the contribution from the $2p_{3/2}^{-1}\,3d_{3/2}(1)$ arrives by 29% at $Z\sim 51$, and the contribution from the $2p_{3/2}^{-1}\,3d_{5/2}(1)$ arrives by 40% at $Z\sim 55$. As we will see below, these mixtures will also cause a series of changes of the corresponding transition probabilities.

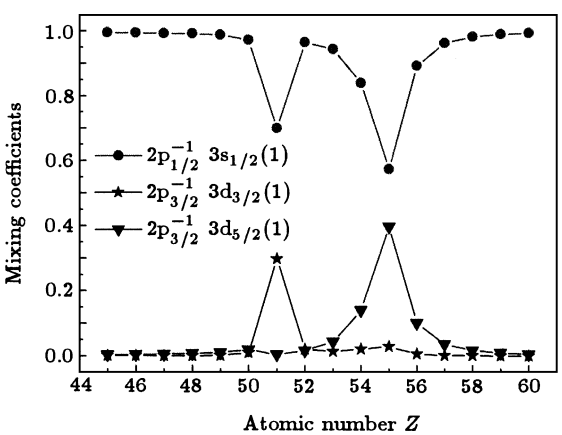


Fig.1. Main wavefunction components of the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ level as a function of Z.

5. Effects of energy crossings on transition probabilities

From the calculated E1 transition probabilities among all the 37 low-lying levels, the Z-dependence of the transition probabilities is also studied systematically along the sequence. It is found that the Z-dependence features become very irregular at some particular Z regions where exist energy crossings: some of them are enhanced, and the others are weakened; at the same time, as a direct result of strong configuration interactions caused by the energy crossings, some of so-called two-electron and one-photon (TEOP) transitions become also very strong in some neon-like ions. In order to illustrate such complicated features, three typical examples are shown below.

In Fig.2, we plot the E1 transition probabilities from the seven excited levels with $J^P=1^-$ (see Table 1 or 2) to the ground state along the neon-like sequence. From the figure, we can see that the radiative transition rates change dramatically at certain ions for some lines, where it is often associated with the energy-crossing or strong configuration mixing (see Table 3). For example, the radiative decay rate of the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ state rises rapidly to a maximum near Z=55, and then falls steeply and vanishes near Z=58. On the other hand, the radiative decay rate of the $2p_{3/2}^{-1}\,3d_{5/2}(1)$ state decreases to a minimum near Z=55, and after that it rises slowly with Z. Similar situations can also be found for the radiative decay rates of the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ and $2p_{3/2}^{-1}\,3d_{3/2}(1)$ states near Z=51, and the $2s_{1/2}^{-1}\,3p_{1/2}(1)$ and $2p_{1/2}^{-1}\,3d_{3/2}(1)$ states near Z=70. Comparing the present calculations with the results from Quinet *et al*[5] and Ivanova *et al*,[3] we find that the trends of transition rates along the neon-like sequence is in good agreement. In addition, we also notice that there are two minima for the radiative decay rates of the $2p_{3/2}^{-1}\,3d_{3/2}(1)$ and $2s_{1/2}^{-1}\,3p_{1/2}(1)$ at Z=46 and Z=67 respectively, what the origin of these is still puzzles us and needs to be studied further, because there are no energy crossings or strong configuration interactions in that special Z region.

In Fig.3, we show the trends of transition probabilities as functions of Z for the five transitions from the $2p^{-1}3s$ and $2p^{-1}3d$ to the $2p_{3/2}^{-1}\,3p_{1/2}(1)$, in which there are very strong configuration interactions among the upper levels (see Table 3 and Fig.1). We can see from the figure that the transition probabilities are extremely sensitive to the configuration mixing. As a result, once one transition is diminished due

to the decrease of the corresponding main wavefunction component, the other one is always increased accordingly. For example, the two strongest peaks of the $2p_{1/2}^{-1}\,3s_{1/2}(1) - 2p_{3/2}^{-1}\,3p_{1/2}(1)$ transitions at Z=51 and 55 are caused due to the weakening of the $2p_{3/2}^{-1}\,3d_{3/2}(1) - 2p_{3/2}^{-1}\,3p_{1/2}(1)$ transition at Z=51 and $2p_{3/2}^{-1}\,3d_{5/2}(1) - 2p_{3/2}^{-1}\,3p_{1/2}(1)$ transition at Z=55, respectively.

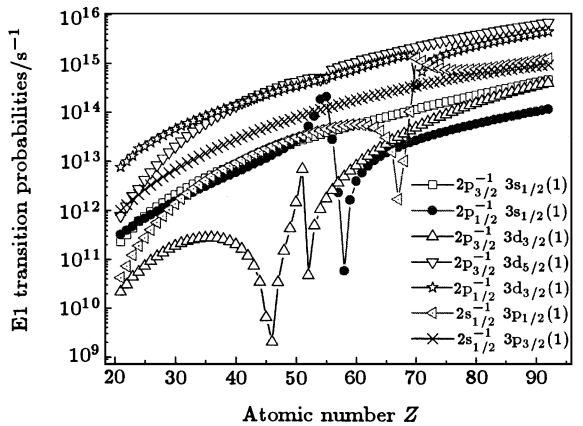


Fig.2. E1 transition probabilities (s^{-1}) from the upper levels with $J^P = 1^-$ to the ground state as functions of Z.

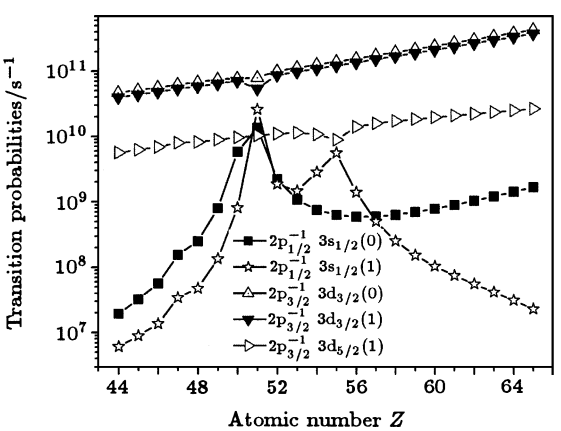


Fig.3. E1 transition probabilities (s^{-1}) from the upper levels with energy-crossings to the $2p_{3/2}^{-1}\,3p_{1/2}(1)$ as functions of Z.

In Fig.4, the E1 transition probabilities from the two upper levels $2s_{1/2}^{-1}\,3d_{3/2}(1)$ and $2s_{1/2}^{-1}\,3d_{3/2}(2)$ to the lower level $2p_{1/2}^{-1}\,3s_{1/2}(1)$ are shown further as functions of Z. We can see that there are two peaks around Z=51 and 55. As we know, these transitions are usually unallowed because of a change of two electrons. But due to the strong configuration interactions between the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ and $2p_{3/2}^{-1}\,3d_{3/2}(1)$ at Z=51 and between the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ and $2p_{3/2}^{-1}\,3d_{5/2}(1)$ at Z=55, the transition to the lower level $2p_{1/2}^{-1}\,3s_{1/2}(1)$ includes some important components of the $2p^{-1}\,3d(1)$ states in these ions. As a result, these transitions become not only possible, but also very strong, even can be comparable to some strong E1 transitions. This is so called two-electron and one-photon (TEOP) transition.[15,16] We hope these transitions from the neon-like ions will contribute to the understanding of the TEOP transition, and can be tested in the future.

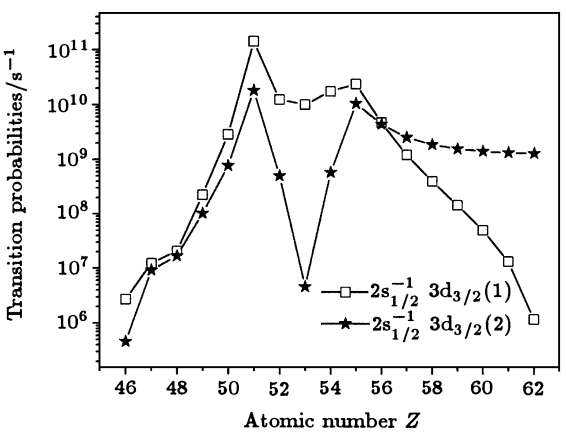


Fig.4. E1 transition probabilities (s^{-1}) from the excited states $2s^{-1}3d$ to the $2p_{1/2}^{-1}\,3s_{1/2}(1)$ as functions of Z.

6. Conclusion

In summary, the 37 low-lying energy levels and the related transition probabilities in the neon-like ions from Z=21 to 92 have been calculated by using the MCDF method. By comparison with some available experimental and theoretical results, it is found that a good agreement between them can be obtained usually for ions with low- , middle- and high-Z along the sequence.

Based on the systematic calculations, all possible energy-crossings among the same J^P level groups have also been presented along the whole isoelectronic sequence. It is found that there are several level-crossings for some particular energy levels in different Z regions, those crossings have resulted in great changes of the transition probabilities even for some strong lines. Some of them are diminished and the others are enhanced accordingly. Especially, several strong TEOP transitions have been found in some of the neon-like ions, which should be observed in experiment.

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