Energy levels in the resonant photoionization of heliumlike Ne^{8+}

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The diagonalization approximation is applied to the photoionization process of Ne^{8+} to determine the energies of autoionizing states converging to the $n=3,4,5$ thresholds of the residual ion. The calculations are carried out for $^{1,3}P^o$ states. The results are compared with available results obtained by other theoretical approaches.

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INTRODUCTION

In the last two decades, interest in experimental and theoretical studies of resonant photoionization of heliumlike ions and properties of autoionizing states has been renewed [1–14] by the advent of high-energy resolution spectrometers using synchrotron radiation and the appearance of multiply charged ions sources like electron cyclotron resonance (ECR) or electron-beam ion source (EBIS) and by the various methods using different approaches of this problem. Now, investigations on autoionizing states receive a great deal of attention with the availability of new short-pulse lasers [15,16].

Like other heliumlike multiply charged ions, the experimental study of doubly excited states of Ne^{8+} ions is related to experimental investigations on capture processes after collision between Ne^{10+} and He or H_2 targets (Bordenave-Montesqiueu *et al.* [17], Frémont *et al.* [18], Martin *et al.* [19]). Bordenave-Montesqiueu *et al.* [17] observed the excitation of $Ne^{8+}(3lnl')$ ^1L Rydberg series by high resolution electron spectroscopy after double capture process at low collision velocity. They show that in the n range where the double capture process populates the symmetrical $4l4l'$ states ($n>9$), an enhancement of the intensities of the $3lnl'$ Rydberg lines is observed. So the transfer of population from the $4l4'$ to the $3lnl'$ states is found to be favored against a direct autoionization into the $n=2$ continuum. In a more recent experimental study of single and double electron capture in low-energy Ne^{10+}-He collisions, the total and differential cross sections for single-electron capture onto the levels $n=3$, 4, 5, and 6 of Ne^{9+} (nl) and double-electron capture onto a series of doubly excited states $(3,n)$ and $(4,n)$ with $n=4$, 5, and 6 of Ne^{8+} have been obtained by Fléchard *et al.* [20]. From the theoretical side, Sanchez and Bachau [21] have reported the positions and widths for $^1D^e(4,4)$ and $(3, n=5-12)$ states of Ne^{8+} ions, on the basis of the Feshbach approach and L^2 discretization method. Doubly excited $^{1,3}F^o$ resonances in Ne^{8+} below the $n=3$ and 4 thresholds of the hydrogenic ion have been calculated by Bhatia and Ho [22] using the complex rotation method.

For $^{1,3}P^o$ resonant states of Ne^{8+} which are in our interest, any of the experimental results have been done with our knowledge and only a few theoretical results have been reported. Those are the calculations of Ho [23] using the complex rotation method, Bachau [24,25] using the truncated diagonalization method (TDM), Van der Hart [26] using the TDM with B-splines basis, and Merabet *et al.* [27] using the Hartree-Fock code by Cowan [28]. Whereas much theoretical work has been reported concerning doubly-excited states in highly-charged ions below the $n=2$ and $n=3$ thresholds, the $4lnl'$ states have been studied to a much lesser extent and the first more complete study was reported by Van der Hart *et al.* [26].

For resonant states lying under the $n=4$, Ho [23] and Bachau [25] reported only the energies of the lowest $4l4l'$ states. While, Van der Hart [26] extended the calculations to the energies of the 10 lowest $4lnl'$ states.

In the present work, we apply the diagonalization approximation to calculate the energies of the $^{1,3}P^o$ resonant states in Ne^{8+} below the $n=3$, $n=4$, and $n=5$ thresholds of the residual ion. This approximation has already been used with success for the description of autoionizing resonances in helium and heliumlike ([26,27]) and in our previous papers [11–14]. Extensive calculations have been done here, and we report a complete set of data for singlet and triplet states of the resonant $3lnl'$, $4lnl'$, and $5lnl'$ states.

CALCULATIONS

Basics formulas of the diagonalization approximation

In the diagonalization approximation, the final state of the ion plus photoelectron system is expanded in the subspaces of closed and open channels as follows:

$$\Psi_{Ej}(\boldsymbol{r}_1,\boldsymbol{r}_2)=\hat{A}\sum\Psi_k(\boldsymbol{r}_1)U_{kj}(E,\boldsymbol{r}_2)+\sum\Lambda_\mu(E)\Phi_\mu(\boldsymbol{r}_1,\boldsymbol{r}_2), \tag{1}$$

where $\hat{A}$ is the operator of antisymmetrization, k represents a set of quantum numbers that characterize the ion plus photoelectron system in the subspace of open channels; $U_{kj}(E,\boldsymbol{r}_2)$ is an unknown function describing the motion of the photoelectron, $\Psi_k(\boldsymbol{r}_1)$ is the eigenfunction of the residual ion.

The determination of the function Ψ_{Ej} $(\boldsymbol{r}_1,\boldsymbol{r}_2)$ is equivalent to the calculation of the coefficients $\Lambda_\mu(E)$ and $U_{kj}(E,\boldsymbol{r}_2)$. Detailed calculations of these coefficients have been reported by [11,29,30]. The functions $\Phi_\mu(\boldsymbol{r}_1,\boldsymbol{r}_2)$ are obtained by unitary transformation of the Hamiltonian in the

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TABLE I. Energies $[-E(\mathrm{eV})]$ of the $^1P^o$ resonances of the Ne^{8+} ion associated with the $n=3$ hydrogenic threshold.

States	Present	Bachau [24,25]	Merabet [27]	Ho [23]
$3s\ 3p$	285.63	285.65		285.70
$3p\ 3d$	273.33	273.43		273.98
$3s\ 4p$	227.35	226.24	228.20	
$4s\ 3p$	223.93	224.12	224.77	
$4p\ 3d$	223.64	224	224.53	
$3d\ 4f$	216.77	217.56	217.85	
$3p\ 4d$	216.23	216.55	216.68	
$3s\ 5p$	198.76			
$5p\ 3d$	196.57			
$5s\ 3p$	196.39			
$3d\ 5f$	191.94			
$3p\ 5d$	191.14			

subspace of closed channels which are the autoionizing states,

$$\Phi_\mu(\boldsymbol{r}_1,\boldsymbol{r}_2) = \hat{A}\sum_{kl} \alpha_\mu(k,l)\Phi_k(\boldsymbol{r}_1)\Phi_l(\boldsymbol{r}_2), \tag{2}$$

with the diagonalization condition

$$\langle \Phi_\mu(\boldsymbol{r}_1,\boldsymbol{r}_2)|\boldsymbol{H}|\Phi_\nu(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle = E_\mu \delta_{\mu\nu}. \tag{3}$$

$\boldsymbol{H}$ is the Hamiltonian operator; the coefficients $\alpha_\mu(k,l)$ which are the statistical weight of the autoionizing states are found by solving the system of linear algebraic equations,

$$\sum_\nu [(E_\mu - E_0)\delta_{\mu\nu} - \langle \chi_\mu|\boldsymbol{V}|\chi_\nu\rangle]\alpha_\nu = 0, \tag{4}$$

where E_μ is the energy of the autoionizing level μ; $\boldsymbol{V}$ is the operator of electrostatic interaction between electrons; E_0 is the energy eigenvalue of the zero-order Hamiltonian corresponding to the eigenfunctions defined by

TABLE II. Energies $[-E(\mathrm{a.u.})]$ of the $^3P^o$ resonances of the Ne^{8+} ion associated with the $n=3$ hydrogenic thresholds. The states are ordered according to increasing energy in *LS* symmetry.

States	Present	Ho [23]
$^3P^o(1)$	288.6927	288.6981
$^3P^o(2)$	281.2588	281.4017
$^3P^o(3)$	226.6868	
$^3P^o(4)$	225.9300	
$^3P^o(5)$	221.7424	
$^3P^o(6)$	221.3397	
$^3P^o(7)$	217.9575	
$^3P^o(8)$	198.0861	
$^3P^o(9)$	197.8902	
$^3P^o(10)$	195.0603	
$^3P^o(11)$	194.9270	
$^3P^o(12)$	193.1883	

TABLE III. Energies $[-E(\mathrm{a.u.})]$ of the $^1P^o$ resonances of the Ne^{8+} ion associated with the $n=4$ hydrogenic thresholds.

Levels	Present work	Ho [23]	Van der Hart [26]
$4s4p$	5.9458	5.944	5.94335
$4d4f$	5.8165	5.818	5.81411
$4p4d$	5.5561	5.576	5.57497
$4s5p$	4.9355		4.93588
$4p5d$	4.8842		4.88515
$5p4d$	4.8729		4.87875
$5d4f$	4.8019		4.80500
$5s4p$	4.7729		4.78504
$4f5g$	4.6307		4.65718
$4d5f$	4.6246		4.64246
$4s6p$	4.3595		
$6s4p$	4.3249		
$6p4d$	4.3225		
$6d4f$	4.2703		
$4d6f$	4.2606		
$4f6g$	4.1872		
$4p6d$	4.1781		
$4s7p$	4.0162		
$7s4p$	3.9883		
$7p4d$	3.9851		
$7d4f$	3.9398		
$4d7f$	3.9227		
$4p7d$	3.8602		
$4f7g$	3.8167		

$$\chi_\nu = \hat{A}[\Phi_k(\boldsymbol{r}_1)\Phi_l(\boldsymbol{r}_2)]. \tag{5}$$

The partial amplitude that describes the formation of the residual ion and photoelectron in a definite state has been defined by the following expression:

$$T_j(E) = \langle \varphi_j(E)|\boldsymbol{D}|\Psi_i\rangle + \frac{q+i}{\varepsilon - i}\langle \Phi_\mu|\boldsymbol{V}|\varphi_j(E)\rangle \times \frac{\sum_k \langle \Phi_\mu|\boldsymbol{V}|\varphi_k(E)\rangle\langle \varphi_k(E)|\boldsymbol{D}|\Psi_i\rangle}{\sum_k |\langle \Phi_\mu|\boldsymbol{V}|\varphi_k(E)\rangle|^2}. \tag{6}$$

In (6), $\varphi_j(E)$ is the wave function of the continuous spectrum in the channel j, without resonance interference; $\boldsymbol{D}$ is the dipole momentum operator; q is the profile index of the resonance; and ε is the relative deviation from the resonance and are defined by the following equations:

$$\varepsilon = (E - E_\mu)/(1/2)\Gamma_\mu^{\mathrm{tot}}, \tag{7}$$

$$q = \frac{\langle \Phi_\mu|\boldsymbol{D}|\Psi_i\rangle}{\pi\sum_k |\langle \Phi_\mu|V|\varphi_k(E)\rangle|^2\langle \varphi_k(E)|\boldsymbol{D}|\Psi_i\rangle} \tag{8}$$

with $\Gamma_\mu^{\mathrm{tot}}$ the total width,

TABLE IV. Energies $[-E(\mathrm{eV})]$ of the $^1P^o$ resonances of the Ne^{8+} ion associated with the configurations $4l4l'$. The states are ordered according to increasing energy in *LS* symmetry.

States	Present work	Bachau [24]
$^1P^o(1)$	161.78	161.79
$^1P^o(2)$	158.26	158.28
$^1P^o(3)$	151.20	151.37

$$\Gamma_\mu^{\mathrm{tot}} = 2\pi \sum_j |\langle \Phi_\mu | V | \varphi_j(E) \rangle|^2. \quad (9)$$

RESULTS AND DISCUSSION

We have applied the diagonalization approximation described above to the calculation of energies for the autoionizing states corresponding to the configurations $3lnl'$ (with $l \leq 2$, $l' \leq 3$, and $3 \leq n \leq 5$), $4lnl'$ (with $l \leq 3$, $l' \leq 4$, and $4 \leq n \leq 7$) for Ne^{8+}, and $5lnl'$ (with $l \leq 5$, $l' \leq 6$, and $5 \leq n \leq 8$). The excitation energies and associated wave functions are obtained by diagonalization of the matrix of electrostatic interaction in 12×12, 24×24 or basis 31×31 basis. Configurations are described by antisymmetrized productsof Coulomb wave functions. The wave functions are given with the eigenvector compositions. The weight of the *sp*, *pd*, *df*, and *fg* components allowed us to classify the states according to the main eigenvector components.

Excitation energies for $3lnl'$ $(^1P^o)$ resonant states of Ne^{8+} are reported in Tables I and II In Table I, present energies of $3lnl'$ $(^1P^o)$ are given along with those of Ho [23], Bachau [24,25], and Merabet *et al.* [27]. For triplet $3lnl'$ $(^3P^o)$, energies are reported in Table II with the values of Ho [23], the only available one. Comparison between present results and the theoretical ones in Table I show a good agreement. In Table I, the low discrepancies between the present results and those of Merabet *et al.* [27] may be due to the configuration interactions of $3l4l'$ with $3lnl'$ $(n \geq 5)$ and $4l4l'$. So the mixing of these configurations should be included in the calculations, which is not the case in Merabet *et al.* [27] results because such calculations exceed the abilities of the Cowan code they used.

TABLE V. Energies $[-E(\mathrm{eV})]$ of the $^1P^o$ resonances of the Ne^{8+} ion associated with the configurations $4l5l'$. The states are ordered according to increasing energy in *LS* symmetry.

States	Present work	Van der Hart [26]	Merabet [27]
$^1P^o(1)$	134.2949	134.31	134.94
$^1P^o(2)$	132.8990	132.93	133.53
$^1P^o(3)$	132.5916	132.76	133.20
$^1P^o(4)$	130.6597	130.75	131.28
$^1P^o(5)$	129.8706	130.21	130.34
$^1P^o(6)$	126.0013	127.54	127.10
$^1P^o(7)$	125.8353	126.33	125.40

TABLE VI. Energies $[-E(\mathrm{a.u.})]$ of the $^3P^o$ resonances of the Ne^{8+} ion associated with the $n=4$ hydrogenic thresholds.

States	Present work
$4s\ 4p$	5.9866
$4p\ 4d$	5.8909
$4d\ 4f$	5.7348
$5s\ 4p$	4.9153
$4s\ 5p$	4.9073
$5d\ 4f$	4.8531
$4d\ 5f$	4.8328
$4f\ 5g$	4.7502
$5p\ 4d$	4.7355
$4p\ 5d$	4.6660
$4s\ 6p$	4.3478
$6s\ 4p$	4.3446
$4d\ 6f$	4.3012
$6d\ 4f$	4.2996
$4f\ 6g$	4.2436
$6p\ 4d$	4.2382
$4p\ 6d$	4.2051
$4s\ 7p$	4.0081
$7s\ 4p$	4.0038
$7d\ 4f$	3.9663
$7p\ 4d$	3.9657
$4f\ 7g$	3.9119
$4d\ 7f$	3.9086
$4p\ 7d$	3.8840

In Table III are reported the energies for $4lnl'$ $(^1P^o)$ resonant states along with the theoretical calculations of Ho [23] using the complex rotation method and those of Van der Hart [26] using the TDM with *B*-splines basis. In this table, only the energies of the $4ln'l'$ $(n'=4,5)$ for the three or 10 first states have been given by the others theoretical works. Here we have extended the calculations to $4ln'l'$ $(n'=4-7)$ states and reported the energies for the 24 lowest autoionizing states. Quite good agreement has been found between our results and those of these authors. The small differences between the present results and those of Van der Hart [26] may be due also to the noninclusion of the interaction with $3lnl'$ series in their calculations. This can be seen by the fact that the difference is more pronounced for the highest states of $4l4l'$ lying close to the $n=3$ threshold than for the lowest

TABLE VII. Energies $[-E(\mathrm{Ry})]$ of the three lowest $^3P^o$ resonances of the Ne^{8+} ion associated with the $n=4$ hydrogenic thresholds.

States	Present work	Ho [23]
$4s\ 4p$	11.9732	11.971
$4p\ 4d$	11.7818	11.7785
$4d\ 4f$	11.4696	11.4790

TABLE VIII. Energies $[-E(\mathrm{a.u.})]$ of the $^1P^o$ resonances of the Ne^{8+} ion associated with the $n=5$ hydrogenic thresholds.

States	Present work
$5s\ 5p$	3.81861900
$5d\ 5f$	3.76356400
$5f\ 5g$	3.67828900
$5p\ 5d$	3.51035500
$5s\ 6p$	3.26481600
$5d\ 6f$	3.23899200
$6p\ 5d$	3.23030100
$6f\ 5g$	3.20169400
$6s\ 5p$	3.18139800
$6d\ 5f$	3.14389200
$5f\ 6g$	3.11435300
$5g\ 6h$	3.02600200
$5p\ 6d$	3.02522700
$5s\ 7p$	2.95064800
$7s\ 5p$	2.91462600
$5d\ 7f$	2.89417700
$7p\ 5d$	2.88582900
$7d\ 5f$	2.86637400
$5s\ 8p$	2.84979100
$7f\ 5g$	2.82877900
$5g\ 7h$	2.81457700
$5p\ 7d$	2.77038000
$5f\ 7g$	2.75688100
$5p\ 8d$	2.69242100
$8s\ 5p$	2.68933500
$8p\ 5d$	2.67161900
$5d\ 8f$	2.64617300
$8f\ 5g$	2.62402000
$8d\ 5f$	2.61041500
$5g\ 8h$	2.55715400
$5f\ 8g$	2.53763700

TABLE IX. Energies $[-E(\mathrm{a.u.})]$ of the $^3P^o$ resonances of the Ne^{8+} ion associated with the $n=5$ hydrogenic thresholds.

States	Present work
$5s\ 5p$	3.8379
$5p\ 5d$	3.7938
$5d\ 5f$	3.7303
$5f\ 5g$	3.6297
$5s\ 6p$	3.2541
$5d\ 6f$	3.2481
$6s\ 5p$	3.2239
$6d\ 5f$	3.2088
$6f\ 5g$	3.1791
$6p\ 5d$	3.1580
$5g\ 6h$	3.1081
$5f\ 6g$	3.0953
$5p\ 6d$	3.0507
$5s\ 7p$	2.9223
$5d\ 7f$	2.9060
$7s\ 5p$	2.8841
$7d\ 5f$	2.8825
$7f\ 5g$	2.8502
$7p\ 5d$	2.8470
$5g\ 7h$	2.8099
$5f\ 7g$	2.8052
$5s\ 8p$	2.8025
$5p\ 7d$	2.7822
$5p\ 8d$	2.6934
$8p\ 5d$	2.6820
$5f\ 8g$	2.6611
$8d\ 5f$	2.6397
$8f\ 5g$	2.6304
$8s\ 5p$	2.5950
$5g\ 8h$	2.5894
$5d\ 8f$	2.5688

$4l4l'$ states. In Tables IV and V are shown the $4ln'l'$ $(^1P^o)$ energies. For the lowest states of $4l4l'$, the present results reported in Table IV, are in very good agreement with the Bachau [24]. In Tables VI and VII, are reported energies for $^3P^o$ resonances of the Ne^{8+} ion associated with $n=4$ hydrogenic thresholds. In Table VII, we compare our results with the only available theoretical results of Ho [23] who report only the three lowest members of the series for which both electrons occupy the same shell. Tables VIII and IX show the present results for the 31 lowest singlet and triplet states lying under the $n=5$ hydrogenic threshold.

CONCLUSION

In this work, the diagonalization approximation applied to the photoionization process of Ne^{8+}, has been used to do extensive calculations of the energies of singlet and triplet autoionizing states converging to the $n=3$, 4, 5 thresholds of the residual ion. Quite good agreement was found between present results and those previously obtained with the use of the complex rotation method by Ho [23], truncated diagonalization method (TDM) by Bachau [25], and TDM with *B*-splines basis by Van der Hart [26]. The present results are as expected more close to those calculations using the configuration interaction method with hydrogenic functions as basis orbitals. We present the energies for $5lnl'$ $(^1P^o, ^3P^o)$.

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[1] A. Bordenave-Montesquieu, P. Benoit Cattin, A. Gleizes, A. I. Marrakchi, S. Dousson, and D. Hitz, J. Phys. B **17**, L127 (1984).
[2] P. Benoit-Cattin, A. Bordenave-Montesquieu, M. Boudjema, A. Gleizes, A. I. Marrakchi, S. Dousson, and D. Hitz, J. Phys. B **21**, 3387 (1988).
[3] P. Moretto-Capelle, P. Benoit Cattin, A. Bordenave-Montesquieu, and A. Gleizes, Z. Phys. D: At., Mol. Clusters **21**, S283 (1991).
[4] M. Domke, G. Remmers, and G. Kaindl, Phys. Rev. Lett. **69**, 1171 (1992).
[5] M. Domke, K. Schulz, G. Remmers, G. Kaindl, and D. Wintgen, Phys. Rev. A **53**, 1424 (1996).
[6] Y. K. Ho, Phys. Rev. A **23**, 2137 (1981).
[7] Y. K. Ho, Phys. Rev. A **35**, 2035 (1987).
[8] Y. K. Ho, Phys. Rev. A **45**, 148 (1992).
[9] D. H. Oza, Phys. Rev. A **33**, 824 (1986).
[10] W. H. Hugo and E. H. Jorgen, J. Phys. B **25**, 2267 (1992).
[11] A. Wagué, Z. Phys. D: At., Mol. Clusters **6**, 337 (1987).
[12] N. A. B. Faye and A. Wagué, Z. Phys. D: At., Mol. Clusters **31**, 37 (1994).
[13] N. A. B. Faye and A. Wagué, J. Phys. B **28**, 1735 (1995).
[14] A. S. Ndao, A. Wagué, N. A. B. Faye, and A. Konté, Eur. Phys. J. D **5**, 327 (1999).
[15] H. N. Ereifej and J. G. Story, Phys. Rev. A **60**, 3947 (1999).
[16] H. N. Ereifej and J. G. Story, Phys. Rev. A **62**, 033405 (2000).
[17] A. Bordenave-Montesqiueu, P. Moretto-Capelle, A. Gonzalez, M. Benhenni, H. Bachau, and I. Sanchez, J. Phys. B **27**, 4243 (1994).
[18] F. Frémont, H. Mérabet, J. Y. Chesnel, X. Husson, A. Lepoutre, D. Lecler, G. Rieger, and N. Stolterfoht, Phys. Rev. A **50**, 3117 (1994).
[19] S. Martin, J. Bernard, A. Denis, J. Desesquelles, L. Chen, and Y. Ouerdane, Phys. Rev. A **50**, 2322 (1994).
[20] X. Fléchard, C. Harel, H. Jouin, B. Pons, L. Adoui, F. Frémont, A. Cassimi, and D. Hennecart, J. Phys. B **34**, 2759 (2001).
[21] I. Sanchez and H. Bachau, J. Phys. B **28**, 795 (1995).
[22] A. K. Bhathia and Y. K. Ho, J. Phys. B **31**, 3307 (1998).
[23] Y. K. Ho, J. Phys. B **12**, 387 (1979).
[24] H. Bachau, J. Phys. B **17**, 1771 (1984).
[25] H. Bachau, F. Martin, A. Riera, and M. Yanez, At. Data Nucl. Data Tables **48**, 167 (1991).
[26] H. Wan der Hart, N. Vaeck, and J. E. Hansen, J. Phys. B **28**, 5207 (1995).
[27] H. Merabet, G. Cremer, F. Frémont, J.-Y. Chesnel, and N. Stolterfoht, Phys. Rev. A **54**, 372 (1996).
[28] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
[29] V. V. Balashov, S. I. Grihanova, I. M. Kruglova, and V. S. Senashenko, Opt. Spectrosc. **T28**, 858 (1970).
[30] V. S. Senashenko and A. Wagué, J. Phys. B **12**, L269 (1979).