



Energy Levels and Lifetimes of $1s^2$ and $1snl$ ($n=2-5$) for Neutral Helium

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Abstract

In this paper, we present calculations for some of the lowest energy levels and lifetimes for neutral helium. The FAC (Flexible-Atomic-Code) is a reliable code for calculating 49 energy levels and their lifetimes. The calculation is performed up to $n=5$ including a series of configuration of $1s^2$ and $1snl$. Comparison has been made with similar data published in the NIST database. A good agreement of less than 1% was found for most levels except the $1s2p\ ^3P_2$ level. This proves the reliability of our results. New values for lifetimes are presented for the first time.



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Introduction

Atomic data are very much needed for the modeling of plasmas¹. They are useful for many applications in astrophysics and nuclear fusion Tokamak. Moreover, the ITER project needs accurate atomic data for a wide area of ions. The simplest multi-electron system, He-like can play an important role in providing the needed accurate atomic data. In previous work, we provided calculations of He-like neon².

We just focus on this study in neutral Helium. For this Nobel gas, the atom contains two protons and two electrons. The energy structure of the $1snl$ configuration is mainly dominated by the electron-

nucleus and electron-electron Coulomb interactions. The separations of levels having belonging to the same n multiplicity and having $l = s, p, \text{ or } d$ are mainly determined by Spin-orbit interactions between the electrons. The final state is given by the ^{2S+1}L notation where n, l, S, L are the standard quantum numbers. The quantity $2S + 1$ is the multiplicity of the term. The S and L momentums are coupled to obtain, $J = S + L$, for a given level. The level is denoted as $^{2S+1}L_J$. J being the total angular momentum.

Many experimental and theoretical studies were performed for this element. Energy levels have been published by the National Institute of Standards

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and Technology (NIST) and are available at their website³. Sow *et al.*⁴ performed calculations for the $2s^2\ ^1S$, $2p^2\ ^1D$, $3s^2\ ^1S$, $3p^2\ ^1D$, $3d^2\ ^1G$, $4p^2\ ^1D$, $4d^2\ ^1D$, $4f^2\ ^1I$ doubly excited states of $2 \leq Z \leq 15$. The energy eigen-values of doubly excited $2pnp\ (^1P_o)$ ($n=3-8$) and $2pnp\ (^3P_o)$ ($n=2-7$) bound states of a neutral helium atom were calculated under the weakly coupled plasma screening by K. Saha *et al.*⁵. Doubly excited states in helium are calculated by E. Lindroth⁶ with a finite discrete spectrum for states with electrons in the $n=2$ and $n=3$ states. An approach to calculating the energies and widths of resonances for neutral Helium was developed on the basis of the stabilization method, the energies of 28 resonances of nS symmetry with the spin multiplicities $n=1, 2, 3$, and 4 were calculated by I. A. Misurkin *et al.*⁷

Therefore, in this paper, we just interest on calculations of the singly excited energy levels for neutral Helium, namely He I. We employed the fully relativistic code Flexible Atomic Code (FAC) of Gu⁸. FAC code provides many different atomic parameters such as energy levels, transitions rates and lifetimes. In the rest of paper, we shall give, for He I, energy levels and lifetimes of the lowest 49 levels belonging to $1s^2$ and $1snl$ (with $n \leq 5$; $0 \leq l \leq n-1$).

Theoretical Method

We employed for our calculations the widely used FAC code of Gu⁸. We simply give here a short description of the theoretical method used by FAC.

By diagonalizing the relativistic Hamiltonian H , we get the energy levels of an N electrons atom⁹

$$H = \sum_{i=1}^N H_D(i) + \sum_{i<j}^N \frac{1}{r_{ij}} \quad \dots(1)$$

where $H_D(i)$ is the single-electron Dirac Hamiltonian. The basis states ϕ_{nkm} , which are usually referred to as configuration state functions (CSF), are antisymmetric sums of products of N one-electron Dirac spinors φ_{nkm}

$$\varphi_{nkm} = \frac{1}{r} \left\{ \begin{array}{l} P_{nk}(r) \chi_{km}(\theta, \phi, \sigma) \\ iQ_{nk}(r) \chi_{-km}(\theta, \phi, \sigma) \end{array} \right\} \quad \dots(2)$$

where χ_{km} is the usual spin-angular function. n is the principal quantum number, k is the relativistic angular quantum number and m is the z -component of the total angular momentum j .

The approximate atomic state functions are obtained by mixing the basis states using the same symmetries

$$\Psi = \sum_v b_v \phi_v \quad \dots(3)$$

where b_v are the mixing coefficients obtained from diagonalizing the total Hamiltonian.

Choice of Local Central Potential

To build the Hamiltonian matrix, the one-electron radial orbital must be known. According to the standard Dirac-Fock-Slater method, the large and small components, P_{nk} and Q_{nk} , satisfy the coupled Dirac equation for a local central field $V(r)$

$$\left(\frac{d}{dr} + \frac{\kappa}{r} \right) P_{nk} = \alpha \left(\epsilon_{nk} - V + \frac{2}{\alpha^2} \right) Q_{nk} \quad \dots(4)$$

$$\left(\frac{d}{dr} - \frac{\kappa}{r} \right) Q_{nk} = \alpha (-\epsilon_{nk} + V) P_{nk}$$

where α is the fine structure constant and ϵ_{nk} are the energy eigenvalues of the radial orbitals.

Solution of Dirac Equations

The radial orbitals sought have a direct influence on the potential, so the Eq. (4) requires a self-consistent iteration. In each iteration, the orbitals from the previous step are used to derive the potential. Consequently, solving the eigenvalue problem using known potential is sufficient. As is standard, we convert Eq. (4) into a Schrodinger-like equation in two steps: eliminating the small component and performing the transformation¹⁰

$$P_a = \xi_a(r) F_a(r)$$

$$\xi_a(r) = \sqrt{1 + \frac{\alpha^2}{2} [\epsilon_a - V(r)]} \quad \dots(5)$$

$$Q_a = \frac{\alpha}{2\varepsilon_a^2} \left(\frac{d}{dr} P_a + \frac{\kappa}{r} P_a \right)$$

Under this transformation, we have

$$\frac{d^2}{dr^2} F_a(r) + \left\{ 2[\varepsilon_a - U(r)] - \frac{\kappa(\kappa+1)}{r^2} \right\} F_a(r) = 0 \quad \dots(6)$$

where $U(r)$ is an effective potential defined as

$$U(r) = V(r) - \frac{\alpha^2}{2} \{ [V(r) - \varepsilon_a]^2 - W(r) \} \quad \dots(7)$$

$$W(r) = \frac{1}{4\varepsilon_a^2(r)} \left[\frac{d^2}{dr^2} V(r) + \frac{3\alpha^2}{4\varepsilon_a^2(r)} \left(\frac{d}{dr} V(r) \right)^2 - \frac{2\kappa}{r} \frac{d}{dr} V(r) \right]$$

We use the standard Numerov method to solve Eq. (6). However, it is customary to perform another transformation before seeking the solution

$$t = t(r) \quad \dots(8)$$

$$F_a(r) = \left(\frac{dt}{dr} \right)^{-1/2} G_a(t)$$

where $t(r)$ as a function of radial distance is suitably chosen so that a uniform grid can be used in the new variable t , and the corresponding transformation on the wave function is to bring the differential equation for $G_a(t)$ to a Schrodinger-like form, i.e., without the first derivative term

$$\frac{d^2}{dt^2} G_a(t) = \left(\frac{dt}{dr} \right)^{-2} G_a(t) \left\{ \frac{\kappa(\kappa+1)}{r^2} - 2[\varepsilon_a - U(r)] + \frac{1}{2} \left(\frac{dt}{dr} \right)^{-1} \frac{d^2 t}{dr^2} - \frac{3}{4} \left(\frac{dt}{dr} \right)^{-2} \left(\frac{d^2 t}{dr^2} \right)^2 \right\} \quad \dots(9)$$

However, for free orbitals with sufficiently high energy, solving Eq. (9) in a conventional way becomes impractical. We shall use a different approach for continuum states, namely, the phase amplitude method.

The minimum and maximum radial distances, r_{min} and r_{max} , in setting up the radial grid are chosen as

$$r_{min} = 10^{-6} / Z_{eff} \quad \dots(10)$$

$$r_{max} = 500 / Z_{eff}$$

where Z_{eff} is the residual charge of the atomic ion that the electrons experience at large r . The low- n and high- n states are treated differently. The dividing n_0 is determined by the choice of r_{max} , specifically, $n_0 = 0.5 * \sqrt{Z_{eff} r_{max}}$. For $n \leq n_0$, the orbitals were found by outward and inward integration of Eq. (9) with zero amplitudes at both ends, and matching at the outer classical turning point. Node counting is used to pick out the appropriate solution corresponding to the quantum numbers n and l . The wave functions are then normalized by numerical integration. For $n > n_0$, Eq. (9) is integrated outward until $r = r_{core}$, where the potential has reached its asymptotic Coulomb value. For $r > r_{core}$, the wave function is the exponentially decaying Whittaker function

$$y_5(v, \lambda, \rho) = W_{v, \lambda+1/2}(2\rho/v) \quad \dots(11)$$

where $v^2 = -\frac{1}{2} Z_{eff}^2 / \varepsilon$, $\rho = Z_{eff} r$, and $\lambda = l$ in the non-relativistic limit⁸. In the relativistic case, the asymptotic behavior of the effective potential is modified according to Eq. (7), and corresponds to

$$Z'_{eff} = Z_{eff} (1 + \alpha^2 \varepsilon)$$

$$v^2 = -\frac{Z_{eff}^2}{2\varepsilon(1 + \frac{1}{2} \alpha^2 \varepsilon)} \quad \dots(12)$$

$$\lambda(\lambda+1) = l(l+1) - (Z_{eff} \alpha)^2$$

To normalize the wave function, we note that the correct normalization is given by¹¹

$$F(r > r_{core}) = K(v_n, \lambda) y_5(v_n, \lambda, \rho) \quad \dots(13)$$

where

$$K(v, \lambda) = Z_{eff}^{1/2} \left[\xi(v_n) v_n^2 \Gamma(v_n + \lambda + 1) \Gamma(v_n - \lambda) \right]^{1/2} \quad \dots(14)$$

and

$$\xi(v_n) = 1 + \frac{d\mu}{dv} \quad \dots(15)$$

Table 1. Energy levels [eV] calculated with FAC code and compared to data taken from NIST database. The last column represents the established lifetimes [s⁻¹] for 49 upper levels of neutral Helium.

i	Level	FAC (eV)	NIST (eV)	Difference (%)	Lifetimes (s ⁻¹)
1	1s ² ¹ S ₀	0	0	0.44	-
2	1s2s ³ S ₁	19.90796	19.81961	0.49	-
3	1s2s ¹ S ₀	20.71812	20.61577	0.39	-
4	1s2p ³ P ₂	21.04742	20.96408	1.12	9.69E-08
5	1s2p ¹ P ₁	20.97935	21.21802	0.39	5.48E-10
6	1s2p ³ P ₀	21.04786	20.96421	0.39	9.70E-08
7	1s2p ³ P ₁	21.04765	20.96409	0.49	9.70E-08
8	1s3s ³ S ₁	22.60505	22.71846	0.07	3.77E-08
9	1s3s ¹ S ₀	22.90365	22.92031	0.98	5.28E-08
10	1s3p ³ P ₁	22.78089	23.00707	0.98	1.06E-07
11	1s3p ³ P ₀	22.78091	23.0071	0.98	1.06E-07
12	1s3p ³ P ₂	22.78092	23.00707	0.91	1.06E-07
13	1s3d ³ D ₃	22.86169	23.07365	0.91	1.42E-08
14	1s3d ³ D ₂	22.86169	23.07365	0.91	1.42E-08
15	1s3d ³ D ₁	22.8617	23.07365	0.91	1.42E-08
16	1s3d ¹ D ₂	22.86401	23.07407	0.74	1.56E-08
17	1s3p ¹ P ₁	22.91453	23.08701	0.45	1.63E-09
18	1s4s ³ S ₁	23.70016	23.59395	0.6	7.07E-08
19	1s4s ¹ S ₀	23.81633	23.67357	0.22	7.17E-08
20	1s4p ³ P ₂	23.7607	23.70789	0.22	1.83E-07
21	1s4p ³ P ₁	23.7607	23.70789	0.22	1.83E-07
22	1s4p ³ P ₀	23.76071	23.7079	0.65	1.83E-07
23	1s4d ³ D ₃	23.89074	23.73609	0.65	3.31E-08
24	1s4d ³ D ₂	23.89075	23.73609	0.65	3.31E-08
25	1s4d ³ D ₁	23.89076	23.73609	0.65	3.31E-08
26	1s4d ¹ D ₂	23.89206	23.73633	0.44	3.62E-08
27	1s4f ³ F ₃	23.84329	23.737	0.44	7.24E-08
28	1s4f ³ F ₄	23.84329	23.737	0.44	7.23E-08
29	1s4f ³ F ₂	23.84329	23.737	0.44	7.23E-08
30	1s4f ¹ F ₃	23.8433	23.737	0.31	-
31	1s4p ¹ P ₁	23.81709	23.74207	0.4	3.64E-09
32	1s5s ³ S ₁	24.06811	23.97197	0.47	1.43E-07
33	1s5s ¹ S ₀	24.12503	24.01121	0.31	6.83E-08
34	1s5p ³ P ₂	24.10452	24.02822	0.31	5.31E-07
35	1s5p ³ P ₁	24.10452	24.02822	0.31	5.31E-07
36	1s5p ³ P ₀	24.10453	24.02823	0.68	5.31E-07
37	1s5d ³ D ₃	24.20621	24.04266	0.68	6.93E-08
38	1s5d ³ D ₂	24.20622	24.04266	0.68	6.93E-08
39	1s5d ³ D ₁	24.20623	24.04266	0.68	6.93E-08
40	1s5d ¹ D ₂	24.20697	24.0428	0.43	6.32E-08
41	1s5f ³ F ₃	24.14813	24.04315	0.43	1.40E-07
42	1s5f ³ F ₄	24.14813	24.04315	0.43	1.40E-07
43	1s5f ³ F ₂	24.14813	24.04315	0.43	1.40E-07
44	1s5f ¹ F ₃	24.14814	24.04315	0.44	-
45	1s5g ³ G ₄	24.15056	24.04321	0.44	2.35E-07
46	1s5g ³ G ₅	24.15056	24.04321	0.44	2.35E-07
47	1s5g ³ G ₃	24.15056	24.04321	0.44	2.35E-07
48	1s5g ¹ G ₄	24.15056	24.04321	0.36	-
49	1s5p ¹ P ₁	24.13335	24.0458	0.44	7.27E-09

where μ is the quantum defect. The quantum defect of a Rydberg atom refers to a correction applied to the equations governing Rydberg atom behavior. For a non-hydrogen atom –alkali for example- the binding energy of the Rydberg states is $\varepsilon = R_y / (n - \delta)^2$ where δ is the quantum defect and R_y is the Rydberg constant. For high n states we are concerned with, $(v_n) = 1$ is a very good approximation.

Results and Discussions

The calculation is performed up to $n=5$ which generate up to 49 levels. The $1s^2$, $1snl$ ($n=2-5$) configurations are given in Table 1. We compare in this table our energy levels from FAC code with the level energies published by NIST³. The differences presented by percentage in the Table are very small. Our calculated energy levels agree within 1%, the only case where the difference is larger being for the $1s2p \ ^3P_2$ level. One can see that results from these two calculations match well for most of the levels and proves that our results are consistent. We can state with confidence that the results are in good agreement to the other published values for

the energy levels of He I. New values of lifetimes are presented in the same Table 1.

Conclusion

We have presented in this paper results for energy levels among the lowest 49 levels, for He I. Based on the experimental published results in NIST database, our energy levels are accurate to better than 1%. Moreover, we presented the results for the lifetimes for almost levels of study. Good agreement between our calculated energy levels for He I and the available NIST data reflects the quality of calculation of the wave functions.

As we don't have other results of lifetimes, we expect that the present set of results will be highly useful for comparison with other future experimental work.

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References

1. K. M. Aggarwal, and F. P. Keenan, *Atomic Data and Nuclear Data Tables*, 99, (2012), 156-248.
2. D. E. Salhi, H. Jelassi, *Canadian Journal of Physics*, Atomic data for allowed and forbidden transitions of helium-like neon DOI: <https://doi.org/10.1139/cjp-2017-0391>
3. <http://www.nist.gov/pml/data/asd.cfm>
4. B. Sow, M. Sow, Y. Gning, A. Traore, A. S. Ndao, A. Wague, *Radiation Physics and Chemistry*, 123, (2016), 25-30
5. Jayanta K. Saha, S. Bhattacharyya, T. K. Mukherjee and P. K. Mukherjee, *J. Phys. B: At. Mol. Opt. Phys.* 42 (2009) 245701
6. E. Lindroth, *Physical Review A*, 49, (1994), 6
7. I. A. Misurkin and S. V. Titov, *Russian Journal of Physical Chemistry A*, 81, (2007), 204-209
8. M. F. Gu, *Canadian Journal of Physics*, 86 (2008) 5
9. K. Stabkowska, M. Polasik, E. Szymańska, J. Starosta, Ł. Syrocki, J. Rzakiewicz, N. R. Pereira, *Physica Scripta*, 2014, (2014), T161,
10. L. V. Chernysheva and V. L. Yakhontov, *Comput. Phys. Commun.*, 119, (1999), 232
11. M. J. Seaton, *Mon. Not. R. Astron. Soc.* 118, (1958), 504