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Radiative Plasma Parameters for Several Levels of Cu I

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Abstract

Energy levels, spontaneous radiative decay rates and electron impact collision strengths are calculated for Cu I with the Relativistic Dirac-Fock (RDF) method. Collision strengths are calculated at the incident energies 7, 8, 9, 10, 11 and 30 eV by using the plane wave Born approximation. Electron impact excitation and de-excitation rate coefficients have been evaluated for 15 excited atomic states for Cu I at different plasma temperatures KT_e. The electron densities N_e corresponding to KT_e have also been calculated from the experimental measurements. These coefficients have been determined at an incident electron excitation temperature in the range between 1.07 to 2.29 eV and the corresponding electron densities varying from 0.95 to 3.1 $\times 10^{16}$ cm^{-3}. The population densities have also been calculated at the considered KT_e and the corresponding N_e. The calculations have been performed using the coupled rate simultaneous equation where the quadrupole transition has been introduced in the calculations in addition to the dipole transition. A good fitting has been obtained between the present result and available ones in literatures.

Keywords: radiative transitions, Collision strength, Cu I.

Introduction

The most important plasma diagnostic tools are Thomson scattering, Langmuir prob, spectroscopy, intrferometry, ionospheric heating and incoherent scatter radar. Plasma spectroscopy is the oldest and one of the most established and oldest diagnostic tool in astrophysics and plasma physics [1, 2]. Radiating atoms, molecules and their ions provide an insight into plasma processes and plasma parameters. Radiative plasma parameters are provided by the optical emission spectroscopy (OES). Using OES one

can obtain fundamental information about the plume by looking directly at the emission spectrum and, particularly, on, the transition probabilities.

A quantitative analysis of stellar spectra and a detailed abundance determination in stellar atmospheres depend heavily on both radiative parameters and transition probabilities. Radiative data for Cu I are also needed in other fields of physics. The determination of the transition probabilities for Cu I lines is justified in plasma physics by the extensive use of copper as an electrode material and is also strongly needed in industry applications.

For atomic structure calculations, Cu I is an interesting medium-heavy element for which strong interplay between the relativistic and correlation effects is to be expected and, consequently, these effects cannot be treated independently. In addition, most of the experimental and theoretical data about the transition probabilities and the radiative lifetimes of the excited states of Cu I were devoted to states belonging to low lying electronic configurations. In astrophysics, the Cu abundance in interstellar H I clouds has been derived from Cu I and Cu II transitions [3, 4]. The investigation of the trends of the Cu and Zn abundances in low-metallicity stars has been performed, the nucleosynthesis mechanisms controlling the production of the elements is still nuclear[5]. Additional abundances for Cu in halo and disk stars were provided by different groups [6, 7]. There is also an increasing interest in spectroscopic data of neutral copper for modeling discharges for copper vapor lasers [8]. The determination of transition probabilities for Cu I lines is justified by the extensive use of copper as an electron cyclotron resonance discharge [9]. These data are necessary for computing the rate coefficients for electron collision excitation as well as for obtaining copper plasma densities from the measured absolute line intensities [10, 11].

The aim of the present work is to compute the fine structure energy levels, the radiative transition wavelengths and the dipole transition probabilities of the $3d^{10}4s$ ($^2S_{1/2}$), $3d^{10}4p$ ($^2P_{1/2}$, $^2P_{3/2}$), $3d^{10}5s$ ($^2S_{1/2}$) and $3d^{10}5p$ ($^2P_{1/2}$, $^2P_{3/2}$) lines for Cu I. The calculations have been performed with the Relativistic Dirac-Fock (RDF) by using the code MCDFGME [12, 13] in the calculations for Cu I. The collision strengths of the studied levels for Cu I have been calculated by using the plane wave Born (PWB) at the incident energies 7, 8, 9, 10, 11 and 30 eV. It has been found that the calculated results using the RDF method generally agree well with the experimental measurements and with the available compared data in literature. The excitation and de-excitation rate coefficients have been determined [14] at the incident electron excitation temperature in the range between 1.07 and 2.29 eV and at the corresponding electron densities from 0.95 to 3.1 $\times 10^{16}$ cm^{-3}. The level populations are calculated as functions of the electron density and of the plasma temperature for the configurations $3d^{10}4s$, $3d^{10}4p$, $3d^{10}5s$ and $3d^{10}5p$ of Cu I.

The MCDF method

The general relativistic MCDF code developed by J.P. Desclaux and P. Indelicato [12,13] has been used to calculate the bound-state wave functions and energies. Details of the method, including the Hamiltonian and the processes used to build the wave functions can be found elsewhere [15, 16].

The total wave function is calculated using of the variational principle. The total energy of the atomic system is the eigenvalue of the equation:

$$H\,\Psi_{\prod,J,M}(\dots,r_i\dots.) = E_{\prod,J,M}\Psi_{\prod,J,M}(\dots,r_i\dots.), \quad (1)$$

where $\prod$ is the parity, J is the total angular momentum eigenvalue, and M is its projection on the z axis J_z. In this equation, the hamiltonian is given by:

$$H = \sum_{i=1}^{N} H_D\ (r_i) + \sum_{i<j} V_{ij}\ (|r_{ij}|), \quad (2)$$

where H_D is the one electron Dirac operator and V_{ij} is the operator representing the electron-electron interaction of order one in α. The expression of Vij in Coulomb gauge and in atomic units, is:

$$V_{ij} = \frac{1}{r_{ij}} - \frac{\alpha_i.\alpha_j}{r_{ij}} - \frac{\alpha_i.\alpha_j}{r_{ij}}\left[cos\left(\frac{\omega_{ij}r_{ij}}{c}\right) - 1\right] + c^2(\alpha_i.\nabla_i)(\alpha_j.\nabla_j)\frac{cos\left(\frac{\omega_{ij}r_{ij}}{c}\right)-1}{\omega_{ij}^2 r_{ij}}, \quad (3)$$

where $r_{ij} = |r_i - r_j|$ is the inter-electronic distance, ω_{ij} is the energy of the exchanged photon between the two electrons, α_i are the Dirac matrices and c is the speed of light. The Coulomb gauge has been used to provide energies free from spurious contributions at the ladder approximation level and must be used in many-body atomic structure calculations [12, 13].

The term $\frac{1}{r_{ij}}$ represents the Coulomb interaction while the term $\frac{\alpha_i.\alpha_j}{r_{ij}}$ is the Gaunt (magnetic) interaction, and the last two terms of equation (3) stand for the retardation operator. In this expression the **∇** operators act only on r_{ij} and not on the wave functions.

The MCDF method is defined by the particular choice of a trial function to solve the Dirac equation as a linear combination of configuration state functions (CSF):

$$|\Psi_{\prod,J,M,}> = \sum_{\nu=1}^{n} c_\nu\,|\nu,\prod,J,M>, \quad (4)$$

The CSF are also the eigenfunctions of the parity $\prod$, the total angular momentum J^2 and its projection J_z. The label ν stands for all other numbers (principal quantum number, etc.) necessary to define unambiguously the CSF. The c_ν are the mixing coefficients which are obtained from the diagonalization of the Hamiltonian matrix coming from the minimization of the energy in Eq. (1) with respect to c_ν.

The CSF is antisymmetric products of one-electron wave functions expressed as linear combinations of the Slater determinants of the Dirac 4-spinors

$$|\nu,\prod,\mathrm{J},\mathrm{M}> = \sum_{i=1}^{N\nu} di \begin{bmatrix} \Psi_1^i(r_1) & \cdots & \Psi_m^i(r_1) \\ \vdots & \ddots & \vdots \\ \Psi_1^i(r_m) & \cdots & \Psi_m^i(r_m) \end{bmatrix}, \quad (5)$$

where the Ψ's are the one-electron wave functions and the coefficients d_i are determined by requiring that the CSF is an eigenstate of J^2 and J_z. The d_i coefficients are obtained by requiring that the CSF are eigenstates of J^2 and J_z.

The Multi-Configuration approach is characterized by the fact that a small number of configurations can account for a large amount of correlations.

Electron-impact excitation cross sections have been computed using the first Born approximation following the work of Kim et al. [17, 18]. A Multi-Configuration Dirac-Fock (MCDF) wave function for the atom and a Dirac wave function for the free electron have been used. Only the Coulomb interaction between the free electron and the atomic electrons has been considered. Then, the individual cross sections thus obtained were weighted by the statistical weight g_j of each j level of the configuration, in order to obtain the excitation cross section σ_{ji}.

The relationship between the collision strengths Ω_{ij} for the electron impact excitation and the excitation cross sections σ_{ij} is given by:

$$\Omega_{ij} = \frac{\sigma_{ij} K_i^2 g_i}{\pi a_0^2}, \quad (6)$$

where a_0 is the Bohr radius, g_i is the statistical weight of the initial target level,K_i^2 is the kinetic energy of the incident electron in Rydbergs (Ry).

Results and Discussion

The levels $3d^{10}4s$ and $3d^{10}5s$ have been selected for the even parity while $3d^{10}4p$ and $3d^{10}5p$ for the odd parity.The calculated RDF of energy levels and the fine structure splitting for Cu I are listed in table 1,as well as the values from NIST [19] for comparison. The agreement is within few tens of cm^{-1}.

The calculations of the transition probabilities of the spectral lines belonging to the transition array $3d^{10}4s - 3d^{10}4p$, $3d^{10}4s - 3d^{10}5p$, $3d^{10}5s - 3d^{10}4p$ and $3d^{10}5s - 3d^{10}5p$ of the neutral copper are presented.

Table 1: Calculated fine structure energy levels (in cm^{-1}) by using MCDF for Cu I.

	Level	**E^{DF}(cm-1)**	**E^{NIST}(cm-1)**
1	$4s\ ^2S_{1/2}$	0.0E+00	0.00000E+00
2	$4p\ ^2P_{1/2}$	3.0548384E+04	3.0535302E+04
3	$4p\ ^2P_{3/2}$	3.0796875E+04	3.0783686E+04
4	$5s\ ^2S_{1/2}$	4.3155690E+04	4.3137209E+04
6	$5p\ ^2P_{3/2}$	4.9404107E+04	4.9382950E+04
5	$5p\ ^2P_{1/2}$	4.9404883E+04	4.9383726E+04

The wavelengths and the radiative transition probabilities for the electric dipole transitions are given in table 2.

Table 2: Wavelengths (in Å) and allowed transition probabilities (in s^{-1}) for Cu I.

λ^{DF} (Å)	$\lambda^{[20]}$ (Å)	Transition	A_L^{DF} (1/sec)	Ref. [20]
202.49586	202.5000	4s $^2S_{1/2}$-5p $^2P_{1/2}$	1.22E+07	1.43E+07
202.5006	202.4335	4s $^2S_{1/2}$-5p $^2P_{3/2}$	1.31E+07	1.43E+07
324.84739	324.7540	4s $^2S_{1/2}$-4p $^2P_{3/2}$	1.39E+08	1.67E+08
327.48981	327.3957	4s $^2S_{1/2}$-4p $^2P_{1/2}$	1.37E+08	1.64E+08
793.53069	793.3130	5s $^2S_{1/2}$-4p $^2P_{1/2}$	2.28E+07	1.45E+07
809.48568	809.2634	5s $^2S_{1/2}$-4p $^2P_{3/2}$	4.43E+07	2.81E+07
1601.0113	1601.0000	5s $^2S_{1/2}$-5p $^2P_{1/2}$	1.32E+07	1.16E+07
1601.281	1601.1000	5s $^2S_{1/2}$-5p $^2P_{3/2}$	1.04E+07	1.16E+07

Table 2 shows a comparison of the present results (RDF) with the calculated results of Lindgard et al [20]. The obtained wavelengths in the EUV region are less than 0.03% accuracy with the compared wavelengths. The calculated transition probabilities have shown a good agreement with theose of Lindgard et al [20] values by using the semiempirical numerical coulomb approximation.

The present values for the collision strengths for Cu I based on the plane wave Born approximation (PWB) at the incoming electron energies 7, 8, 9, 10, 11 and 30 eV are given in table 3.

Table 3: Collision strengths (Ω_{ij}) for Cu I.

Transition	6	7	8	9	10	11	30
1-2	1.2951E+01	1.4770E+01	1.6327E+01	1.7688E+01	1.8897E+01	1.9984E+01	3.1170E+01
1-3	2.5390E+01	2.9011E+01	3.2112E+01	3.4822E+01	3.7229E+01	3.9394E+01	6.1679E+01
1-4	1.5189E+01	1.5426E+01	1.5604E+01	1.5742E+01	1.5853E+01	1.5943E+01	1.6516E+01
1-5	1.4385E+00	1.6128E+00	1.7525E+00	1.8682E+00	1.9664E+00	2.0514E+00	2.7907E+00
1-6	7.1938E-01	8.0269E-01	8.6940E-01	9.2457E-01	9.7132E-01	1.0117E+00	1.3617E+00
2-3	9.6737E+00	9.6738E+00	9.6738E+00	9.6738E+00	9.6738E+00	9.6738E+00	9.6738E+00
2-4	2.8916E+01	3.1265E+01	3.3295E+01	3.5081E+01	3.6677E+01	3.8119E+01	5.3224E+01
2-5	1.3765E+00	1.4457E+00	1.4976E+00	1.5380E+00	1.5703E+00	1.5968E+00	1.7642E+00
2-6	1.1141E+01	1.1361E+01	1.1527E+01	1.1655E+01	1.1758E+01	1.1842E+01	1.2375E+01
3-4	6.0810E+01	6.5669E+01	6.9866E+01	7.3561E+01	7.6861E+01	7.9842E+01	1.1107E+02
3-5	3.2067E+01	3.2941E+01	3.3596E+01	3.4105E+01	3.4512E+01	3.4846E+01	3.6957E+01
3-6	1.5045E+00	1.5770E+00	1.6314E+00	1.6737E+00	1.7076E+00	1.7353E+00	1.9107E+00
4-5	3.2115E+02	3.4295E+02	3.6182E+02	3.7846E+02	3.9335E+02	4.0681E+02	5.4838E+02
4-6	1.6367E+02	1.7467E+02	1.8420E+02	1.9260E+02	2.0011E+02	2.0690E+02	2.7834E+02
5-6	6.4172E+01	6.4172E+01	6.4172E+01	6.4172E+01	6.4172E+01	6.4172E+01	6.4172E+01

The evaluation of 15 electron impact excitation and de-excitation coefficients for the excited atomic states in Cu I have been carried out using an empirical formula [21]. The calculations were carried out by introducing all forbidden and allowed transitions. Therefore, in addition to the dipole transitions, the quadrupole transitions has been included in the calculations.

The rate coefficients are determined for $3d^{10}4s$ ($^2S_{1/2}$), $3d^{10}4p$ ($^2P_{1/2}$), $3d^{10}4p$ ($^2P_{3/2}$), $3d^{10}5s$ ($^2S_{1/2}$) and $3d^{10}5p$ ($^2P_{1/2}$) and $3d^{10}5p$ ($^2P_{3/2}$) excited atomic states in Cu I. The calculations were carried out at the different electron temperatures 1.07 eV, 1.15 eV, 1.29 eV, 1.75 eV and 2.29 eV corresponding to the different electron densities 9.5×10^{15} cm^{-3}, 1.3×10^{16} cm^{-3}, 2.1×10^{16} cm^{-3}, 2.6×10^{16} $cm^{-3}$and 3.1×10^{16} cm^{-3}, respectively. Excitation and de-excitation rate coefficients (in cm^3s^{-1}) have been tabulated in tables 4 and 5 at different excitation temperatures.

Table 4: Excitation rate coefficients (in cm^3s^{-1}) at different excitation temperatures.

Transition	1.07 eV	1.15 eV	1.29 eV	1.75 eV	2.29 eV
$3d^{10}4s(^2S_{1/2})$-$3d^{10}4p(^2P_{1/2})$	.9907E-01	.1300D+00	.1940D+00	.4747D+00	.8908D+00
$3d^{10}4s(^2S_{1/2})$-$3d^{10}4p(^2P_{3/2})$	.9728D-01	.1279D+00	.1913D+00	.4708D+00	.8867D+00
$3d^{10}4s(^2S_{1/2})$-$3d^{10}5s(^2S_{1/2})$	.1786D-09	.2552D-09	.4302D-09	.1360D-08	.3003D-08
$3d^{10}4s(^2S_{1/2})$-$3d^{10}5p(^2P_{3/2})$	.7830D-03	.1166D-02	.2084D-02	.7456D-02	.1782D-01
$3d^{10}4s(^2S_{1/2})$-$3d^{10}5p(^2P_{1/2})$	.7318D-03	.1090D-02	.1948D-02	.6969D-02	.1666D-01
$3d^{10}4p(^2P_{1/2})$-$3d^{10}4p(^2P_{3/2})$	.2575D+02	.2489D+02	.2357D+02	.2037D+02	.1788D+02
$3d^{10}4p(^2P_{1/2})$-$3d^{10}5s(^2S_{1/2})$	.1142D+00	.1313D+00	.1621D+00	.2657D+00	.3864D+00
$3d^{10}4p(^2P_{1/2})$-$3d^{10}5p(^2P_{3/2})$	.9009D-07	.1022D-06	.1223D-06	.1777D-06	.2240D-06
$3d^{10}4p(^2P_{1/2})$-$3d^{10}5p(^2P_{1/2})$	.9110D-07	.1033D-06	.1236D-06	.1794D-06	.2260D-06
$3d^{10}4p(^2P_{3/2})$-$3d^{10}5s(^2S_{1/2})$	.2325D+00	.2671D+00	.3288D+00	.5360D+00	.7768D+00
$3d^{10}4p(^2P_{3/2})$-$3d^{10}5p(^2P_{3/2})$	.9311D-07	.1054D-06	.1259D-06	.1823D-06	.2293D-06
$3d^{10}4p(^2P_{3/2})$-$3d^{10}5p(^2P_{1/2})$	.9691D-07	.1097D-06	.1308D-06	.1888D-06	.2369D-06
$3d^{10}5s(^2S_{1/2})$-$3d^{10}5p(^2P_{3/2})$	.6642D+00	.7334D+00	.8539D+00	.1243D+01	.1685D+01
$3d^{10}5s(^2S_{1/2})$-$3d^{10}5p(^2P_{1/2})$	.1973D+00	.2179D+00	.2537D+00	.3693D+00	.5006D+00
$3d^{10}5p(^2P_{3/2})$-$3d^{10}5p(^2P_{1/2})$	.1562D+10	.1507D+10	.1423D+10	.1222D+10	.1068D+10

Table 5: De-excitation rate coefficients (in cm^3s^{-1}) at different excitation temperatures.

Transition	1.07 eV	1.15 eV	1.29 eV	1.75 eV	2.29 eV
$3d^{10}4s(^2S_{1/2})$-$3d^{10}4p(^2P_{1/2})$	.3579D+02	.3672D+02	.3833D+02	.4337D+02	.4886D+02
$3d^{10}4s(^2S_{1/2})$-$3d^{10}4p(^2P_{3/2})$	.1682D+01	.1726D+01	.1801D+01	.2036D+01	.2293D+01
$3d^{10}4s(^2S_{1/2})$-$3d^{10}5s(^2S_{1/2})$	.2316D-07	.2338D-07	.2378D-07	.2528D-07	.2716D-07
$3d^{10}4s(^2S_{1/2})$-$3d^{10}5p(^2P_{3/2})$	.1256D+01	.1256D+01	.1260D+01	.1295D+01	.1356D+01
$3d^{10}4s(^2S_{1/2})$-$3d^{10}5p(^2P_{1/2})$	.2348D+01	.2348D+01	.2356D+01	.2420D+01	.2535D+01
$3d^{10}4p(^2P_{1/2})$-$3d^{10}4p(^2P_{3/2})$	.1233D+01	.1189D+01	.1123D+01	.9643D+00	.8431D+00
$3d^{10}4p(^2P_{1/2})$-$3d^{10}5s(^2S_{1/2})$	.4097D-01	.4259D-01	.4535D-01	.5406D-01	.6370D-01
$3d^{10}4p(^2P_{1/2})$-$3d^{10}5p(^2P_{3/2})$	.4000D-06	.3897D-06	.3741D-06	.3376D-06	.3107D-06
$3d^{10}4p(^2P_{1/2})$-$3d^{10}5p(^2P_{1/2})$	.8092D-06	.7881D-06	.7563D-06	.6820D-06	.6271D-06
$3d^{10}4p(^2P_{3/2})$-$3d^{10}5s(^2S_{1/2})$	.1744D+01	.1813D+01	.1931D+01	.2304D+01	.2717D+01
$3d^{10}4p(^2P_{3/2})$-$3d^{10}5p(^2P_{3/2})$	.8637D-05	.8417D-05	.8088D-05	.7317D-05	.6748D-05
$3d^{10}4p(^2P_{3/2})$-$3d^{10}5p(^2P_{1/2})$	.1798D-04	.1751D-04	.1681D-04	.1516D-04	.1395D-04
$3d^{10}5s(^2S_{1/2})$-$3d^{10}5p(^2P_{3/2})$	.8217D+01	.8628D+01	.9337D+01	.1161D+02	.1417D+02
$3d^{10}5s(^2S_{1/2})$-$3d^{10}5p(^2P_{1/2})$	.4884D+01	.5128D+01	.5550D+01	.6899D+01	.8424D+01
$3d^{10}5p(^2P_{3/2})$-$3d^{10}5p(^2P_{1/2})$	.3125D+10	.3015D+10	.2846D+10	.2444D+10	.2136D+10

The population densities of these previous configurations in Cu I have been calculated [22, 23] at five electron temperatures 1.07 eV, 1.15 eV, 1.29 eV, 1.75 eV and 2.29 eV corresponding to the electron densities 9.5×10^{15} cm^{-3}, 1.3×10^{16} cm^{-3}, 2.1×10^{16} cm^{-3}, 2.6×10^{16} $cm^{-3}$and 3.1×10^{16} cm^{-3}, respectively. The spontaneous decay rate A_{ij} has been calculated using MCDFMGE code [12, 13].

Table 6: Level population densities (in cm^3) at different excitation temperatures.

Transition	1.07 eV	1.15 eV	1.29 eV	1.75 eV	2.29 eV
$3d^{10}4s(^2S_{1/2})$	.9500E+16	.1300E+17	.2100E+17	.2600E+17	.3100E+17
$3d^{10}4p(^2P_{1/2})$	.47996E+13	.1098E+14	.3668E+14	.1207E+15	.2807E+15
$3d^{10}4p(^2P_{3/2})$	.9835E+14	.2255E+15	.7563E+15	.2493E+16	.5793E+16
$3d^{10}4s(^2S_{1/2})$	.79611E+13	.2190E+14	.9380E+14	.4388E+15	.1296E+16
$3d^{10}5p(^2P_{3/2})$	.3939E+12	.1154E+13	.5709E+13	.3331E+14	.1163E+15
$3d^{10}5p(^2P_{1/2})$	.1969E+12	.5767E+12	.2854E+13	.1665E+14	.5817E+14

The population density for each level has been calculated. It has been found that the highest value of the population density is for the $3d^{10}4s(^2S_{1/2})$ level and the lowest value is for the $3d^{10}5p(^2P_{1/2})$ excited level.

Conclusion

In the present paper, atomic data and radiative plasma parameters for the seven fine structure configurations of Cu I have been calculated, in order to provide, the astrophysical community a dataset that allows one to predict a more complete Cu I spectrum. The data were compared with earlier available calculations. it has been found that the highest value of the population density is for the $3d^{10}4s(^2S_{1/2})$ level and the lowest value is for the $3d^{10}5p(^2P_{1/2})$ excited level.

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