Transition Analysis of Ne-like Ge XXIII

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【abstract】*Transition between fine-structure levels arising from the $2p^5 3s$, $2p^5 3p$ and $2p^5 3d$ configurations of highly charged Ne-like ions, obtained from GRASP (General-purpose Relativistic Atomic Structure Program) calculations, are tabulated for Ge XXIII.*

Introduction

Over the past 15 years, substantial efforts have been directed towards understanding the lasing possibilities for certain $2p^5 3s$--$2p^5 3p$ transitions in Ne-like ions. Significant progress has been made during this period and an overview of the results has been provided by Nilsen and Scofield[1]. Transition between fine-structure levels arising from the $2p^5 3s$, $1s^2 2s^2 2p^5 3p$ and $2p^5 3d$ configurations of highly charged Ne-like ions have recently attracted large interest in connection with attempts to achieve amplification of radiation at short wavelengths [2,3]. They also have a considerable astrophysical interest, as they can be used for diagnostic purposes in high-temperature plasmas [4,5]. Identification of the spectra of all these above mentioned systems is practically impossible without corresponding theoretical analysis. In this situation, accurate theoretical wavelength predictions can be of great value.

In this work, transition wavelengths of Ne-like Ge XXIII are calculated by means of GRASP code[6]. Theoretical calculation can provide transition wavelengths, energy level lifetimes and so on for experimentation . Such calculations could be done prior to the corresponding experimental observations or after them to help to explain the interesting phenomena found in experimental analyzing. GRASP presented by I.P. Grant[7] extends the previously published program which solved the atomic orbital wavefunctions and energy levels. Two types of the charge distribution (point charge distribution and Fermi two-parameter distribution) in nucleus were adopted to calculate wavelengths of highly stripped ions. Making use of GRASP one can be in a position to perform calculations of the energy spectra, transition probabilities of all atoms of the Periodical Table and ions of any ionization degree.

1 Theory

Relativistic atomic structure theory is ultimately based on quantum electro-dynamics. The GRASP approximation for the calculation of atomic stationary states and transitions among them has been described in the literature [8~10]. Only a brief outline of the theory is given in this paper.

From the theoretical point of view the atom is considered to be a many-body system. As described more fully in Ref.[11] we construct atomic state functions (ASF) from a linear combination of configuration state functions (CSF) which are eigenfunctions of J^2,J_z and parity. These in turn are built from single-electron Dirac equation.

All the dominant interactions in the highly stripped ions are included in the Dirac-Coulomb Hamiltonian,

$$\hat{\mathrm{H}}^{\mathrm{DC}} = \sum_{i=1}^{N} \hat{\mathrm{H}}_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left| \hat{r}_i - \hat{r}_j \right|^{-1} \tag{1}$$

in the first term (in atomic units) ,

$$\hat{\mathrm{H}}_{\hat{i}} = c \sum_{j=1}^{3} \alpha_j p_j + (\beta - 1)c^2 + V_{\mathrm{nuc}}(r), \tag{2}$$

is the one-body contribution for an electron due to its kinetic energy and interaction with the nucleus—the rest energy; c^2, has been subtracted out; r is the position vector of the electron; c is the velocity of light; $p \equiv -\mathrm{i}\nabla$ is the momentum operator. The nuclear potential energy, $V_{\mathrm{nuc}}(r)$, takes the two types of the charge distribution in nucleus. First, takes the Coulomb form or point charge distribution in nucleus, $V_{\mathrm{nuc}} = -Z/r$ (where Z denotes the atomic number of the system). Second, takes the Fermi two-parameter distribution,

$$\rho_{nuc}(r) = \frac{\rho_0}{1 + \mathrm{e}^{(r-c1)/a}}, t = (4 \ln 3)a \tag{3}$$

the parameter c1 is the "half-charge radius", the value of r for which $\rho_{nuc}(r)=0.5\rho_0$; it thus provides a measure of the nuclear radius. The surface thickness t, which measures the distance over which the density falls from 0.9 ρ_0 to 0.1 ρ_0. For A (nuclear numbers of system)＞12 , there is a central region of fairly uniform charge density given by $\rho_0=0.17\ fm^{-3}$, α=0.54 fm[12]. The nuclear potential can be calculated from the identity[7]

$$-rV_{nuc}(r)=4\pi(\int_0^r \rho(s)s^2 ds + r\int_r^\infty \rho(s)s ds)$$

2 Results

From the paper[13] we know that GRASP is an available program for researching the atomic structure. Wavelengths of highly ionized atoms Ne-like Ge XXIII are computed by means of GRASP code with two types of the charge distribution in nucleus. Table 1 give out the comparison of transition wavelengths between theoretical calculation performed by this work and experimental data taken from experimentation performed in the Department of Nuclear Physics of the China Institute of Atomic Energy (CIAE)[14,15]. From Table 1 we can see that seven new 3s—3p transition experimental values in Ge XXIII have been obtained by CIAE group. In Table 1, Model 1 for point charge distribution in nucleus, Model 2 for Fermi two-parameter distribution in nucleus.

From these comparisons we can see that there are differences of wavelengths between theory and experiment for highly ionized atoms Ne-like Ge XXIII, but no differences or small differences of wavelengths between theoretical calculations with two types of the charge distribution in nucleus. In this work, the main differences come from correlation effects not being considered completely. We will improve the GRASP code to include more correlation effects completely in the future.

Table 1 Wavelength comparison between calculated & measured data for Germanium XXIII (Ge^{22+})

Transition	Wavelength(in Å [2])		
	Exp.(CIAE)	Model 1	Model 2
$3p(3/2,1/2)_1$----$3d(3/2,3/2)_2$	179.73[1]	179.06	179.06
$3p(1/2,1/2)_1$----$3d(1/2,3/2)_2$	186.71[1]	186.83	186.83
$3p(1/2,3/2)_1$----$3d(1/2,5/2)_2$	206.54[1]	206.78	206.78
$3p(3/2,3/2)_3$----$3d(3/2,5/2)_4$	209.08[1]	209.27	209.27
$3s(3/2,1/2)_2$----$3p(3/2,3/2)_2$	221.32[1]	221.53	221.55
$3s(3/2,1/2)_3$----$3p(3/2,3/2)_3$	238.36	238.22	238.24
$3s(3/2,1/2)_2$----$3p(3/2,1/2)_2$	269.94[1]	269.68	269.71
$3s(3/2,1/2)_1$----$3p(3/2,1/2)_2$	286.43[1]	286.86	286.88

1) measured data are published first time in the world; 2) 1Å=10^{-10}m.

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