J. Astrophys. Astr. (2008) **29,** 367–378

Investigation of the Effects of Expectation Values for Radii on the Determination of Transition Probabilities using WBEPM Theory

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Received 2007 February 8; accepted 2008 June 24

Abstract. Transition probabilities for some excited s–p and p–s transition arrays of neutral nitrogen have been calculated using the weakest bound electron potential model theory (WBEPMT) for the investigation of effects of expectation values of radii. We have used both numerical non-relativistic Hartree-Fock (NRHF) wave functions and numerical Coulomb approximation (NCA) wave functions to calculate expectation values of radii. The transition probability results obtained using the parameters determined with two different wave functions agree well with each other and accepted values taken from NIST for low values of transition probability. However, the NRHF wave functions present better results for p–s transitions, while NCA wave functions are better in s–p transitions for large values of transition probability.

Key words. Neutral nitrogen—atomic data—transition probabilities—WBEPM theory.

1. Introduction

The optical properties of carbon, nitrogen and oxygen atoms are important in both atmospheric and astrophysical applications. Accurate atomic data such as transition probabilities, oscillator strengths and life-times are essential in various fields of astrophysics. Absorption lines observed in sun light related to the transitions between fine structure levels may contain very important information about far stars in galaxy. Moreover, the lighter elements have been proving ground of truly many-electron methodologies. Numerous experimental and theoretical studies have been published over the last 40 years for these elements. Atomic nitrogen is abundant in higher parts of the atmosphere, and its spectrum is apparent in the dayglow. Due to the abundance of atomic nitrogen in stellar atmospheres, spectral lines of NI are prominent features in their absorption spectra, and therefore are becoming increasingly important for all kinds of quantitative analyses (Baclawski *et al.* 2002). The determination of the nitrogen abundance in hot stars is also strongly dependent upon the atomic transition probabilities (Hibbert *et al.* 1991). The accuracy and reliability of radiative transition probabilities for some spectral lines are thus

very important, not only for testing of theoretical models and experimental techniques in atomic systems, but also for possible applications in plasma diagnostics and astrophysical applications. In spite of their extreme importance in atmospheric physics and astrophysics, the multiplet transitions in NI has been examined up until now by applying many theoretical and experimental methods (Beck & Nicolaides 1976).

In this work, in order to investigate the effects of parameters on the transition probabilities, the WBEPM theory has been applied to some excited s–p and p–s transitions in the neutral nitrogen. We employed both NRHF wave functions and NCA wave functions for determination of relevant parameters.

2. Theoretical approximation

The determination of some parameters corresponding to individual energy levels, especially for high lying levels in multi-electron atoms or ions are always a difficult problem for both experimental and theoretical studies. While the calculation procedure for the systems with a few electrons can be carried out easily, the calculations became more difficult and complex in the case of increasing number of electrons. Especially, for the excited states of many-electron atomic or ionic systems, more configurations or basis sets must be considered. Therefore, the calculations became more complicated. Many of the physical properties in multi-electron systems have been studied using some powerful methods such as Multiconfigurational Hartree-Fock (MCHF) (Tong *et al.* 1994; Tachiev & Fischer 2002), Configuration Interaction (CI) (Hibbert *et al.* 1991; Bell *et al.* 1995), Multiconfigurational Dirac-Fock (MCDF) (Indelicato *et al.* 1988) and R-Matrix method (Seaton 1987; Bell & Berrington 1991). In the well known theoretical methods, atomic wave functions are obtained using many basis-set orbital functions and configurations. The reliability and accuracy of the results depend on the number of basis-set orbital functions chosen. It is difficult to deal with many configuration and orbital basis-set functions and not practicable in calculations. For highly excited states of many electron atoms, it is difficult to obtain appropriate basis-set orbital functions and configurations. Because of the difficulties mentioned above, generally, many of the used methods have considered transitions belong to multiplet levels instead of fine structure transitions and the transitions belong to low lying states rather than highly excited states.

The weakest bound electron potential model theory (WBEPMT) is an efficient method especially for transitions between low excited and highly excited levels. In this method, the determination of some parameters is sufficient for the calculation of the spectroscopic data. The calculations for transition probabilities belong to both low and highly excited levels can be obtained easily and in a shorter time (Zheng *et al.* 2000; Fan & Zheng 2004; Zheng & Wang 2004; Zheng *et al.* 2004). Recently, Çelik *et al.* (2006a) have studied effects of expectation values of radii in some p–d and d–p transitions of neutral nitrogen and this study has shown that changes in the expectation values of radii considerably affect the transition probability results.

The WBEPM theory was proposed by Zheng and he has suggested a new model potential to describe the electronic motion in a multi-electron atom or ion (Zheng 1988).

Zheng *et al.* have employed the WBEPM theory to calculate the energy levels, ionization potentials, transition probabilities, oscillator strengths and lifetimes in many electron atomic or ionic systems. They have obtained very satisfactory physical parameters (Zheng *et al.* 2000a; Fan & Zheng 2004; Zheng & Wang 2004; Zheng *et al.* 2004). The WBEPM theory, based on the idea that electrons in a system can be divided into two groups of electrons; to be the weakest bound electron and non-weakest bound electrons. The weakest bound electron in a given many-electron system is most weakly bound electron to the system compared to the other electrons. By the separation of the electrons in a given system, complex many-electron problem can be simplified as the single electron problem and so can be solved easily (Zheng *et al.* 2004). According to the WBEPM theory, electronic radial wave functions are presented as a function of Laguerre polynomial in terms of some parameters which are determined using the experimental energy data and the expectation values of radii (Zheng *et al.* 2000a),

$$R_{nl}(r) = \left(\frac{2Z^*}{n^*}\right)^{l^*+3/2} \left[\frac{2n^*}{(n-l-1)!}\Gamma(n^*+l^*+1)\right]^{-1/2}$$

$$\times \exp\left(-\frac{Z^*r}{n^*}\right) r^{l^*} L_{n-l-1}^{2l^*+1}\left(\frac{2Z^*r}{n^*}\right). \tag{1}$$

Here, Z^*, n^*, l^* quantities are defined to be effective nuclear charge, effective principal quantum number, effective azimuthal quantum number, respectively, and d is an adjustable parameter. Moreover, n^* and l^* parameters have been given to be (Zheng *et al.* 2000a; Zheng & Wang 2002, 2004; Zheng *et al.* 2004; Fan & Zheng 2004):

$$n^* = n + d, \qquad l^* = l + d. \tag{2}$$

In the WBEPM theory, these parameters are obtained by solving two equations in equation (3) together.

$$I = -\varepsilon = \frac{Z^{*2}}{2n^{*2}}, \qquad \langle r\rangle = \frac{3n^{*2} - l^*(l^*+1)}{2Z^*}. \tag{3}$$

Here, I is the ionization energy and $\langle r\rangle$ is the expectation value for radius of weakest bound electron. The ionization energies and expectation values for radii of all states must be known for the parameters Z^*, n^*, l^* to be determined. It is well known that some difficulties in obtaining the parameters directly from theory are still present. Therefore, Zheng *et al.* suggest that the values of ionization energy can be taken from the experimental atomic data in the literature and expectation value of radius of the weakest bound electron $\langle r\rangle$ can be obtained by different theoretical methods.

The most important quantity in the calculation of transition probabilities is determination of radial transition integral or radial matrix elements. In this work, we have employed the weakest bound electron potential model theory for determination

Table 1. The parameters obtained using two different wave functions.

Level	n	l	NCA		NRHF		Energy (cm^{-1}) Ralchenko *et al.* (2006)
			d	Z^*	d	Z^*	
$2p^2(^3P)3s^4P$	3	0	−1.165497	1.019477	−1.026685	1.096618	33890.102
$2p^2(^3P)3s^4P_{1/2}$	3	0	−1.166581	1.019649	−1.025417	1.098157	33941.63
$2p^2(^3P)3s^4P_{3/2}$	3	0	−1.165871	1.019536	−1.026248	1.097149	33907.87
$2p^2(^3P)3s^4P_{5/2}$	3	0	−1.164886	1.019380	−1.027399	1.095752	33861.08
$2p^2(^3P)3p^4S$	3	1	−0.967354	0.878000	−0.987073	0.869483	20474.86
$2p^2(^3P)3p^4S_{3/2}$	3	1	−0.967354	0.878000	−0.987073	0.869483	20474.86
$2p^2(^3P)3p^4P$	3	1	−1.057978	0.863903	−0.914685	0.927647	21715.843
$2p^2(^3P)3p^4P_{1/2}$	3	1	−1.060374	0.863523	−0.912676	0.929278	21750.39
$2p^2(^3P)3p^4P_{3/2}$	3	1	−1.059100	0.863725	−0.913745	0.928410	21732.01
$2p^2(^3P)3p^4P_{5/2}$	3	1	−1.056428	0.864149	−0.915981	0.926594	21693.55
$2p^2(^3P)3p^4D$	3	1	−1.103459	0.856627	−0.942736	0.929222	22387.919
$2p^2(^3P)3p^4D_{1/2}$	3	1	−1.107858	0.855916	−0.939026	0.932288	22454.82
$2p^2(^3P)3p^4D_{3/2}$	3	1	−1.106374	0.856156	−0.940279	0.931251	22432.21
$2p^2(^3P)3p^4D_{5/2}$	3	1	−1.103913	0.856554	−0.942354	0.929538	22394.81
$2p^2(^3P)3p^4D_{7/2}$	3	1	−1.100550	0.857096	−0.945180	0.927205	22343.88
$2p^2(^3P)4s^4P$	4	0	−1.134515	1.006234	−1.061183	1.031985	13531.82
$2p^2(^3P)4s^4P_{1/2}$	4	0	−1.140992	1.006603	−1.054343	1.037111	13603.19
$2p^2(^3P)4s^4P_{3/2}$	4	0	−1.136948	1.006372	−1.058622	1.033903	13558.54
$2p^2(^3P)4s^4P_{5/2}$	4	0	−1.130711	1.006020	−1.065172	1.028999	13490.22
$2p^2(^3P)4p^4P$	4	1	−0.915302	0.940991	−0.837940	0.964590	10211.742

$2p^2(^3P)4p^4P_{1/2}$	4	1	−0.921791	0.940549	−0.831999	0.967985	10245.22
$2p^2(^3P)4p^4P_{3/2}$	4	1	−0.918781	0.940754	−0.834758	0.966408	10229.668
$2p^2(^3P)4p^4P_{5/2}$	4	1	−0.910800	0.941297	−0.842043	0.962247	10188.631
$2p^2(^3P)4p^4D$	4	1	−0.951765	0.938506	−0.866069	0.964891	10402.368
$2p^2(^3P)4p^4D_{1/2}$	4	1	−0.963857	0.937681	−0.854953	0.971315	10466.969
$2p^2(^3P)4p^4D_{3/2}$	4	1	−0.960201	0.937931	−0.858325	0.969365	10447.363
$2p^2(^3P)4p^4D_{5/2}$	4	1	−0.953433	0.938930	−0.864541	0.965773	10411.241
$2p^2(^3P)4p^4D_{7/2}$	4	1	−0.943206	0.939090	−0.873873	0.960390	10357.065
$2p^2(^3P)4p^4S$	4	1	−0.828160	0.946902	−0.909403	0.922648	9780.078
$2p^2(^3P)4p^4S_{3/2}$	4	1	−0.828160	0.946902	−0.909403	0.922648	9780.078
$2p^2(^3P)5s^4P$	5	0	−1.122025	1.003044	−1.078360	1.014338	7341.491
$2p^2(^3P)5s^4P_{1/2}$	5	0	−1.38945	1.003551	−1.060930	1.023828	7413.467
$2p^2(^3P)5s^4P_{3/2}$	5	0	−1.128571	1.003237	−1.071652	1.017987	7369.18
$2p^2(^3P)5s^4P_{5/2}$	5	0	−1.111900	1.002751	−1.088652	1.008747	7299.039
$2p^2(^3P)5p^4P$	5	1	−0.834685	0.967605	−0.817246	0.971656	5921.82
$2p^2(^3P)5p^4P_{1/2}$	5	1	−0.848169	0.967098	−0.804571	0.977254	5954.104
$2p^2(^3P)5p^4P_{3/2}$	5	1	−0.842317	0.967318	−0.810085	0.974817	5940.056
$2p^2(^3P)5p^4P_{5/2}$	5	1	−0.825034	0.967969	−0.826253	0.967686	5898.902
$2p^2(^3P)5p^4D$	5	1	−0.872337	0.966193	−0.840934	0.973544	6012.758
$2p^2(^3P)5p^4D_{1/2}$	5	1	−0.900389	0.965147	−0.814340	0.985405	6082.133
$2p^2(^3P)5p^4D_{3/2}$	5	1	−0.891720	0.965469	−0.822610	0.981711	6060.542
$2p^2(^3P)5p^4D_{5/2}$	5	1	−0.875979	0.966057	−0.837509	0.975068	6021.684
$2p^2(^3P)5p^4D_{7/2}$	5	1	−0.852619	0.966931	−0.859346	0.965363	5964.827

Table 2. Atomic transition probabilities between some excited levels for nitrogen.

Lower state (L)	Upper state (U)	L	U	Wavelength (Å)	Statistical weight		This work (NCA)	This work (NRHF)	NIST values Wiese (2006)
$2s^2 2p^2 (^3P) 3s$	$2s^2 2p^2 (^3P) 3p$	^4P	^4P	8214.05	12	12	3.21e-01	3.79e-01	3.10e-01[B+]
				8187.111	4	6	9.7e-02	1.14e-01	8.58e-02[B+]
				8190.263	2	4	1.34e-01	1.59e-01	1.27e-01[B+]
				8202.611	2	2	5.3e-02	6.3e-02	4.95e-02[B+]
				8212.98	4	4	4.29e-02	5.05e-02	4.84e-02[B+]
				8218.60	6	6	2.25e-01	2.65e-01	2.23e-01[B+]
				8225.40	4	2	2.67e-01	3.14e-01	2.64e-01[B+]
				8244.66	6	4	1.43e-01	1.68e-01	1.36e-01[B+]
$2s^2 2p^2 (^3P) 3s$	$2s^2 2p^2 (^3P) 3p$	^4P	^4D	8694.00	12	20	2.74e-01	3.22e-01	2.47e-01[B+]
				8682.666	6	8	2.75e-01	3.23e-01	2.46e-01[B+]
				8721.232	6	6	8.17e-02	9.58e-02	6.75e-02[B+]
				8749.771	6	4	1.34e-02	1.58e-02	1.04e-02[B+]
				8685.788	4	6	1.92e-01	2.26e-01	1.86e-01[B+]
				8714.096	4	4	1.45e-01	1.70e-01	1.28e-01[B+]
				8731.298	4	2	4.51e-02	5.30e-02	3.76e-02[B+]
				8688.535	2	4	1.14e-01	1.34e-01	1.09e-01[B+]
				8705.637	2	2	2.27e-01	2.67e-01	2.10e-01[B+]
$2s^2 2p^2 (^3P) 3p$	$2s^2 2p^2 (^3P) 4s$	^4P	^4P	12218.9	12	12	6.55e-02	7.52e-02	9.62e-02[B]
				12190.17	6	6	4.5e-02	5.32e-02	7.11e-02[B]
				12292.55	6	4	2.94e-02	3.31e-02	3.76e-02[B]
				12133.29	4	6	1.9e-02	2.31e-02	2.95e-02[B]
				12234.711	4	4	8.7e-03	9.9e-03	1.52e-02[B]
				12301.91	4	2	5.4e-02	6.10e-02	7.41e-02[B]
				12207.26	2	4	2.73e-02	3.13e-02	4.08e-02[B]
				12274.16	2	2	1.09e-02	1.22e-02	1.43e-02[B]

$2s^2 2p^2(^3P)3p$	$2s^2 2p^2(^3P)4s$	^4D	^4P	11291.7	20	12	1.12e-01	1.35e-01	1.35e-01[B]
				11294.76	8	6	8.95e-02	1.08e-01	1.08e-01[B]
				11230.16	6	6	2.01e-02	2.48e-02	2.09e-02[B]
				11316.99	6	4	7.10e-02	8.44e-02	9.02e-02[B]
				11183.19	4	6	2.24e-03	2.19e-03	2.01e-03[C+]
				11269.29	4	4	3.61e-02	4.34e-02	4.13e-02[B]
				11326.281	4	2	5.66e-02	6.65e-02	7.36e-02[B]
				11240.66	2	4	5.64e-03	6.83e-03	6.00e-03[B]
				11297.35	2	2	5.67e-02	6.70e-02	6.92e-02[B]
$2s^2 2p^2(^3P)3p$	$2s^2 2p^2(^3P)4s$	^4S	^4P	14402.9	4	12	1.93e-02	1.55e-02	1.24e-02[C]
				14317.13	4	6	1.93e-02	1.58e-02	1.33e-02[C]
				14458.55	4	4	1.92e-02	1.52e-02	1.18e-02[C]
				14552.51	4	2	1.90e-02	1.40e-02	1.10e-02[C]
$2s^2 2p^2(^3P)3p$	$2s^2 2p^2(^3P)5s$	^4S	^4P	7614.19	4	12	7.51e-03	7.05e-03	6.94e-03[D+]
				7589.660	4	6	7.6e-03	7.24e-03	7.01e-03[D+]
				7630.280	4	4	7.4e-03	6.90e-03	6.90e-03[D+]
				7656.151	4	2	7.31e-03	6.73e-03	6.83e-03[D+]
$2s^2 2p^2(^3P)3p$	$2s^2 2p^2(^3P)6s$	^4S	^4P	6294.33	4	12	5.17e-03	5.08e-03	3.72e-03[D+]
				6277.248	4	6	5.2e-03	4.71e-03	3.75e-03[D+]
				6305.658	4	4	5.0e-03	4.7e-03	3.70e-03[D+]
				6323.259	4	2	4.9e-03	4.6e-03	3.67e-03[D+]

(*Continued*)

Table 2. (*Continued*)

Lower state (L)	Upper state (U)	L	U	Wavelength (Å)	Statistical weight		This work (NCA)	This work (NRHF)	NIST values Wiese (2006)
$2s^2 2p^2(^3P)4s$	$2s^2 2p^2(^3P)4p$	^4P	^4D	31954	12	20	3.24e-02	3.41e-02	3.06e-02[D+]
				31916.7	6	8	3.27e-02	3.42e-02	3.07e-02[D+]
				32478.3	6	6	9.36e-03	9.74e-03	8.74e-03[D+]
				32863.9	6	4	1.51e-03	1.56e-03	1.41e-03[D+]
				31773.3	4	6	2.3e-02	2.42e-02	2.18e-02[D+]
				32142.2	4	4	1.7e-02	1.78e-02	1.60e-02[D+]
				32346.0	4	2	5.22e-03	5.47e-03	4.92e-03[D+]
				31687.4	2	4	1.37e-02	1.45e-02	1.31e-02[D+]
				31885.5	2	2	2.70e-02	2.85e-02	2.57e-02[D+]
$2s^2 2p^2(^3P)4s$	$2s^2 2p^2(^3P)4p$	^4P	^4S	26654	12	4	5.06e-02	5.81e-02	4.14e-02[D+]
				26953.1	6	4	2.47e-02	2.81e-02	2.00e-02[D+]
				26465.8	4	4	1.71e-02	1.98e-02	1.41e-02[D+]
				26156.7	2	4	8.75e-03	1.02e-02	7.29e-03[D+]
$2s^2 2p^2(^3P)5s$	$2s^2 2p^2(^3P)5p$	^4P	^4D	75260	12	20	8.07e-03	8.31e-03	7.07e-03[D+]
				74950.6	6	8	8.20e-03	8.43e-03	7.15e-03[D+]
				78286.8	6	6	2.2e-03	2.21e-03	1.88e-03[D+]
				80743.0	6	4	3.38e-04	3.35e-04	2.86e-04[D+]
				74211.7	4	6	5.83e-03	6.06e-03	5.16e-03[D+]
				76415.3	4	4	4.12e-03	4.22e-03	3.60e-03[D+]
				77697.2	4	2	1.23e-03	1.25e-03	1.07e-03[D+]
				73913.9	2	4	3.48e-03	3.64e-03	3.11e-03[D+]
				75112.6	2	2	6.68e-03	6.94e-03	5.92e-03[D+]

Note: Estimated accuracy rates from NIST: B+ $\leq$ 7%, B $\leq$ 10%, C+ $\leq$ 18%, D+ $\leq$ 40%.

of radial transition integrals. According to the WBEPM theory, the radial transition integral for transitions between two excited levels is given as (Zheng *et al.* 2000a),

$$\langle n_i, l_i | r^k | n_f, l_f \rangle = \int_0^\infty r^{k+2} R_{n_i l_i}(r) R_{n_f l_f}(r) dr$$

$$= (-1)^{n_f+n_i+l_f+l_i} \left(\frac{2Z_f^*}{n_f^*}\right)^{l_f^*} \left(\frac{2Z_i^*}{n_i^*}\right)^{l_i^*} \times \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*}\right)^{-l_f^*-l_i^*-k-3} x$$

$$\times \left[\frac{n_f^{*4}\Gamma(n_f^*+l_f^*+1)}{4Z_f^{*3}(n_f-l_f-1)!}\right]^{-1/2} x \left[\frac{n_i^{*4}\Gamma(n_i^*+l_i^*+1)}{4Z_i^{*3}(n_i-l_i-1)!}\right]^{-1/2}$$

$$\times \sum_{m_1=0}^{n_f-l_f-1} \sum_{m_2=0}^{n_i-l_i-1} \frac{(-1)^{m_2}}{m_1! m_2!} \left(\frac{Z_f^*}{n_f^*} - \frac{Z_i^*}{n_i^*}\right)^{m_1+m_2} \times \left(\frac{Z_f^*}{n_f^*} + \frac{Z_i^*}{n_i^*}\right)^{-m_1-m_2} x$$

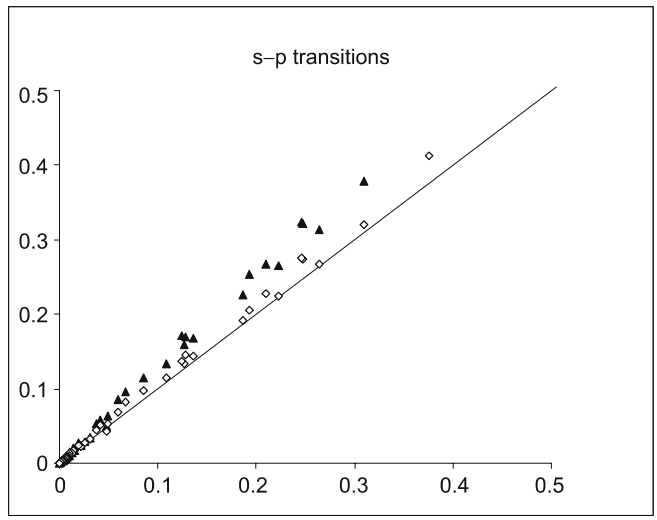
$$\times \Gamma(l_f^*+l_i^*+m_1+m_2+k+3) \times \sum_{m_3=0}^{S} \binom{l_i^*-l_f^*+k+m_2+1}{n_f^*-l_f^*-1-m_1-m_3}$$

$$\times \binom{l_f^*-l_i^*+k+m_1+1}{n_i^*-l_i^*-1-m_2-m_3} \times \binom{l_i^*+l_f^*+k+m_1+m_2+m_3+2}{m_3}, \quad (4)$$

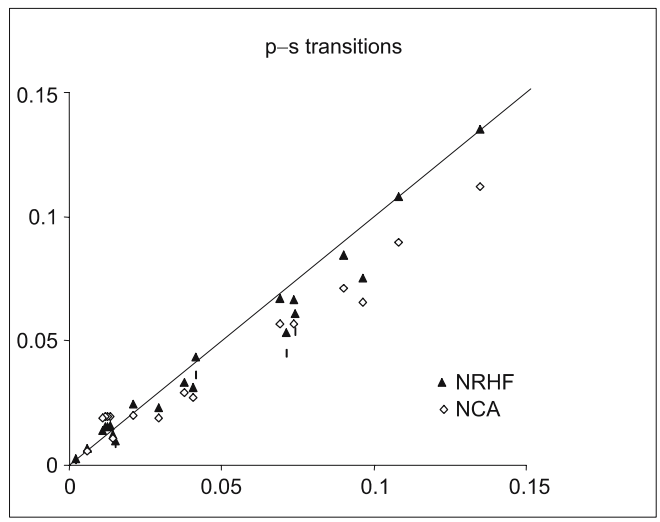
where $S = \min\{n_f - l_f - 1 - m_1, n_i - l_i - 1 - m_2\}$ and $k > -l_f^* - l_i^* - 3$. In this work, expectation values of radii for all excited states have been calculated both by NCA wave functions (Lindgard & Nielsen 1977) and by numerical NRHF wave functions (Gaigalas & Fischer 1996) in determination of parameters required for the transition probability calculations. The necessary experimental energy values have been taken from NIST (Ralchenko *et al.* 2006). The parameters obtained by using the two different wave functions are presented in Table 1. Then, making use of these parameters, transition probabilities have been calculated in neutral nitrogen.

3. Results and conclusions

In order to investigate the effects of expectation values for radii, the transition probabilities have been calculated for some s–p and p–s transitions of excited atomic nitrogen in the WBEPM theory framework. The results obtained in this work are presented in Table 2. Expectation values of radii for all states have been calculated by using both the NCA wave functions and the numerical NRHF wave functions to determine the Z^* and d parameters required for the calculation of the transition probabilities. The results of transition probability have been compared with each other and accepted values are taken from NIST (Wiese 2006) which contains recommended values for many transitions. The NIST values are given together with their accuracy rating in relevant columns of tables. The estimated uncertainties of accepted values are ±7% for 3s–3p transitions, ±10–40% for 3p–4s, 5s, 6s transitions and ±40% for



(a)



(b)

Figure 1. Transition probability results calculated with parameters obtained using NRHF and NCA wave functions *versus* accepted values taken from NIST for neutral nitrogen. **(a)** s–p transitions **(b)** p–s transitions.

4s–4p and 5s–5p. It can be seen from Table 2 that there is an agreement between data obtained in the present work and the accepted values from NIST. Experimental and theoretical data for comparison are quite limited for some excited transitions. On the other hand, some data have not been sensitively tested for both the multiplet values and the individual lines, especially in transitions belonging to highly excited levels. Therefore, the results obtained from our calculations have been compared to only

NIST data. It is well known from literature that the WBEPM theory is an efficient method especially for transitions between excited and highly excited levels. Accuracy and reliability of the spectroscopic data results obtained from the WBEPM theory strongly depend on the accuracy and reliability of the expectation values of radii and experimental ionization energies which are used to determine Z^*, n^* and l^* parameters. Since experimental ionization energy data are very precise, the determination of the expectation values of the radii is more crucial than energy values in the WBEPM theory. Zheng *et al.* have employed only NCA method in all the calculations carried out using the WBEPM theory for the expectation values of radii. In this study, we have employed more sophisticated numerical NRHF wave functions than the NCA wave functions which are commonly employed in the traditional WBEPM theory procedure. Previously, we employed numerical NRHF wave functions for the determination of relevant parameters in atomic nitrogen (Çelik *et al.* 2006a, 2007), lithium (Çelik 2007) and fluorine (Çelik *et al.* 2006b) and obtained very satisfactory transition probability and oscillator strength results by using the WBEPM theory.

In order to observe the effects of expectation values for radii, we have plotted transition probability results calculated with parameters obtained using NRHF and NCA wave functions *versus* accepted values taken from NIST in both some s–p transitions and p–s transitions. It can be seen clearly from Table 2 and Fig. 1 that our results are in agreement with the accepted values taken from NIST. It can be concluded that, according to Fig. 1, our results obtained by using both NRHF wave functions and NCA wave functions for low values of transition probability are in agreement with NIST data. The parameters obtained from NRHF wave functions present better results in p–s transitions, while the parameters obtained from NCA wave functions present better results in s–p transitions for large values of transition probability.

The obtained results indicate that accuracy of transition probabilities in the WBEPM theory framework strongly depends on the accuracy and reliability of the expectation values for radii. In the WBEPM theory, although relativistic effects are neglected except for the observed binding energies, many of the spectroscopic data results are in very good agreement with the results obtained from theoretical methods and experimental measurements in the literature. By courtesy of this method, physical parameters can be calculated for both highly excited states and low lying states without any increase of complexity in calculation process. The transitions between individual lines in both low and highly excited levels have a great importance in many areas of the physics, especially in astrophysics. The calculations of spectroscopic data will be better, if the expectation values of radii belonging to the levels are accurate enough.

Acknowledgements

The authors gratefully acknowledge Prof. Ulfet ATAV for his help and the Selçuk University Scientific Research Projects (BAP) Coordinating Office for financial support.

References

Baclawski, A., Wujec, T., Musielok, J. 2002, *Phys. Scr.*, **65**, 28.
Beck, D. R., Nicolaides, C. A. 1976, *J. Quant. Radiat. Transfer*, **16**, 297.
Bell, K. L., Berrington, K. A. 1991, *J. Phys. B: At. Mol. Opt. Phys.*, **24**, 933.

Bell, K. L., Hibbert, A., Stafford, R. P. 1995, *Phys. Scr.*, **52**, 240.
Çelik, G. 2007, *J. Quant. Spectrosc. Radiat. Transfer*, **103**, 578.
Çelik, G., Akın, E., Kılıç, H. Ş. 2006a, *Eur. J. Phys. D*, **40**, 325.
Çelik, G., Kılıç, H. Ş., Akın, E. 2006b, *T. J. Phys.*, **30**, 165.
Çelik, G., Akın, E., Kılıç, H. Ş. 2007, *Int. J. Quant. Chem.*, **107**, 495.
Fan, J., Zheng, N. W. 2004, *Chem. Phys. Lett.*, **400**, 273.
Gaigalas, G., Fischer, C. F. 1996, *Comput. Phys. Commun.*, **98**, 255.
Hibbert, A., Biemont, E., Godefroid, M., Vaeck, N. 1991, *Astron. Astrophys. Suppl. Ser.*, **88**, 505.
Indelicato, P., Gorceix, O., Desclaux, J. P. 1988, *J. Phys. B: At. Mol. Phys.*, **20**, 651.
Lindgard, A., Nielsen, S. E. 1977, *At. Data Nucl. Data Tables*, **19**, 533.
Ralchenko, Y., Jou, F. C., Kelleher, D. E., Kramida, A. E., Musgrove, A., Reader, J., Wiese, W. L., Olsen, K. 2006, *NIST Atomic Spectra Database* (version 3.0.1). URL: http://physics.nist.gov, National Institute of Standards and Technology, Gaithersburg, MD.
Seaton, M. J. 1987, *J. Phys. B*, **20**, 6363.
Siegel, W., Migdalek, J. 1998, *At. Data Nucl. Data Tables*, **68**, 303.
Tachiev, G. I., Fischer, C. F. 2002, *Astron. Astrophys.*, **385**, 716 and Vanderbilt University, Nashville, TN http://www.vuse.vanderbilt.edu/∼cff/mchf. collection
Tong, M., Fischer, C. F., Sturesson, L. 1994, *J. Phys. B: At. Mol. Opt. Phys.*, **27**, 4819.
Wiese, W. L. 2006, Atomic transition probabilities (Web Version 2.0). [Online] Available: URL: http://physics.nist.gov/PhysRefData/datarefs/IAU/WG2/report2.html National Institute of Standards and Technology, Gaithersburg, MD.
Zheng, N. W. 1988a, A new outline of atomic theory (Jiang Su Education Press).
Zheng, N. W. 1988b, *Chin. Sci. Bull.*, **33**, 916.
Zheng, N. W., Wang, T., Yang, R. Y. 2000a, *J. Chem. Phys.*, **113**, 6169.
Zheng, N. W., Wang, T., Yang, R. Y., Wu, Y. G. 2000b, *J. Chem. Phys.*, **112**, 7042.
Zheng, N. W., Wang, T. 2002, *Astrophys. J. Suppl. Ser.*, **143,** 231.
Zheng, N. W., Wang, T., Ma, D. X., Zhou, T., Fan, J. 2004, *Int. J. Quant. Chem.*, **98**, 281.
Zheng, N. W., Wang, T. 2004, *Int. J. Quant. Chem.*, **98**, 495.