Volume 9, Number 1 January, 2000
1009-1963/2000/09(01)/0013-06 CHINESE PHYSICS © 2000 Chin. Phys. Soc.

CALCULATION OF THE TRANSITION ENERGIES OF THE Ne-LIKE IONS WITH THE CORRECTION OF CORE POLARIZATION*

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(Received 20 November 1998; revised manuscript received 4 May 1999)

The transition energies between $n = 3$ and $n = 2$ of the Ne-like ion Ge^{22+}, Se^{24+}, Zr^{30+}, Rh^{35+}, Ag^{37+}, Sb^{41+}, Xe^{44+}, La^{47+}, Nd^{50+} and Eu^{53+} are calculated by adding polarization in the core. The systematic errors in multi-configuration Dirac-Fock calculation are greatly reduced and a good agreement is obtained between the theory and the experiment. This study shows that introducing the polarization of core orbitals is a good method to calculate the atomic structure, and there is a close relation between polarizability and nucleus charge.

PACC: 3220R; 3130; 3150

I. INTRODUCTION

Recently there has been considerable interest in the transition energy of Ne-like ions. Because of its close-shell configuration, the Ne-like charge-state is relatively stable, and consequently is the dominant charge-state over a wide range of plasma parameters. As a result, Ne-like ions of medium and high Z are present in a variety of high-temperature plasma sources. So the spectra of neon isoelectronic sequences play an important role in the research of high-temperature plasma. Spectra from Ne-like ions may provide diagnostic information on plasma electron temperature, electron density, charge-state abundance, or ion temperature, etc. Recent experiments have demonstrated amplification and lasing in the soft-X-ray region involving Ne-like ions. A population inversion was achieved between the $2p^53p$ and $2p^53s$ in Ne-like selenium ($Z = 34$) by making use of the fact that the radiative decay rates to the $2p^6$ ground state are different greatly for the two levels due to the dipole selection rules. Subsequent experiments using Ne-like yttrium ($Z = 39$) and Ne-like molybdenum ($Z = 42$) obtained lasing at shorter wavelengths.[1] Another reason for studying the Ne-like ions is that the energy levels of Ne-like ions provide important tests and understanding of relativistic and quantum electrodynamics (QED) correction in multi-electron system. At the same time, the study of Ne-like ions can bring about development in the theory of quantum mechanics and the calculation method of multi-electron systems.

During the past decades, a lot of works have been done in both theory and experiments.[1—12] These include various theoretical calculation methods, such as z-expansion method (MZ), model potential method (MPM or PW), basic method (BAS), multi-configuration Dirac-Fock method (MCDF), etc.[2] In the calculation of highly stripped atoms, it is worthy to point out that different methods are available only in different ranges of atoms. The MCDF method produces good results in the range of $47 \leq Z \leq 60$.[2] The development of equipment and the improvement of experimental accuracy not only give the theoretical researchers reliable foundation, but also bring them some new problems.

In the course of calculation of the neon isoelectronic sequences Ag^{37+}, Xe^{44+}, La^{47+}, Nd^{50+} and Eu^{53+}, although the agreement is generally excellent, small yet significant differences have been found.[3,4] The measurement shows systematic discrepancies between observed and calculated wavelengths, which depend on the type of transition. It was found that the experimental wavelengths of the 3p, 3s→2p transitions were shorter than the values predicated by a relativistic atomic structure calculation. The experimental wavelengths of the 3d→2p transitions were determined to be slightly longer, and those of the 3p→3s transitions considerable longer than the predicated values. In order to understand these discrepancies, some authors made a simple estimate of the residual electron correlation energy arising from electron ground-state correlation and from (super-)Coster-Kronig-type fluctuations. This correlation actually reduces the differences between theoretical and experimental wave-

* Project supported by the Foundation of China Academy of Engineering Physics (Grant No. 98020207).

lengths for many transitions. However, the residual electron correlation energy cannot account for all differences, and considerable discrepancies remain for some type of transitions. Just like other theoretical workers, we also think the discrepancies come from the rough estimates of all kinds of correlation energy including QED effects (especially the self-energy). But, to focus on the correlation may not be the only way to solve this problem. It should be noticed that most of the correlation energies are related to the original model chosen to solve the problem.

Polarization is not a new concept in discussing the atomic structure. In classical atomic physics, the core polarization has been used to explain the atomic structure of alkaline metals and by making use of the classical theory the polarizability of the core has been calculated. Temkin[12] introduces the discussion of atomic polarization using the full quantum mechanics in 1957. In his research of the collision between an electron and an atom, Temkin took the action of incident electron on the atomic orbitals into account and then introduced the polarization of atomic orbital.[12] Afterwards, researches were done on the polarization of atoms and ions that were exposed in the external electronic field, and obtained a few polarized features of some simple atoms and ions.[13—15] The works in calculation of the atomic structures by using the polarized orbital are not so popular. However, in recent years the calculations of the atomic structure by adding the polarization to orbitals arouse much interest. By means of polarized orbitals the ionization potential for some atoms[16,17] and the energy levels structure of some simple 2- or 3-electron atoms are calculated.[18,19] More information about the orbital polarization can be found in Refs.[20—22].

In this paper, starting from the orbital polarization of the core electrons, we calculate the transition energies of neon isoelectronic sequences by adding the polarization to the orbital $2p^5$. The results are satisfactory and basically cancel the systematic errors appearing in MCDF method, which have been mentioned above.

Ⅱ. THEORY

The calculations are based on a fully relativistic multi-configuration Dirac-Fock self-consistent-field treatment. The details of theory have been described in Ref.[23]. Here we only give a brief introduction to the relativistic Dirac-Fock method. The relativistic Dirac-Fock Hamiltonian is taken to be (in a.u.)

$$\widehat{H} = \sum_{i=1}^{N} \widehat{H}_i + \sum_{i<j}^{N} |\hat{r}_i - \hat{r}_j|^{-1}\,, \tag{1}$$

where all the dominant interactions in an N-electron atom or ion are included, H_i is the relativistic Dirac-Fock Hamiltonian of the ith electron in atomic units(a.u.). Using the standard notation, H_i is given by

$$\widehat{H}_i = c\alpha \cdot \widehat{P} + (\beta - 1)c^2 + V_{\rm nuc}(r)\,, \tag{2}$$

where $V_{\rm nuc}(r)$ is the nuclear potential at $r = r_i$ due to nucleus, α and β are the Dirac-Fock scalar and vector matrices, respectively, $\widehat{P}$ is the relativistic parity operator and c is the velocity of light in vacuum.

The central field Dirac orbital of a single electron is given by

$$\langle \hat{r}|nkm\rangle = \frac{1}{r}\begin{bmatrix} P_{nk}(r) & \chi_{km}(\hat{r}/r) \\ {\rm i}Q_{nk}(r) & \chi_{-km}(\hat{r}/r) \end{bmatrix}, \tag{3}$$

where $P_{nk}(r)$ and $Q_{nk}(r)$ are the large and small components of the radial wave functions, respectively, and the function $\chi_{km}(\hat{r}/r)$ is the spinor spherical harmonics. A configuration state function (CSF), $|\gamma PJM\rangle$, of an N-electron system is formed by taking linear combinations of Slater determinants of order N constructed from orbitals (3) so as to obtain normalized eigenfunctions of the parity operator $\widehat{P}$, and total angular momentum operators $\hat{J}^2$ and $\hat{J}_Z$. Atomic state function (ASF) is a linear combination of CSF sharing common values of P, J and M. Then the energy of atomic state Γ is $E_\Gamma^{\rm DC} = \langle \Gamma PJM|H^{\rm DC}|\Gamma PJM\rangle$.

An important physical effect, including the polarization of core electron orbitals, has been ignored in standard Hamiltonian equation. This polarization produces an additional potential on the valence electron. Now we treat a general N-electron atom in which one of the electrons is in excited state. The other $(N-1)$ electrons form the core. There are two distinct parts in our procedure. In the first place, we must obtain the orbital wave function that describes the core electrons which, in contrast with the usual procedure, are now influenced by the adiabatic field of the valence electron. The polarized core orbitals form the basis of our polarization potential that is used to derive the valence electron orbital in the second stage. In this paper, we employ the following optical potential $V_{\rm pol} = \dfrac{\alpha_1}{r_N^4} + \dfrac{6\beta_1 - \alpha_2}{r_N^6}$, which will be added to the Dirac-Fock equation. The symbols α_1 and α_2 are

dipole and quadrupole polarizability respectively. We only take account of the dipole approximation.

Ⅲ. CALCULATION RESULTS

Based on the discussion above, we employ the MCDF procedure and take into account the QED effect (including vacuum polarization (VP) and self-energy (SE)) and Breit correction. In the course of calculation, we choose the Fermi nucleus model and the extended average level calculation procedure. And finally, we add the orbital polarization to $2p^5$. After careful choice of configurations, we calculate the transition energies of Ne-like ions between $n = 3$ and $n = 2$. The results are listed in Tables 1, 2, 3, 4, and 5. All of the transition energies are in units of eV.

Table 1. Comparison between theoretical (including our calculation and other authors calculation) and experimental energies of Ag^{37+} and Xe^{44+}.

	$\|Ag^{37+}$					$\|Xe^{44+}$				
Transitions	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$
$(2p^5_{3/2}3s_{1/2})J{=}2{\rightarrow}$gs(M2)	3077.7256	3080.5862	3080.7761	3079.49	+0.1899	4206.7166	4210.0402	4210.1882	4208.88	+0.1488
$(2p^5_{3/2}3s_{1/2})J{=}1{\rightarrow}$gs(3G)	3082.9196	3085.2546	3085.2992	3084.12	+0.0446	4212.3153	4215.6408	4215.6279	4214.44	−0.0128
$(2p^5_{3/2}3p_{1/2})J{=}2{\rightarrow}$gs(E2L)	3156.4612	3159.2033	3158.8747	3158.23	−0.3286	4301.9515	4305.2729	4305.2131	4304.29	−0.0597
$(2p^5_{3/2}3p_{3/2})J{=}2{\rightarrow}$gs(E2M)	3207.2772	3210.1411	3209.8230	3209.11	−0.3181	4395.6943	4399.0232	4398.8446	4397.93	−0.1786
$(2p^5_{1/2}3s_{1/2})J{=}1{\rightarrow}$gs(3F)	3260.0038	3262.6951	3262.5275	3261.59	−0.1676	4540.6137	4543.7274	4543.6028	4542.42	−0.1246
$(2p^5_{3/2}3d_{5/2})J{=}1{\rightarrow}$gs(3D)	3331.1311	3335.9999	3334.8350	3334.53	−1.1649	4555.8556	4559.1323	4557.8000	4557.75	−1.3323
$(2p^5_{1/2}3p_{3/2})J{=}2{\rightarrow}$gs(E2U)	3383.7211	3386.4066	3386.5733	3385.36	+0.1667	4725.0561	4728.1055	4728.4937	4726.92	+0.3882
$(2p^5_{1/2}3d_{3/2})J{=}1{\rightarrow}$gs(3C)	3494.0342	3496.7142	3495.8083	3495.07	−0.906	4854.8597	4857.8855	4857.4274	4856.20	−0.4581
$(2s_{1/2}3p_{1/2})J{=}1{\rightarrow}$gs(3B)	3597.7097	3597.9283	3598.1726	3599.59	+0.2443	4949.4056	4949.6407	4949.1391	4951.60	−0.5015
$(2s_{1/2}3p_{3/2})J{=}1{\rightarrow}$gs(3A)	3646.3442	3646.5557	3646.2132	3648.18	−0.3425	5039.9382	5040.1524	5039.8696	5042.03	−0.2827
$(2s_{1/2}3d_{5/2})J{=}2{\rightarrow}$gs(E2S)	3757.2272	3757.4121	/	/	/	5179.0654	5179.2524	5178.8036	5181.22	−0.4488
$(2p^5_{3/2}3d_{3/2})J{=}1{\rightarrow}$gs(3E)	3294.6136	3297.4518	3297.6710	/	+0.2192	/	/	/	/	/

Table 2. Comparison between theoretical (including our calculation and other authors calculation) and experimental energies of La^{47+} and Nd^{50+}.

	$\|La^{47+}$					$\|Nd^{50+}$				
Transitions	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$
$(2p^5_{3/2}3s_{1/2})J{=}2{\rightarrow}$gs(M2)	4740.6295	4744.2270	4744.4163	4743.04	+0.1893	5303.7204	5307.6245	5307.8399	5306.39	+0.2154
$(2p^5_{3/2}3s_{1/2})J{=}1{\rightarrow}$gs(3G)	4746.6421	4750.2416	4750.4151	4749.02	+0.169	5310.1570	5314.0631	5314.2099	5312.79	+0.1468
$(2p^5_{3/2}3p_{1/2})J{=}2{\rightarrow}$gs(E2L)	4843.3813	4846.9773	4846.9833	4845.98	+0.006	5414.2255	5418.1288	/	/	/
$(2p^5_{3/2}3p_{3/2})J{=}2{\rightarrow}$gs(E2M)	4962.5954	4966.1994	/	/	/	5564.1993	5568.1112	/	/	/
$(2p^5_{1/2}3s_{1/2})J{=}1{\rightarrow}$gs(3F)	5170.0819	5173.3536	5173.6213	5172.06	+0.2676	5842.3976	5845.9009	5846.7336	5844.46	+0.8327
$(2p^5_{3/2}3d_{5/2})J{=}1{\rightarrow}$gs(3D)	5133.6736	5137.2765	5136.3284	5135.73	−0.9481	5752.3874	5756.3064	5755.2724	5754.75	−1.034
$(2p^5_{1/2}3p_{3/2})J{=}2{\rightarrow}$gs(E2U)	5382.6589	5385.9178	5386.2389	5384.62	+0.3211	6093.5640	6097.0631	/	/	/
$(2p^5_{1/2}3d_{3/2})J{=}1{\rightarrow}$gs(3C)	5520.7876	5524.0061	/	/	/	6239.8908	6243.3139	/	/	/
$(2s_{1/2}3p_{1/2})J{=}1{\rightarrow}$gs(3B)	5605.7999	5606.0558	/	/	/	6311.3223	6311.6198	/	/	/
$(2s_{1/2}3p_{3/2})J{=}1{\rightarrow}$gs(3A)	5721.2817	5721.5017	5721.2788	5723.49	−0.2229	6456.8548	6457.0828	/	/	/
$(2s_{1/2}3d_{5/2})J{=}2{\rightarrow}$gs(E2S)	5874.2938	5874.4858	5873.8787	5876.58	−0.6071	6625.0517	6625.2507	/	/	/
$(2p^5_{3/2}3d_{3/2})J{=}1{\rightarrow}$gs(3E)	/	/	/	/	/	/	/	/	/	/

Table 3. Comparison between theoretical (including our calculation and other authors calculation) and experimental energies of Sb^{41+} and Rh^{35+}.

	$\|Sb^{41+}$					$\|Rh^{35+}$				
Transitions	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$
$(2p^5_{3/2}3s_{1/2})J$=2→gs(M2)	3702.4605	3704.4733	/	/	/	2785.9187	2789.0858	/	/	/
$(2p^5_{3/2}3s_{1/2})J$=1→gs(3G)	3707.6378	3709.6517	3710.1512	3709.9291	+0.4995	2936.5434	2939.5399	2940.3879	2938.3314	+0.848
$(2p^5_{3/2}3p_{1/2})J$=2→gs(E2L)	3790.4501	3792.4629	/	/	/	2859.9883	2863.1511	/	/	/
$(2p^5_{3/2}3p_{3/2})J$=2→gs(E2M)	3863.2748	3865.2932	/	/	/	2902.1526	2905.3231	/	/	/
$(2p^5_{1/2}3s_{1/2})J$=1→gs(3F)	3964.1460	3966.1493	3965.5770	3965.8968	−0.5723	2790.3256	2793.4954	2793.2915	2792.1593	−0.2039
$(2p^5_{3/2}3d_{5/2})J$=1→gs(3D)	4006.7208	4008.7375	4006.1337	4008.4651	−2.6038	3019.6947	3022.8709	3021.3917	3021.2445	−1.4792
$(2p^5_{1/2}3p_{3/2})J$=2→gs(E2U)	4118.0087	4119.8764	/	/	/	3047.2039	3050.1938	/	/	/
$(2p^5_{1/2}3d_{3/2})J$=1→gs(3C)	4239.2261	4241.0829	4239.7016	4241.1518	−1.3813	3151.9704	3154.9581	3152.6096	3153.2511	−2.3485
$(2s_{1/2}3p_{1/2})J$=1→gs(3B)	4340.0196	4340.1669	4339.1136	/	−1.0533	3255.5298	3255.9802	3255.0757	3258.9258	−0.7045
$(2s_{1/2}3p_{3/2})J$=1→gs(3A)	4410.0608	4410.2000	/	/	/	3295.6179	3295.8624	3294.8667	3296.4435	−0.9957
$(2s_{1/2}3d_{5/2})J$=2→gs(E2S)	4536.4499	4536.5702	/	/	/	3399.2979	3399.5119	/	/	/
$(2p^5_{3/2}3d_{3/2})J$=1→gs(3E)	3959.9108	3961.8994	3961.96	3962.6013	+0.0606	2984.6729	2987.8141	/	2986.4590	/

Table 4. Comparison between theoretical (including our calculation and other authors calculation) and experimental energies of Zr^{30+} and Se^{24+}.

	$\|Zr^{30+}$					$\|Se^{24+}$				
Transitions	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$
$(2p^5_{3/2}3s_{1/2})J$=2→gs(M2)	2117.4593	2121.3126	/	/	/	1432.7561	1435.1138	/	/	/
$(2p^5_{3/2}3s_{1/2})J$=1→gs(3G)	2121.2121	2125.0692	2125	2125.9573	−0.0692	1435.7527	1438.1133	1438.3501	1438.6845	+0.2368
$(2p^5_{3/2}3p_{1/2})J$=2→gs(E2L)	2180.4811	2184.3304	/	/	/	1483.0177	1485.3731	/	/	/
$(2p^5_{3/2}3p_{3/2})J$=2→gs(E2M)	2205.5462	2209.2364	/	/	/	1495.9119	1498.2743	/	/	/
$(2p^5_{1/2}3s_{1/2})J$=1→gs(3F)	2207.3676	2211.0624	2211	2209.2985	-0.0624	1476.9786	1479.2708	1479.5445	1479.5445	+0.2737
$(2p^5_{3/2}3d_{5/2})J$=1→gs(3D)	2303.6989	2307.5600	2307	2307.5718	−0.56	1572.0129	1574.3713	1573.4243	1574.6232	−0.947
$(2p^5_{1/2}3p_{3/2})J$=2→gs(E2U)	2290.9923	2294.6809	/	/	/	1536.2255	1538.5142	/	/	/
$(2p^5_{1/2}3d_{3/2})J$=1→gs(3C)	2381.7135	2385.4072	2385	2382.9681	−0.407	1610.4949	1612.7969	1610.2056	1612.7189	−2.5913
$(2s_{1/2}3p_{1/2})J$=1→gs(3B)	2481.1982	2481.5390	2482	2480.7089	+0.461	1699.0278	1699.2734	1696.1126	1699.6002	−3.1608
$(2s_{1/2}3p_{3/2})J$=1→gs(3A)	2505.0539	2505.3925	2506	2501.2272	+0.6075	1710.9070	1711.1554	/	/	/
$(2s_{1/2}3d_{5/2})J$=2→gs(E2S)	2591.9967	2592.2920	/	/	/	1779.4915	1779.7083	/	/	/
$(2p^5_{3/2}3d_{3/2})J$=1→gs(3E)	22806106	2284.4422	2284	2282.0878	−0.4422	/	/	/	/	/

Table 5. Comparison between theoretical (including our calculation and other authors calculation) and experimental energies of Ge^{22+} and Eu^{53+}.

	$\|Ge^{22+}$					$\|Eu^{53+}$				
Transitions	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$	$E^{a)}_{theo}$	$E^{b)}_{theo}$	$E^{c)}_{expt}$	$E^{d)}_{theo}$	$\Delta E^{e)}$
$(2p^5_{3/2}3s_{1/2})J$=2→gs(M2)	1233.4795	1236.4059	/	/	/	5895.99	5899.7227	5899.8731	5898.22	+0.1504
$(2p^5_{3/2}3s_{1/2})J$=1→gs(3G)	1236.2371	1239.1673	1238.6197	1238.6197	−0.5476	5902.85	5906.5965	5906.9001	5905.05	+0.3036
$(2p^5_{3/2}3p_{1/2})J$=2→gs(E2L)	1279.5849	1282.5043	/	/	/	6014.53	6018.2652	/	/	/
$(2p^5_{3/2}3p_{3/2})J$=2→gs(E2M)	1289.6739	1292.6029	/	/	/	6201.23	6205.1180	/	/	/
$(2p^5_{1/2}3s_{1/2})J$=1→gs(3F)	1267.4638	1270.3208	1270.3466	1269.8262	+0.0258	6564.98	6569.0403	/	/	/
$(2p^5_{3/2}3d_{5/2})J$=1→gs(3D)	1358.9921	1361.9167	1360.9861	1361.1355	-0.9306	6407.34	6411.3491	/	/	/
$(2p^5_{1/2}3p_{3/2})J$=2→gs(E2U)	1320.0394	1322.8883	/	/	/	6860.66	6864.6856	/	/	/
$(2p^5_{1/2}3d_{3/2})J$=1→gs(3C)	1389.1280	1392.0051	1391.5357	1391.0673	-0.4694	7014.56	7018.6242	/	/	/
$(2s_{1/2}3p_{1/2})J$=1→gs(3B)	1472.6821	1473.0013	1472.5158	1473.3907	-0.4855	7068.25	7068.8698	/	/	/
$(2s_{1/2}3p_{3/2})J$=1→gs(3A)	1481.9349	1482.2599	1481.3122	1482.7294	-0.9477	7249.25	7249.9296	/	/	/
$(2s_{1/2}3d_{5/2})J$=2→gs(E2S)	1544.6795	1544.9665	/	/	/	7434.29	7434.7483	/	/	/
$(2p^5_{3/2}3d_{3/2})J$=1→gs(3E)	1341.9613	1344.8556	1344.7487	1345.3324	−0.1069	/	/	/	/	/

a) Our calculation of the transition energies without orbital polarazation. b) Our calculation of the transition energies with orbital polarazation. c) Experimental transition energies.[2,3,7,9] d) The other calculation of the transition energies.[1,2,4,8] e) $\Delta E^{e)} = E^{c)}_{expt} - E^{b)}_{theo}$.

IV. DISCUSSION

1. In comparison with those in Refs. [1] and [4], our results are considerably better than the calculations reported in the literature and the agreement with experiments is greatly improved. After introducing the orbital polarization to $2p^5$, it can easily be seen from Tables 1, 2 and 5 that the systematic differences are fundamentally eliminated for Ag^{37+}, Xe^{44+}, La^{47+}, Nd^{50+} and Eu^{53+}. Tables 3, 4 and 5 show that the results of other elements can also be compared with the results by other calculation methods, and some of our results are even better than the results from the literature. However, the improvements for the lines 3D and 3C are little. Relatively great discrepancies still exist in these lines. The transition energies of 3D and 3C are all larger than those obtained in experiments. In Refs.[1] and [4], the authors specifically employed the optimum level (OL) approach for 3D and 3C and got excellent results. This indicates that the OL approach is better than the extended average level (EAL) calculation for the lines 3D and 3C. The EAL calculation at least has certain deficiencies for 3D and 3C. Meanwhile, we found that the MCDF procedure is extremely available in the atomic range $47 \leq Z \leq 60$. We can infer from these tables that the transition energies of M2, 3G, 3F, E2L, E2M, E2U, 3E and 3A obtained by polarized orbital method are reliable. To the two lines 3D and 3C, our differences are in the range of 0 to 2.6 eV, most are in 0 to 1.5 eV. Since we cannot make calculation by using the OL approach, we can only predict from Refs.[1] and [4] that if the OL procedure is adopted for the calculation of 3D and 3C, the results can be improved. For the line 3B of Se^{24+} we have no good explanation for the difference -3.1608 eV (the difference is -3.4876 eV in Refs.[8]). Maybe, in Se^{24+}, there are still some correlations we have not given sufficient estimate.

2. By analyzing the polarization of the orbital $2p^5$, we find that the polarizabilty of $2p^5$ decreases with the increase of the atomic number Z. It is because the bonding force of the core is great when the atomic number is large. So the core of a heavy atom is difficult to be distorted under the external field. And then its polarizabilty is small. This relation is also found in the classic atomic polarization of the core. Figure 1 shows the relationship between the dipolarizability α_1 and the atomic number Z. In the range of $47 \leq Z \leq 60$, the curve can be taken as a line. From $Z = 32$ to $Z = 63$, the contribution of the polarization to the transition energies ranges from 0→3 eV. It includes the change of all correlation energies after inducing the orbital polarization, such as the change of Breit correction, vacuum polarization and self-energy correction.

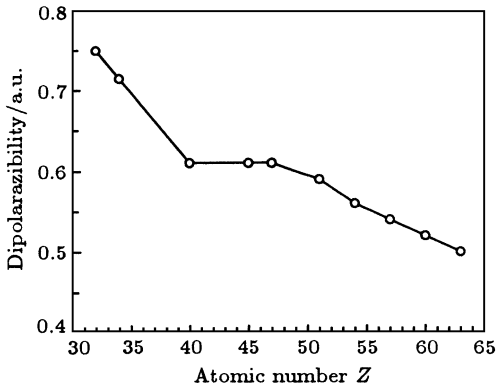


Fig.1. The dipolarizability vs atomic number curve.

3. In recent discussion about the orbital polarization, the orbital polarization of the core is considered to originate from the Coulomb interaction of the valence electron only. In our opinion, in addition to the Coulomb repulsion, there are other two facts that possibly are the causes for the orbital polarization: (a) Under the central field approach, the core with $(N-1)$ electrons has a spherical symmetry and the $2p^5$ in the configuration $1s^2 2s^2 2p^5 nl$ is equally treated as spherical symmetry. However, when the $2p^6$ loses an electron and changes into $2p^5$, the $2p^5$ will lose its spherical symmetry. Then $2p^5$ will polarize under the classical conditions. (b) The valence electron moves in the field of the other electrons. Due to the Coulomb repulsion, it is impossible for the valence electron to stay with other electrons in the same position and even in a small space. This is the so-called Coulomb hole effect. The Coulomb hole effect will destroy the symmetrical properties of the distribution of the core electrons. Hence the orbital polarization of the core electrons occurs. This kind of polarization is especially notable for the valence electron in the low and medium exciting states.

4. As the affect of polarization on transition en-

ergies is concerned, we can employ a simple model to obtain a similar result in the experiment. In the transitions from $1s^2 2s^2 2p^5 3l$ to the ground state, due to the polarization of $2p^5$, the screen effect of $2p^5$ on nucleus is decreased. So the effective-charge $Z_{\rm effp}$ of the valence electron 3l in the core polarization approximation is greater than the effective-charge $Z_{\rm effc}$ of the valence electron 3l in the central field approach, i.e., $Z_{\rm effp} > Z_{\rm effc}$. Using H-like model, the energy of valence electron can be expressed approximately as $E = Z_{\rm eff}^2/N^2$ ($Z_{\rm eff}$ is the effective-charge of valence electron). For the two states of N_1 and N_2, the transition energy between N_1 and N_2 is $\Delta E = Z_{\rm eff}^2 \left(\frac{1}{N_2^2} - \frac{1}{N_1^2}\right)$. It is clear that the transition energy is proportional to $Z_{\rm eff}^2$. Since $Z_{\rm effp} > Z_{\rm effc}$, the transition energies obtained in experiment are greater than those calculated in the central field approach. This is why the experimental wavelengths of the 3p, 3s→2p transitions are shorter than the values predicated in the central field approach. In the transition from $1s^2 2s 2p^6 3l$ to the ground state, the spherical symmetry is unchanged when $2s^2$ changes into 2s, then there is no polarization on 2s due to the destroy of the spherical symmetry. Since the 2s electron is an inner-shell electron and then far from the 3l electron, the force between 2s and 3l are relatively small. The 2s has no distinct polarization. Because $2p^6$ is full shell structure and has spherical symmetry, it also has no remarkable polarization. Finally, the polarization of the core $1s^2$ 2s $2p^6$ is small. This means that the experimental results are generally equal to the theoretical results. This is just what we have got in our calculation.

5. Since we have chosen ten elements uniformly distributed in $32 \leq Z \leq 63$, it can be inferred that we can obtain accurate results for other atoms in this range of $32 \leq Z \leq 63$ by using orbital polarization correction. Particularly, for the atoms in the range of $47 \leq Z \leq 60$ we can firstly get their polarizability according to the proportional relation shown in Fig.1, and then calculate the transition energies. The results must be more reliable.

V. CONCLUSION

By adding the polarization in $2p^5$, we have systematically calculated ten of the Ne-like ions transitions from $n = 3$ to $n = 2$ and got satisfactory results, indicating that the method of adding polarization to the orbital is feasible in calculating atomic structures. In our calculation we have got all of the Briet correction, vacuum polarization and self-energy correction, which have not been listed, here.

REFERENCES

[1] P. Beiersdorfer, M. Bitter, R. S. Walling *et al., Phys. Rev.*, **A34**(1986), 1297.

[2] E. V. Aglitskii, E. P. Ivanova, L. A. Vainshtein, *Phys. Scripta*, **40**(1989), 601.

[3] P. Beiersdorfer, M. H. Chen, R. E. Marrs, *Phys. Rev.*, **A41**(1990), 3453.

[4] P. Beiersdorfer, S. von Goeler, M. H. Chen *et al., Phys. Rev.*, **A37**(1988), 4153.

[5] T. N. Lee, E. A. McLean, R. C. Elton, *Phys. Rev. Lett.*, **59**(1987), 1185.

[6] D. D. Dietrich, G. A. Chandler, R. J. Fortner, *Phys. Rev. Lett.*, **54**(1985), 1008.

[7] M. D. Rosen, P. L. Hagelstein, D. L. Matthews, *Phys. Rev. Lett.*, 54(1985), 106.

[8] P. G. Burkhalter, D. J. Nagel, R. D. Cowan, *Phys. Rev.*, **A11**(1975), 782.

[9] E. Kallne, J. Kallne, R. D. Cowan, *Phys. Rev.*, **A27**(1983), 2682.

[10] J. E. Rice, K. B. Fournier, J. L. Terry, *Phys. Rev.*, **A53**(1996), 3953.

[11] E. Avgoustoglou, W. R. Johnson, Z. W. Liu, *Phys. Rev.*, **A51**(1995), 1196.

[12] A. Temkin, *Phys. Rev.*, **A 107**(1957), 1004.

[13] T. Kwong *et al., Phys. Rev.*, **A152**(1966), 35.

[14] G. N. Bhattacharya, P. K. Mukherjee, H. P. Roy, *Phys. Rev.*, **A22**(1980), 363.

[15] W. R. Johnson, K. T. Cheng, *Phys. Rev.*, **A53**(1996), 1375.

[16] R. P. McEachran, A. D. Stauffer, *J. Phys.*, **B23**(1990), 4605.

[17] R. P. McEachran, M. Cohen, *J. Phys.*, **B16**(1983), 3125.

[18] R. J. Drachman, *Phys. Rev.*, **A26**(1982), 1228.

[19] A. K. Bhatia, R. J. Drachman, *Phys. Rev.*, **A45**(1992), 7752.

[20] C. K. Au, K. L. Poon, K. Young, *J. Phys.*, **B24**(1991), 4671.

[21] A. W. Yau, R. P. McEachran, A. D. Stauffer, *J. Phys.*, **B11**(1978), 2097.

[22] R. P. McEachran, D. L. Morgan, A. G. Ryman *et al., J. Phys.*, **B10**(1977), 663.

[23] J. Sucher, *Phys. Rev.*, **A22**(1980), 384.