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THEORETICAL ATOMIC PHYSICS CODE DEVELOPMENT AT LOS ALAMOS

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Recently, several computer codes for calculation of various types of atomic physics data have been developed at the Los Alamos National Laboratory. The purpose of the code development was to provide a set of codes that are very easy to use, will provide results for any ion or atom, use the best possible theory within the constraints of reasonable running time, and provide great flexibility to the user. The codes relevant to this meeting are the CATS[1] atomic structure code based on Cowan's[2] Hartree-Fock method, the ACE[3] collisional excitation code which can calculate collisional data in the distorted wave approximation (DWA) of Mann[4] or via first order many body theory (FOMBT), and the TAPS[5] code which can display various quantities from CATS and ACE and can provide differential cross sections (DCS) and electron impact coherence parameters (EICP).

For the three codes, CATS, ACE, and TAPS, a brief description of the theory will be presented. Following this will be a presentation of the method of using the codes. Finally, several examples of DCS and EICP calculations using various approximations available in ACE will be given.

The atomic structure code, CATS, is based on Cowan's[2] Hartree-Fock method. Radial wave functions are calculated in the single configuration Hartree-Fock approximation. Configuration interaction and intermediate coupling mixing is brought in through perturbation theory. The calculation of the radial wave functions is a non-relativistic calculation except that the mass and Darwin terms can be included. Quantities calculated by the CATS code include the radial wave functions, energy levels, oscillator strengths and, optionally, plane wave Born collision strengths. The CATS code is run via commands. The following set of commands will generate atomic structure data for neutral barium:

```
opend bal
ion 56 1
ref
6s2
6p2
6s1 6p1
6p1 5d1
/
run
end
```

All data calculated by CATS is placed on a random access file for easy retrieval by the ACE and TAPS codes.

The collisional excitation code, ACE, reads the atomic structure data from the random access file prepared by the CATS code. The radial wave functions for the target states can be generated in the Hartree-Fock or Hartree-statistical-exchange approximations of Cowan[2] with or without the inclusion of the mass and Darwin terms. The ACE code

also contains subroutines to generate hydrogenic bound state wave functions for comparison purposes. The continuum wave functions can be calculated in the DWA method of Mann[4] or via FOMBT[6,7] theory. Subroutines are available to calculate Coulomb functions for comparison purposes. A variety of local exchange potentials are available. Unitarization of the reactance matrix can be turned on and off. Mixing in the target states is included. If requested, the scattering amplitude will be written to a file for use in the TAPS code for DCS and EICP calculations. The ACE code is also run by commands. The following set of commands will calculate cross-section data for neutral barium:

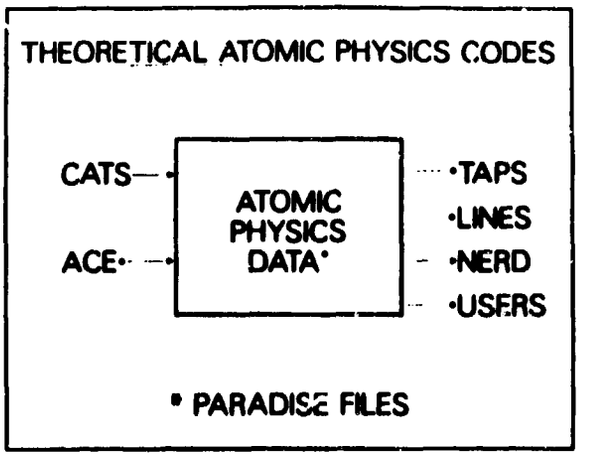
```
files bal
seq 4
setl 1 5
setle 1 5
0.0
2.24
eunits ev
e 20 50
lmax 250
dcs t
thetalin 37 0 180
go
end
```

All data from the ACE code is also written to a random access file.

The display code, TAPS, reads data generated from the CATS and ACE codes. It displays selected data in either text or graphic form. Sums and averages over fine structure levels and LS terms can be performed to provide data for LS terms and configurations. The TAPS code can use the scattering amplitude generated by the ACE code to calculate DCS's and EICP's. Various sets of EICP's are written to different files which are named Blum, Fano, Hertel, and Stokes for obvious reasons.[8-11] The TAPS code is also run by commands. The following set of commands will genetrate DCS's and EICP's for barium:

```
file adam
ion 56 1 4
dcs
cop
end
```

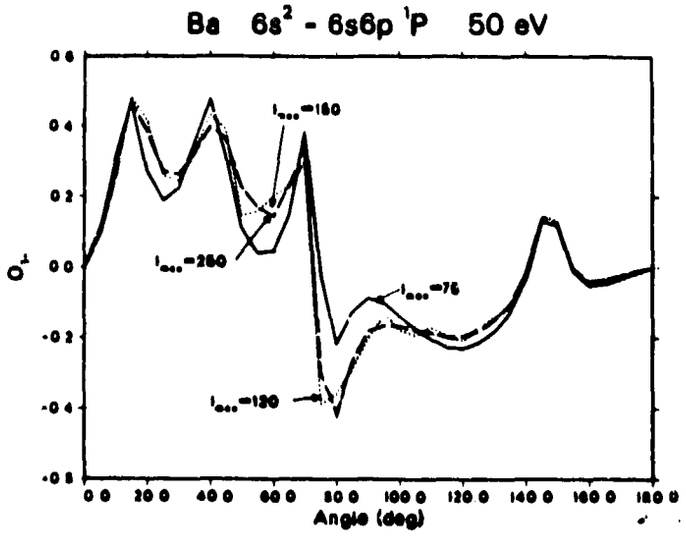
The following figure shows a schematic diagram of the system of codes:



Central to the system is the data file. The arrows indicate that the CATS code writes data to the file, the ACE code reads and writes data, and the other codes read various data. The LINES code generates synthetic spectra and the NERD code is a non LTE code; these two codes will not be discussed further here.

The sets of commands can be sent to the CATS, ACE, and TAPS codes either through interactive use of the computer terminal or through a text file. Full descriptions of all commands are available in the manuals.[1,3,5] Running the three codes with these sets of commands will ultimately produce DCS's and EICP's for the $6s^2$-$6s6p\ ^1P_1$ transition in neutral barium. The CATS run takes $\sim$ 30 sec,

ACE takes ~ 180 sec and TAPS takes ~ 1 sec of Cray-1 time for this test case. Scattering calculations were performed at 20 and 50 eV with 250 partial waves at each energy. The setl command in ACE was used to select the $6s^2$-6s6p $^1P_1$ transition. Other level to level transitions may easily be selected. Tables 1-4 show samples of the EICP's for bariuim. Table 1 shows the EICP's from the blum file for 50 eV. Table 3 shows the corresponding fano file; Table 3 shows the hertel file; Table 4 shows the stokes file. The transition energy for barium $6s^2$-6s6p $^1P_1$ is 2.4 eV so that 50 eV electron energy corresponds to over 20 times the threshold energy. This requires a large number of partial waves for convergence. The following figure shows the orientation parameter for different numbers of partial waves for this case.



Excitation to a specific magnetic sublevel can also be calculated from our codes. From these, polarization fractions can be obtained. Table IV is taken from Ref. 12. It shows collision strengths to magnetic sublevels for neon-like molybdenum (Mo^{+32}) calculated with the fully relativistic code of Zhang et al.[12] compared with the present results. The collision strengths and cross section are related by

$$Q = \frac{\pi a_o^2}{w_i E(R_y)} \Omega$$

where Q is the cross section, a_o is the Bohr radius, w_i is the statistical weight of the initial state, $E(R_y)$ is the impact electron energy in rydbergs and Ω is the collision strength.

In summary, we have developed a set of computer codes for atomic physics calculations at Los Alamos. These codes can calculate a large variety of data with a minimum of effort on the part of the user. In particular, DCS's and EICP's can be readily obtained for arbitrary ions or atoms. Currently, the theory consists of non-relativistic Hartree-Fock structure calculations and non relativistic DWA or FOMBT collisional calculations.

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Table 1. Blum file for barium at 50 eV.

start	i1,i2,e=	1	5	5.0000e+01	
c theta	lambda	chi	cos delta	cos eps	
0.0000e+00	1.0000e+00	0.0000e+00	0.0000e+00	0.0000e+00	
5.0000e+00	4.4039e-02	-5.0521e-01	1.0000e+00	1.0000e+00	
1.0000e+01	7.7861e-02	-1.6153e+00	1.0000e+00	1.0000e+00	
1.5000e+01	3.3075e-01	-1.4757e+00	9.9999e-01	9.9999e-01	
2.0000e+01	4.7757e-01	-8.8734e-01	1.0000e+00	9.9999e-01	
2.5000e+01	4.1853e-01	-5.8229e-01	1.0000e+00	1.0000e+00	
3.0000e+01	3.9709e-01	-5.6558e-01	9.9998e-01	9.9999e-01	

Table 2. Fano file for barium at 50 eV.

start	i1,i2,e=	1	5	5.0000e+01	
c theta	e1-	a1+	a0	a2+	
0.0000e+00	0.0000e+00	0.0000e+00	-1.0000e+00	0.0000e+00	
5.0000e+00	9.9306e-02	1.7955e-01	4.3394e-01	-4.7798e-01	
1.0000e+01	2.6769e-01	-1.1917e-02	3.8321e-01	-4.6197e-01	
1.5000e+01	4.6835e-01	4.4672e-02	3.8755e-03	-3.3462e-01	
2.0000e+01	3.8731e-01	3.1542e-01	-2.1635e-01	-2.61[illegible]-01	
2.5000e+01	2.7129e-01	4.1202e-01	-1.2780e-01	-2.907[illegible]e-01	
3.0000e+01	2.6221e-01	4.1310e-01	-9.5639e-02	-3.0145e-01	

Table 3. Hertel file for barium at 50 eV.

start	i1,i2,e=	1	5	5.0000e+01			
c theta	rho00	p1 +	gamma(rad)	gamma(deg)	1 perp +	1 perp	
0.0000e+00	9.5363e-10	1.0000e+00	-4.3672e-05	-2.5022e-03	0.0000e+00	0.0000e+00	
5.0000e+00	4.5688e-08	9.8008e-01	-1.3832e+00	-7.9253e+01	1.9861e-01	1.9861e-01	
1.0000e+01	7.0877e-07	8.4461e-01	1.5567e+00	8.9191e+01	5.3538e-01	5.3538e-01	
1.5000e+01	2.5547e-06	3.5009e-01	-1.4418e+00	-8.2607e+01	9.3671e-01	9.3671e-01	
2.0000e+01	1.7246e-06	6.3243e-01	-8.2089e-01	-4.7034e+01	7.7462e-01	7.7461e-01	
2.5000e+01	9.3473e-07	8.4000e-01	-8.8300e-01	-5.0592e+01	5.4259e-01	5.4259e-01	
3.0000e+01	2.0884e-06	8.5145e-01	-9.0747e-01	-5.1994e+01	5.2442e-01	5.2442e-01	

Table 4. Stokes file for barium at 50 eV.

start	i1,i2,e=	1	5	5.0000e+01
c theta	p1	p2	p3	
0.0000e+00	1.0000e+00	-8.7344e-05	0.0000e+00	
5.0000e+00	-9.1192e-01	-3.5910e-01	-1.9861e-01	
1.0000e+01	-8.4428e-01	2.3834e-02	-5.3538e-01	
1.5000e+01	-3.3850e-01	-8.9344e-02	-9.3671e-01	
2.0000e+01	-4.4860e-02	-6.3084e-01	-7.7462e-01	
2.5000e+01	-1.6294e-01	-8.2404e-01	-5.4259e-01	
3.0000e+01	-2.0581e-01	-8.2621e-01	-5.2442e-01	

TABLE IV. Comparisons of results for the collision strengths for excitation from the ground level to the magnetic sublevels M_f of the excited odd parity levels with $n = 3$ and $J_f = 1$ in neon-like molybdenum. In each case upper entries are the present fully relativistic results and the second entries are from the code of Ref. 13. Numbers in square brackets designate powers of 10 by which adjacent entries should be multiplied.

Excited Level	M_f	E_f(Ry)				
		10	50	200	500	1000
$2p3s\ ^1P_1$ or $(2p_{3/2}3s_{1/2})_1$	0	3.43[-4] 3.47[-4]	4.65[-4] 4.80[-4]	8.99[-4] 9.20[-4]	1.48[-3] 1.46[-3]	2.00[-3] 1.87[-3]
	1	1.11[-4] 1.08[-4]	1.28[-4] 1.29[-4]	2.30[-4] 2.36[-4]	4.85[-4] 5.03[-4]	8.85[-4] 9.13[-4]
$2p3s\ ^3P_1$ or $(2p_{1/2}3s_{1/2})_1$	0	2.36[-4] 2.67[-4]	3.06[-4] 3.56[-4]	5.61[-4] 6.60[-4]	9.17[-4] 1.05[-3]	1.24[-3] 1.36[-3]
	1	1.19[-4] 1.23[-4]	1.23[-4] 1.32[-4]	1.65[-4] 1.89[-4]	3.00[-4] 3.56[-4]	5.31[-4] 6.32[-4]
$2p3d\ ^3P_1$ or $(2p_{3/2}3d_{3/2})_1$	0	2.14[-4] 2.06[-4]	1.76[-4] 1.67[-4]	1.08[-4] 9.86[-5]	6.90[-5] 5.77[-5]	5.25[-5] 3.81[-5]
	1	7.94[-4] 8.03[-4]	6.30[-4] 6.35[-4]	3.13[-4] 3.11[-4]	1.25[-4] 1.19[-4]	5.72[-5] 4.93[-5]
$2p3d\ ^3D_1$ or $(2p_{3/2}3d_{5/2})_1$	0	1.36[-2] 1.37[-2]	1.61[-2] 1.62[-2]	2.33[-2] 2.31[-2]	3.11[-2] 2.99[-2]	3.75[-2] 3.43[-2]
	1	6.03[-3] 5.91[-3]	6.61[-3] 6.50[-3]	8.95[-3] 8.84[-3]	1.37[-2] 1.37[-2]	2.06[-2] 2.06[-2]
$2p3d\ ^1P_1$ or $(2p_{1/2}3d_{3/2})_1$	0	1.15[-2] 1.18[-2]	1.36[-2] 1.39[-2]	1.97[-2] 1.99[-2]	2.65[-2] 2.62[-2]	3.22[-2] 3.03[-2]
	1	5.00[-3] 4.97[-3]	5.49[-3] 5.46[-3]	7.44[-3] 7.44[-3]	1.14[-2] 1.16[-2]	1.73[-2] 1.76[-2]
$2s3p\ ^3P_1$ or $(2s_{1/2}3p_{1/2})_1$	0	2.30[-4] 2.22[-4]	3.37[-4] 3.01[-4]	6.45[-4] 5.79[-4]	1.08[-3] 9.47[-4]	1.48[-3] 1.26[-3]
	1	1.56[-4] 1.45[-4]	1.57[-4] 1.44[-4]	1.93[-4] 1.73[-4]	3.31[-4] 3.00[-4]	5.82[-4] 5.35[-4]
$2s3p\ ^1P_1$ or $(2s_{1/2}3p_{3/2})_1$	0	6.30[-4] 7.75[-4]	8.78[-4] 1.05[-3]	1.74[-3] 2.00[-3]	2.97[-3] 3.25[-3]	4.13[-3] 4.30[-3]
	1	1.93[-4] 2.62[-4]	2.33[-4] 2.80[-4]	4.17[-4] 4.89[-4]	8.59[-4] 9.97[-4]	1.58[-3] 1.82[-3]