

CALCULATION OF DETAILED ATOMIC DATA USING PARAMETRIC POTENTIALS

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RESUMEN. Los potenciales paramétricos que consisten de una suma de términos de Yukawa más una cola coulombica de largo alcance, pueden proveer datos atómicos de precisión comparable a la que se obtiene en cálculos de campo auto-consistente, de una sola configuración y con correcciones relativísticas. El método se utiliza para generar potenciales efectivos pre-ajustados para las secuencias isoelectrónicas hasta el zinc, no sólo para los electrones de valencia sino también para las configuraciones múltiplemente excitadas y las excitaciones internas del core. Se presentan comparaciones con experimentos y otros cálculos teóricos.

ABSTRACT. Parametric potentials consisting of a sum of Yukawa terms plus a long-ranged Coulomb tail can provide atomic data of accuracy comparable to single-configuration, self-consistent field calculations with relativistic corrections. The method is used to generate prefitted effective potentials for isoelectronic sequences up to zinc, not only for valence electrons but also for multiply excited configurations as well as inner-core excitations. Comparisons to experimental and other theoretical calculations are presented.

Key words: ATOMIC PROCESSES - PLASMAS - TRANSITION PROBABILITIES

1. INTRODUCTION

The calculation of plasma radiative properties is a complex problem that is currently being addressed by several groups. This was prompted, in part, by discrepancies between existing theories and astronomical observations whose description require accurate opacities as input to the stellar models. In order to evaluate the relative merits of the various opacity efforts, it is important to know what physics principles are incorporated into each code. Here, the atomic physics in the OPAL code developed by the authors is described. Although the parametric potential approach has already been presented in Rogers, Wilson, and Iglesias (1988, hereafter RWI), it is included in this volume since improvements in atomic physics have been shown to have significant impact on astrophysical opacities (Iglesias, Rogers, and Wilson 1987; 1990; Iglesias and Rogers 1991b; Rogers and Iglesias 1992; Rosznayai 1989).

The OPAL code uses the method of detailed configuration accounting; that is, ion stages and the electron configurations of those ions are considered explicitly. In addition, the OPAL code considers the detailed energy-level structure of the configurations. This approach requires atomic photoabsorption data for all possible transitions from each occupied level. The parametric potential method is attractive because it is possible to produce quickly atomic data of accuracy comparable to single-configuration, self-consistent field (SCF) calculations with relativistic corrections. It was chosen, in part, because stored data from atomic structure codes may constrain opacity calculations to regions of low density where isolated-ion data may be inadequate. With the ability to generate data quickly, any density effects on the wave functions could be incorporated as needed.

II. PARAMETRIC POTENTIALS

In the past it has been shown that experimental atomic properties can be reasonably well represented by independent particle models and that optimized potentials yield wave functions which are almost the same as those from SCF methods. Klapisch (1971) has used an analytic effective potential involving Yukawa terms modified by

polynomials and advocated adjusting parameters to reproduce experimental data or *ab initio* calculations. However, all free parameters in the potential were optimized and no simple fitting to the parameters are available. Interestingly, an effective potential similar to Klapisch's has been postulated by approximating the Hartree-Fock set of equations in momentum space with a local operator (Lassetre 1985).

We are interested in finding effective potentials for arbitrary configurations and ion stages for all elements with atomic number less than 31. In particular, we have developed a procedure for calculating a large and varied amount of atomic data from a small number of prefitted parameters. Physically motivated corrections to the parameters are used to extend to regions where there are no reliable experiments and we then depend on SCF calculations for guidance.

When discussing the parametric potentials in OPAL, it is convenient to define an electron configuration as having two components. The first component is a "parent" configuration consisting of all electrons in a given configuration except one. The excluded electron defines the second component or "running" electron. The parent configuration defines the potential for all subshells and scattering states available to the running electron. In order to incorporate the shell structure of the parent configuration, Rogers (1981) introduced a potential with a Yukawa term for each occupied shell in the parent configuration,

$$V = -\frac{2}{r} \left[(Z-v) + \sum_{n=1}^{n^*} N_n e^{-\alpha_n r} \right] \quad (1)$$

(in Rydbergs), where

$$v = \sum_{n=1}^{n^*} N_n \quad (2)$$

is the number of electrons for a parent ion, N_n the number of electrons in the shell with principal quantum number n , n^* the maximum value of n for the parent configuration, and α_n the screening parameter for the electrons in shell n . The screening parameters in Eq. (1) are determined by iteratively solving a spin-averaged Dirac equation and matching the eigenvalues to the experimentally observed one electron configuration-averaged ionization energies.

At this point, it is useful to discuss an example. Consider the configuration $1s^2 2s^2 2p^4$. For the ionization of a $2p$ electron, the system is defined by the parent $1s^2 2s^2 2p^3$ plus a running electron. In fact, this parent describes all transitions of the form

$$1s^2 2s^2 2p^3 n_1 l_1 \quad \text{to} \quad 1s^2 2s^2 2p^3 (n_1 l_1)' \quad \text{or to} \quad 1s^2 2s^2 2p^3 \epsilon l_1'$$

where $n_1 l_1$ and $(n_1 l_1)'$ denote the set of orbitals $2p, 3s, 3p, \dots$ and ϵ the energy of the scattering states, so that photoionization and bremsstrahlung can be considered. Similarly the parent $1s^2 2s^2 2p^4$ describes transitions of the form

$$1s^2 2s^2 2p^4 n_2 l_2 \quad \text{to} \quad 1s^2 2s^2 2p^4 (n_2 l_2)' \quad \text{or to} \quad 1s^2 2s^2 2p^4 \epsilon l_2'$$

where now $n_2 l_2$ includes the $1s$ but not the $2p$ orbital. If we assign $n_1 l_1 = 2p$ and $n_2 l_2 = 1s$ in these examples, then the initial configurations are identical. However, it is important to note that the effective potentials are different since the parent configurations are different. In contrast, a SCF potential uses the same set of orbital wave functions for the initial configurations in both sets of transitions above. It follows that the effective potential is not an independent particle parametrization of a SCF potential. In OPAL, transition energies are assumed to be differences between eigenvalues of the running electron. The eigenvalues of the parent-configuration closed shells have no physical interpretation. In contrast, the interpretation in SCF eigenvalues as ionization energies (neglecting orbital relaxation) is a consequence of Koopmans' theorem.

The simplest configurations involve a closed core plus an open valence subshell for which there exists good experimental data. Screening parameters are obtained systematically for varying nuclear charge in each

isoelectronic sequence. Starting with two electron ions (one electron parents), a spin-averaged Dirac equation was solved iteratively to find the screening parameter for the K-shell that best reproduces experimental ground configuration ionization energies. The procedure continues by adding one electron to the parent configuration at a time. Note, however, that matching the experimental energies is simplified since only the optimization of the outer-most shell screening parameter is necessary. The parameters for the inner shells are fixed at the closed shell value.

It was found that each shell parameter could be fitted accurately along an isoelectronic sequence with the simple form

$$\alpha_n = (\xi_n + 1) \sum_{j=0}^3 \frac{a_j(v_n)}{\xi_n^j} \quad (3)$$

Each screening parameter is fitted by coefficients which depend on the occupancy of the parent up to that shell,

$$v_n = \sum_{n=1}^n N_n \quad (4)$$

and by the net charge at the shell, $\xi_n = Z - v_n$, for the parent-configuration ion. The resulting set of a_j 's is relatively small (total of 106 entries) and is given in RWI.

These one-open valence shell configurations comprise only a small subset of all the transitions that must be considered in an opacity calculation. For example, configurations involving inner shell excitations (underlined subshells indicate running electron jumps)

$$1s^2 2s^2 2p^2 \quad \text{to} \quad 1s^2 2s^2 2p^2 \underline{np} \quad \text{and} \quad 1s^2 \underline{2s}^2 2p^2 \quad \text{to} \quad 1s^2 2s^2 \underline{2p}^2 np.$$

must be included. Multiply excited configurations also need to be considered,

$$1s^2 2s^2 \underline{2p}^2 nl \quad \text{to} \quad 1s^2 2s^2 nl (\underline{nl})' \quad \text{and} \quad 1s^2 \underline{2p}^4 \quad \text{to} \quad 1s^2 2p^3 \underline{nl}$$

and, of course, combinations of the above

$$1s^2 \underline{2s}^2 2pnl \quad \text{to} \quad 1s^2 2s^2 pnl (\underline{nl})'.$$

In these example (as well as in the parametric potential model) the atomic structure is assumed to be described by single configurations when obviously a very accurate description would require configuration interactions. Although this may appear to be a limitation of the approach, in particular when comparing to spectroscopic data, for opacity calculations it does not seem to be an issue. On the flip side of the coin, approaches based on atomic structure calculations which include configuration interactions must be certain that they include all the necessary data of which there are vast amounts. Probably the optimal approach would be accurate data bases supplemented by quick, reasonably accurate methods such as parametric potentials to obtain a complete data set.

In RWI it was shown how it is possible to generate from the simpler one-open valence shell parent configurations screening parameters for more complicated situations such as multiply excited ions and inner core excitations. The procedure involves simple scaling laws based on physical arguments. In deriving the scaling laws it was necessary to resort to atomic structure codes since for these more complicated configurations experimental data is limited.

The parametric potentials in Eq. (1) provide the configuration-averaged energies and a set of radial wave functions, $\{\psi_{nl}\}$. In order to obtain reasonable agreement with spectral data, it is necessary to consider the energy level structure of configurations. In OPAL, the calculation is done in the single-configuration approximation of the Slater-Condon theory of atomic structure (Cowan 1981). All results here assume the pure LS coupling scheme (Cowan 1981). The term energies can be obtained using Racah algebra and involve Slater integrals which in turn depend on the set $\{\psi_{nl}\}$. As mentioned above, the one-electron binding energies for each subshell of a configuration is computed from a distinct parent-configuration effective potential. Consequently, the set $\{\psi_{nl}\}$ to be used in the configuration

structure calculation is not uniquely defined. For simplicity, $\{\psi_{nl}\}$ is chosen from the parent associated with both initial and final configurations of a given transition. For example, for the transition $1s^22s2p^2$ to $1s^22p^23p$ where the running electron makes a $2s$ to $3p$ jump, the appropriate parent configuration is $1s^22p^2$.

Calculations with the parametric potentials, which accurately reproduce ionization energies, do not *a priori* guarantee accurate oscillator strengths since these quantities involve expectation values that weight different regions of the radial wave functions. Furthermore, the photoionization cross sections require scattering states and again there is no *a priori* reason for the scattering wave functions to be accurate. Nevertheless, the parametric potentials model both the long-ranged and the inner structure of atoms for both discrete and continuum states so that the resulting photoabsorption data are comparable to SCF calculations. Below, we show some comparisons.

III. COMPARISONS

Comparisons of the parametric potential method to experiment and other theoretical calculations have been given in RWI. There, typical as well as worst case situations were presented that demonstrated the relatively good accuracy of the parametric potential approach. Here, we repeat some of those comparisons but also add a few new examples. We begin with Table 1 where the oscillator strengths of neutral lithium from the parametric potential are shown to be in excellent agreement with close-coupling calculations (Peach, Saraph, and Seaton 1988).

TABLE 1
Comparison of *gf* Values for Neutral Lithium^a

| Transition | Peach et al. | OPAL ^b | Transition | Peach et al. | OPAL ^b |
|------------|--------------|-------------------|------------|--------------|-------------------|
| 2s-2p | 1.495 | 1.49 | 3s-2p | 0.664 | 0.656 |
| 2s-3p | 9.61(-3) | 9.45(-3) | 3s-3p | 2.430 | 2.42 |
| 2s-4p | 8.60(-3) | 9.57(-3) | 3s-4p | 9.83(-5) | 1.84(-4) |
| 2s-5p | 5.14(-3) | 5.63(-3) | 3s-5p | 2.60(-3) | 2.88(-3) |
| 2s-6p | 3.15(-3) | 3.40(-3) | 3s-6p | 2.26(-3) | 2.44(-3) |
| 4s-2p | 7.73(-2) | 7.61(-2) | 5s-2p | 2.60(-2) | 2.54(-2) |
| 4s-3p | 1.339 | 1.32 | 5s-3p | 0.156 | 0.155 |
| 4s-4p | 3.282 | 3.26 | 5s-4p | 2.015 | 1.908 |
| 4s-5p | 1.92(-3) | 1.93(-3) | 5s-5p | 4.106 | 4.06 |
| 4s-6p | 5.73(-4) | 8.78(-4) | 5s-6p | 6.89(-3) | 4.92(-3) |
| 6s-2p | 1.23(-2) | 1.20(-2) | 6s-5p | 2.690 | 2.62 |
| 6s-3p | 5.32(-2) | 5.30(-2) | 6s-6p | 4.916 | 4.85 |
| 6s-4p | 0.232 | 0.231 | | | |

^aNumbers in parentheses represent powers of 10.

^bParametric potential

In Table 2 we compare OPAL results for neutral silicon with experiments. The agreement for configuration-averaged energies is very good even for these more complicated cases. There is some loss in accuracy for the high Rydberg levels. This difficulty is also present in SCF calculations since small discrepancies in total energies correspond to appreciable errors in the ionization energies. However, the configuration level structure in silicon is sensitive to configuration interactions and there are problems with some of the terms. For example, the configuration $[\text{Ne}]3s3p^3$ is poorly described (RWI). We emphasize that such problems reduce rapidly with increasing ion charge. Even singly ionized phosphorus shows much improved agreement with experiment (RWI). From the point of view of astrophysical Rosseland mean opacity calculations, neutral atoms play a very minor part so that discrepancies in neutrals will not be important.

TABLE 2
Configuration-Averaged Energies (Ry) for the Outermost Electron in Neutral Silicon^a

| Configuration | Experiment | Parametric Potential | %Error |
|-----------------|------------|----------------------|--------|
| 3p ² | 0.56983 | 0.57210 | +0.4 |
| 3p4p | 0.15471 | 0.15511 | +0.3 |
| 3p5p | 0.076855 | 0.079113 | +2.9 |
| 3p4s | 0.23340 | 0.23191 | -0.6 |
| 3p5s | 0.10216 | 0.10181 | -0.3 |
| 3p6s | 0.057326 | 0.056049 | -2.3 |
| 3p3d | 0.13015 | 0.12534 | -3.6 |
| 3p4d | 0.071375 | 0.069515 | -2.7 |

^aNote that all these configurations have the same parent

Errors in ionization energies could lead to problems in equation of state calculations. For photon absorption the relative energy difference between the levels in a transition is more important. In Table 3 we compare oscillator strengths for neutral silicon with experiments and with single-configuration SCF calculations (Cowan and Griffin 1976). The transition energies are in reasonable agreement with experiment and the oscillator strengths agree well with the single configuration SCF code.

TABLE 3
Transition Energies and Oscillator Strengths for Neutral Silicon

| Transition | Multiplet | Transition Energy (Ry) | | f values | |
|-----------------------|-----------|------------------------|-------------------|---------------------------|-------------------|
| | | Experiment | OPAL ^a | Cowan et al. ^b | OPAL ^a |
| 3p ² -3p4s | 3P-3P | 0.3619 | 0.3538 | 0.234 | 0.215 |
| | 1D-1P | 0.3159 | 0.3177 | 0.196 | 0.193 |
| | 1S-1P | 0.2330 | 0.2309 | 0.130 | 0.140 |
| 3p4s-3p4p | 1P-1S | 0.0971 | 0.1006 | 0.219 | 0.184 |
| | 1P-1P | 0.0576 | 0.0438 | 0.320 | 0.240 |
| | 1P-1D | 0.0841 | 0.0803 | 0.919 | 0.730 |
| | 3P-3S | 0.0869 | 0.0795 | 0.164 | 0.145 |
| | 3P-3P | 0.0745 | 0.0880 | 0.558 | 0.482 |
| | 3P-3D | 0.0756 | 0.0711 | 0.733 | 0.649 |
| | 3P-3F | 0.0756 | 0.0711 | 0.733 | 0.649 |
| 3p4p-3p4d | 1P-1D | 0.084 | 0.0970 | 0.045 | 0.043 |
| | 1P-1P | 0.105 | 0.112 | 0.046 | 0.040 |
| | 3D-3F | 0.085 | 0.0909 | 0.117 | 0.108 |

^aParametric potential method

^bSingle-configuration SCF calculations using Cowan and Griffin (1976)

Results are given for oscillator strengths of carbon-like oxygen in Table 4. The comparisons are to the Cowan et al. SCF calculations, experimental data, and close-coupling results by Luo et al. (1988). In general, the agreement between SCF and parametric potential is good. For some 2s to 2p transitions, both the parametric potential and SCF agree poorly with the experiments. These transitions are subject to configuration interaction and the close-coupling results show much better agreement with the experimental values. However, except for some $\Delta n=0$ transitions, the parametric potential compares favorably to the experiment.

TABLE 4
Oscillator Strengths for Carbon-Like Oxygen.

| Transition | Multiplet | OPAL ^a | SCF ^b | Close-Coupling ^c | Experiment ^d |
|------------------------------------|-----------|-------------------|------------------|-----------------------------|-------------------------|
| 2p ² -2s2p ³ | 3P-3D | 0.185 | 0.206 | 0.107 | 0.11 |
| | 3P-3D | 0.130 | 0.142 | 0.137 | 0.14 |
| | 3P-3S | 0.254 | 0.268 | 0.188 | 0.18 |
| | 1D-1D | 0.492 | 0.521 | 0.294 | |
| | 1D-1P | 0.184 | 0.194 | 0.240 | 0.23 |
| | 1S-1P | 0.617 | 0.652 | 0.237 | 0.27 |
| 2s2p ³ -2p ⁴ | 3D-3P | 0.132 | | 0.166 | |
| | 3P-3P | 0.112 | | 0.055 | |
| | 1D-1D | 0.233 | | 0.262 | |
| | 1P-1D | 0.096 | | 0.060 | |
| | 3S-3P | 0.202 | | 0.253 | |
| 2p ² -2p3s | 3P-3P | 0.074 | 0.094 | 0.083 | 0.075 |
| | 1P-1P | 0.070 | 0.088 | 0.041 | 0.064 |
| | 1S-1P | 0.062 | 0.078 | 0.150 | |
| 2p ² -2p3d | 3P-3D | 0.487 | 0.448 | 0.471 | |
| | 3P-3P | 0.163 | 0.155 | 0.160 | |
| | 1D-1D | 0.091 | 0.085 | 0.161 | |
| | 1D-1F | 0.524 | 0.494 | | |
| | 1D-1P | 0.006 | 0.006 | 0.002 | |
| | 1S-1P | 0.566 | 0.531 | 0.616 | |
| | 3P-3D | 0.340 | | 0.346 | 0.39 |
| 2p3s-2p3p | 3P-3S | 0.077 | | 0.072 | 0.082 |
| | 3P-3P | 0.288 | | 0.276 | 0.28 |
| | 1P-1P | 0.139 | | 0.145 | 0.15 |
| | 1P-1D | 0.489 | | | 0.51 |
| | 1P-1S | 0.123 | | | 0.13 |
| | 3D-3F | 0.493 | | | 0.51 |
| 2p3p-2p3d | 3P-3D | 0.349 | | | 0.42 |
| | 3D-3D | 0.096 | | 0.089 | 0.097 |
| | 3P-3P | 0.124 | | 0.104 | 0.14 |
| | 3S-3P | 0.614 | | | 0.59 |
| | 1D-1F | 0.413 | | | 0.41 |
| | 1P-1D | 0.458 | | 0.419 | 0.59 |
| | 1P-1P | 0.203 | | 0.160 | 0.19 |

^aParametric potential method

^bSingle-configuration SCF calculations (Cowan and Griffin 1976)

^cLuo et al.(1989)

^dSmith and Wiese (1971)

As mentioned earlier, inner shell excitations are important in opacity calculations (e.g., Iglesias and Rogers 1991a). Figure 1 shows a comparison of parametric potential results and experimental ionization energies for the 2s electron as a function of atomic number for neutral atoms. The errors are within 5% and tend to improve for charged ions.

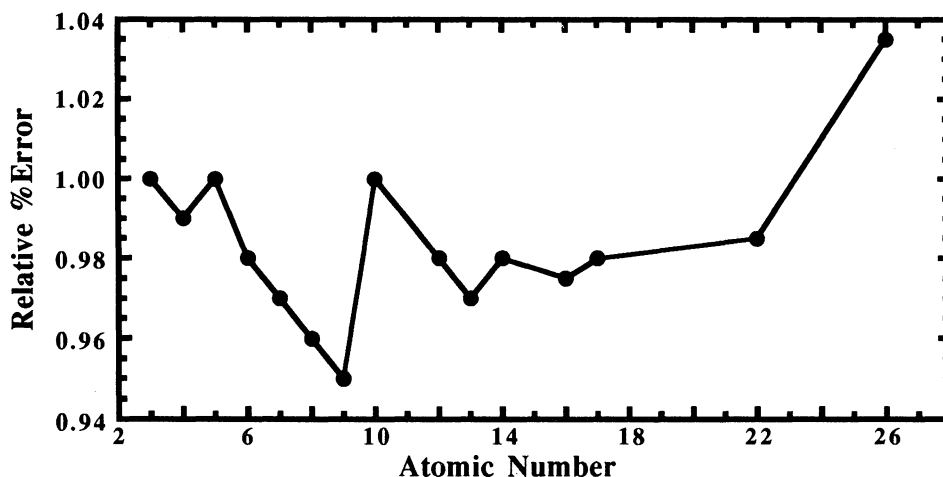


Fig. 1 --- Comparison OPAL and experimental 2s electron ionization energies for neutral atoms.

Comparisons are offered in Table 5 for sodium-like iron, except now the comparisons are to the relativistic SCF code by Grant, McKenzie, Norrington, Mayers, and Pyper (1980). Sodium-like systems are not complicated by configuration term structure and the results for the transition strengths reflect the quality of the one-electron wave functions in an element with higher atomic number.

TABLE 5
Transition Energies and Oscillator Strengths for Sodium-Like Iron.

| Transition | Energy (eV) | | | f value | |
|------------|-------------|------------------|-------------------|------------------|-------------------|
| | Experiment | SCF ^a | OPAL ^b | SCF ^a | OPAL ^b |
| 3s-3p | 36.1 | 35.7 | 34.6 | 0.397 | 0.376 |
| 3s-4p | 246 | 245 | 245 | 0.217 | 0.229 |
| 3s-5p | 337 | 336 | 336 | 0.067 | 0.070 |
| 3p-3d | 47.9 | 48.4 | 48.4 | 0.286 | 0.286 |
| 3p-4s | 195 | 195 | 196 | 0.065 | 0.063 |
| 3p-4d | 227 | 227 | 228 | 0.308 | 0.307 |
| 3p-5s | 294 | 294 | 295 | 0.0128 | 0.0125 |
| 3p-5d | 310 | 308 | 310 | 0.098 | 0.098 |
| 3d-4p | 162 | 162 | 162 | 0.040 | 0.041 |
| 3d-4f | 187 | 186 | 187 | 0.925 | 0.930 |
| 3d-5p | 253 | 253 | 253 | 0.0064 | 0.0066 |
| 3d-5f | 266 | 264 | 266 | 0.170 | 0.171 |
| 4s-4p | 14.4 | 14.4 | 14.7 | 0.573 | 0.545 |
| 4s-5p | 106 | 106 | 105 | 0.230 | 0.242 |
| 4p-4d | 17.5 | 17.7 | 18.1 | 0.452 | 0.464 |
| 4p-5s | 84.1 | 84.6 | 84.8 | 0.110 | 0.107 |
| 4p-5d | 99.8 | 99.2 | 100 | 0.266 | 0.258 |
| 4d-4f | 7.4 | 7.3 | 7.2 | 0.110 | 0.102 |
| 4d-5p | 73.8 | 73.8 | 73.4 | 0.089 | 0.092 |
| 4d-5f | 86.0 | 85.8 | 85.6 | 0.724 | 0.725 |

^aGrant et al. (1980)

^bParametric potential

We present results for configuration level energies of Fe XII in Table 6. Here, the comparison is to experimental data and to the close-coupling calculations. Again the parametric potential energies are in reasonable agreement with the close-coupling results as well as experiment.

TABLE 6
Configuration Term Energies for Fe XII^a

| Configuration | Term | Close-Coupling ^b | OPAL ^c | Experiment ^d | |
|---|-----------------------------------|-----------------------------|-------------------|-------------------------|--|
| 3s ² 3p ³ | 4S ^o | 0. | 0. | 0. | |
| | 2D ^o | 0.4194 | 0.4258 | 0.4034 | |
| | 2P ^o | 0.6868 | 0.7097 | 0.7142 | |
| 3s3p ⁴ | 4P | 2.4023 | 2.399 | 2.551 | |
| | 2D | 2.9816 | 3.180 | 3.108 | |
| | 2P | 3.5080 | 3.893 | 3.551 | |
| | 2S | 3.6005 | 3.606 | 3.591 | |
| 3s ² 3p ² (³ P)3d | 4F | 3.9468 | 4.032 | | |
| | 2F | 4.0760 | 4.174 | | |
| | 4D | 4.0799 | 4.178 | | |
| (1D)3d | 2G | 4.5221 | 4.568 | | |
| | (³ P)3d | 2P | 4.6024 | 4.212 | |
| (1D)3d | 4P | 4.7135 | 4.574 | 4.694 | |
| | 2D | 4.8597 | 4.703 | 4.860? | |
| | 2D | 5.0773 | 5.009 | 5.052 | |
| | 2S | 5.2866 | 5.129 | 5.282 | |
| | 2P | 5.2996 | 5.186 | 5.238 | |
| | 2F | 5.3317 | 5.373 | | |
| 3s3p ³ (⁵ S ^o)3d | 6D ^o | 5.4969 | 5.548 | | |
| 3s ² 3p ² (¹ S)3d | 2D | 5.5343 | 5.546 | 5.509? | |
| 3p ⁵ | 2P | 5.6089 | 5.651 | | |
| 3s3p ³ (³ P ^o) | 4D ^o | 6.0238 | 6.196 | | |
| | 2S ^o | 6.4234 | 6.780 | | |
| | 4G ^o | 6.4368 | 6.626 | | |
| | 2G ^o | 6.6732 | 6.984 | | |
| | (⁵ S ^o)3d | 4D ^o | 6.8781 | 6.983 | |
| | (³ P ^o)3d | 2D ^o | 6.8916 | 7.049 | |
| | | 4F ^o | 6.9284 | 6.760 | |
| | | 4P ^o | 7.0499 | 7.046 | |
| | | 4S ^o | 7.0623 | 7.337 | |
| | | 2P ^o | 7.3136 | 7.121 | |
| | 2F ^o | 7.4177 | 7.543 | | |

^aThe ? indicate questionable term assignment from experiment

^bSeaton (private communication ,1991)

^cParametric potential

^dNBS tables

Finally, in Fig. 2 we compare the photoionization cross section from neutral sodium to the results from Weisheit (1972) which agreed well with experiments. Clearly, the parametric potential reproduces the so-called Cooper minimum. It also reproduces the high energy cross section very well. The good agreement suggests that the scattering wave functions from the parametric potential method are reasonably accurate, in particular when considering that the present case is a neutral atom.

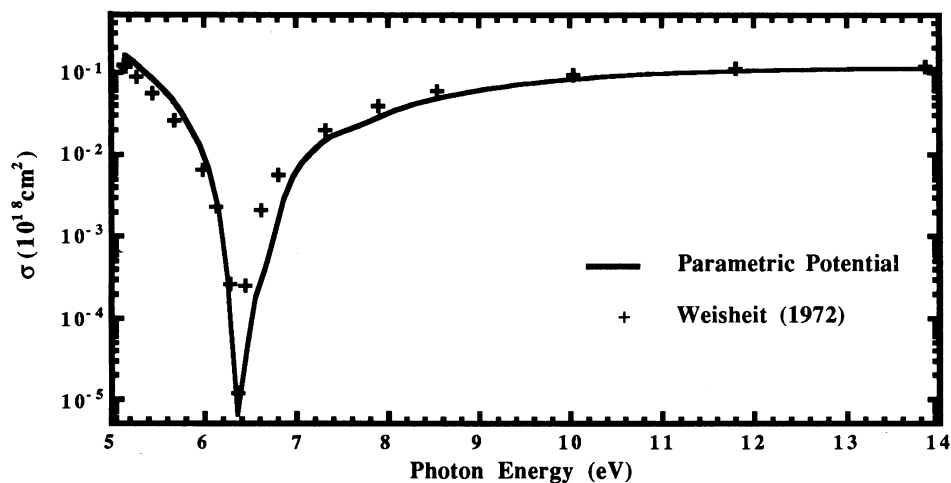


Figure 2 --- Photoionization cross section of 3s electron in neutral sodium

Before closing the Section, we remind the reader that autoionizing lines are included in the OPAL opacity calculations. What is ignored is the interference effects present in calculations with configuration interaction. That is, after combining the photoionization cross sections from all possible configurations, the single configuration calculation will approximately reproduce the resonant structure of close-coupling calculations, but it can not reproduce the correct shape of those resonances (the Fano profiles). However, the close-coupling results are for isolated atoms which ignores any possible density effects such as plasma electric fields. The latter may have a pronounced effect on the very sensitive interference processes (e.g., Kelleher (1989), Gallagher and Jones (1989), Rzazewski *et al.* 1989)

IV. CONCLUSIONS

We have reviewed a parametric potential method for generating atomic data necessary in astrophysical equation of state and radiative opacity calculations. The effective potentials are analytic and consist of a Yukawa term for each occupied shell in a parent configuration plus a long-ranged Coulomb tail. The screening parameters were obtained by iteratively solving a spin-averaged Dirac equation until the ground-state eigenvalue matched the experimental configuration-averaged ionization energy.

An important feature of the method is that the screening parameters were fitted by a simple function and are available for all ion stages of elements through the zinc isoelectronic sequence. It is also important to note that the parametric potentials can be scaled for treating multiply excited configurations and inner shell excitations necessary in opacity calculations.

The results were compared to experiments and atomic structure codes. For the configuration-averaged energies, the agreement with respect to experiment is better than a few percent. The configuration level structure, oscillator strengths, and photionization cross sections are comparable in accuracy to single-configuration, SCF calculations with relativistic corrections.

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