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Accurate model-potential methods for the prediction of energy spectra and oscillator strengths in one- and two-valence-electron atomic systems

ABSTRACT

Model-potential methods which include long-range polarisation terms are briefly reviewed. Transition wavelengths and oscillator strengths for dipole allowed transitions in some one- and two-valence-electron ions are presented. An alternative form of the dipole operator for use with the Coulomb approximation is introduced. Fine-structure splittings and intercombination transitions are also considered.

INTRODUCTION

Transition wavelengths and oscillator strengths are fundamental quantities in atomic spectroscopy and are essential for the interpretation of solar and stellar spectra and for diagnostic spectroscopy of fusion plasmas. Accurate experimental measurements of oscillator strengths are not usually available, and thus there is a great need for precise theoretical values.

Model-potential methods, in which the effects of the core electrons of an atomic system are represented by effective operators, present an attractive approach for describing the valence-electron properties (such as energy spectra and transition rates) of few-valence-electron systems. By explicitly including only the optical electrons in the calculations they simplify the computational tasks dramatically and, in favourable cases, they provide highly accurate results. They also provide a simple physical picture of the system.

An extensive number of model-potential approaches have been employed and it is not our intention to review these here (see Hibbert (1982) and Laughlin and Victor (1988) for recent reviews). Instead we concentrate on our approach to the problems of predicting transition wavelengths and oscillator strengths in alkali- and alkaline-earth-like systems and illustrate the high accuracy that may be achieved. But first we revisit the simplest model-potential method, the Coulomb approximation, which has been widely used to calculate oscillator strengths since the early applications to lithium and sodium by Trumpy (1930) and to a variety of one- and two-electron systems by Bates and Damgaard (1948).

THE COULOMB APPROXIMATION FOR OSCILLATOR STRENGTHS

For a one-valence-electron ion consisting of a nucleus of charge Z and $N+1$ electrons, the optical electron is considered to move in the Coulomb potential $(Z-N)/r$ with energy E, where $-E$ is the experimental ionisation potential. Because the wave functions thus determined are irregular at the origin, they are set equal to zero close to the nucleus, say $0 \leq r \leq r_c$, and the length form $\mathbf{r}$ of the electric dipole operator is used to emphasise the asymptotic region far from the nucleus where the approximation should be good. For the method to be successful in practice it is clear that dipole matrix elements should not be sensitive to the choice of r_c. An interesting question is: can we find a form of the electric dipole operator which has longer range than the length form $\mathbf{r}$? One such form may be derived quite simply from the commutator

$$[H, r^2\mathbf{r}] = -2\mathbf{r} - r\nabla r - 2\mathbf{r}\frac{\partial}{\partial r}r \qquad (1)$$

which gives (Laughlin, 1989a)

$$\langle\psi_1|\mathbf{r}|\psi_2\rangle = \langle r\psi_1|\mathbf{b}|r\psi_2\rangle, \qquad (2)$$

where

$$\mathbf{b} = -\tfrac{1}{2}\left[(E_1-E_2)\mathbf{r} + \nabla + 2\hat{\mathbf{r}}\frac{\partial}{\partial r}\right]. \qquad (3)$$

When ψ_1 and ψ_2 are approximate wave functions, $\langle\psi_1|\mathbf{r}|\psi_2\rangle$ will *not* be equal to $\langle r\psi_1|\mathbf{b}|r\psi_2\rangle$ and the latter expression apparently provides an attractive alternative long-range form of the dipole operator for use with Coulomb wave functions. In practice, however, no real advantage seems to be gained with this formulation. In fig. 1 we show how the 3d–4p transition matrix element for the sodium atom varies with r_c. Generally, there is little to choose between $\mathbf{r}$ and $r\mathbf{b}r$ as far as sensitivity to r_c is concerned. A problem with $r\mathbf{b}r$ is that it is not Hermitian and, in fact, the mean of $\langle r\psi_1|\mathbf{b}|r\psi_2\rangle$ and $\langle r\psi_2|\mathbf{b}|r\psi_1\rangle^*$ is $\langle\psi_1|\mathbf{r}|\psi_2\rangle$, even for approximate (differentiable) wave functions ψ_1 and ψ_2.

FORM OF THE MODEL POTENTIAL

Many forms of model potential have been used in practice (see, for example, Hibbert (1982) and Szasz (1985), and references therein). Our formulation (Laughlin *et al*, 1978, Fairley and Laughlin, 1984) is based on a core potential derived from Hartree-Fock orbitals plus long-range polarisation terms. For a 1-valence-electron system the model Schrödinger equation is

$$\left(-\tfrac{1}{2}\nabla^2 + V_M\right) = \varepsilon_{nl}\phi_{nl}, \qquad (4)$$

where, in atomic units,

$$V_M = -\frac{Z}{r} + V_{HF} - \frac{\alpha_d}{2r^4}W_1\left(\frac{r}{r_c}\right) + U(r). \qquad (5)$$

Here, α_d is the static dipole polarisability of the core (quadrupole and dynamical correction terms may also be

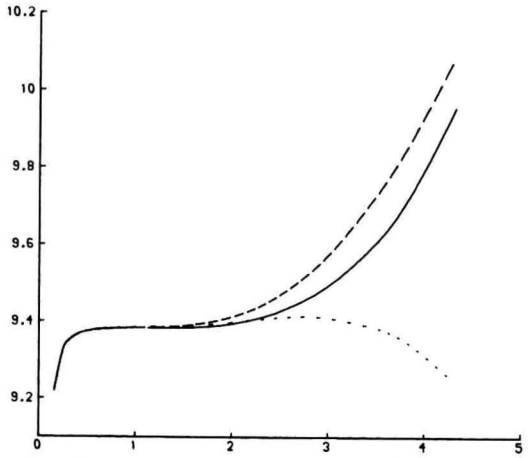

Fig. 1. Variation of the sodium atom 3d–4p transition matrix element (vertical axis) with the cut-off radius r_c for the Coulomb wave functions (horizontal axis) calculated with various dipole operators: ——————— $\mathbf{r}$; - - - - - - - $r\mathbf{b}r$; ——————— $r\mathbf{b}^{\dagger}r$.

included; see, for example, Peach (1983)) and the polarisation potential $\alpha_d/2r^4$ is cut off for small r by the function $W_1(r/r_c)$, where r_c is an effective core radius. $U(r)$ is a short-range correction chosen empirically so that the eigenvalues ε_{nl} of equation (1) give very precise values for the observed ionisation energies. If the Hartree-Fock core potential V_{HF} contains only the static interactions with the fixed Hartree-Fock core orbitals then V_M is a local potential, whereas if exchange terms are included in V_{HF} then V_M will be non-local. Higher accuracy is achieved when a non-local potential is employed.

For a 2-valence-electron system we adopt the equation

$$\left[-\tfrac{1}{2}\nabla_1^2-\tfrac{1}{2}\nabla_2^2+V_M(1)+V_M(2)+\frac{1}{r_{12}} - \frac{\alpha_d}{r_1^2 r_2^2}P_1(\hat{\mathbf{r}}_1\cdot\hat{\mathbf{r}}_2)W_2\left(\frac{r_1}{r_c},\frac{r_2}{r_c}\right)\right]\Psi = E\Psi, \qquad (6)$$

where the final term in the square brackets is the so-called "dielectric" term (Chisholm and Öpik, 1964) modified by a cut-off function W_2. The eigenfunctions Ψ and eigenvalues E of equation (6) are calculated variationally by expanding Ψ in terms of properly anti-symmetrised and angular-momentum coupled products of the 1-electron functions ϕ_{nl} of equation (4).

POLARISATION CORRECTIONS TO THE DIPOLE OPERATOR

Consider an electric dipole transition between 2 states with model-potential wave functions Ψ_a and Ψ_b, each of which satisfy equation (6). In lowest order in the valence electron–core electron interaction, the dipole matrix element is $\langle\Psi_a|\mathbf{r}_1+\mathbf{r}_2|\Psi_b\rangle$. Since a dipole moment is induced on the core by the valence electrons a corrected dipole operator $\mathbf{d}_1+\mathbf{d}_2$ replaces $\mathbf{r}_1+\mathbf{r}_2$, where

$$\mathbf{d} = \mathbf{r}\left(1-\frac{\alpha_d(\omega)}{r^3}\right), \qquad (7)$$

$\alpha_d(\omega)$ being the dipole polarisability of the core at the transition frequency $\omega = |E_a - E_b|$ (Bersuker, 1957; Hameed *et al*, 1968). It has recently been shown (Laughlin, 1989b) that the next correction to $\mathbf{r}$ is of order r^{-6} and can be written in terms of the dipole-quadrupole interaction $\nabla\frac{1}{r}\cdot\nabla\nabla\frac{1}{r}$. This latter correction has not yet been included in any actual calculations.

OSCILLATOR STRENGTH RESULTS

Rather few oscillator strengths are known to high accuracy, even for the relatively simple alkali-like systems. For Li and Na, however, Gaupp *et al* (1982) have carried out precise beam-laser measurements on the resonance transitions and we can use these experimental values as a check on the accuracy of the model-potential calculations. Some comparisons are presented in Table 1. It may be observed that the model-potential values calculated with the corrected form of the dipole operator (equation (7)) are very close to the measured values, though they fall outside the experimental error bars of Gaupp *et al* (1982). We note that this discrepancy also exists for other recent theoretical values (Froese Fischer, 1988). The Coulomb approximation also provides reliable values.

Accurate data are also available in the helium isoelectronic sequence of ions (Schiff *et al*, 1971; Kono and Hattori, 1984). The excited states of these systems may be treated in the model-potential framework by constructing an effective potential to represent the *K*-shell electron and it has been found that model-potential oscillator strengths for triplet transitions in ions up to Ne IX agree to better than 1% with the very extensive *ab initio* calculations of Schiff *et al* (1971) and Kono and Hattori (1984), even for weak transitions. Some specimen results are also included in Table 1.

Turning now to 2-valence-electron systems, where accurate solution of equation (6) is more difficult, the situation is less favourable. However, the evidence suggests that reliable oscillator strength values can be obtained with model-potential methods without undue computational effort. As examples, we present some specimen results for beryllium sequence ions in Table 2. Results are also available for the magnesium sequence (Victor *et al*, 1976a), the calcium sequence (Victor *et al*, 1976b) and the copper and zinc sequences (Victor and Taylor, 1983).

In the case of the $2s^2\,{}^1S - 2s2p\,{}^1P^o$ resonance transitions in the beryllium sequence, agreement between the model-potential values and the results of Reistad and Martinson (1986), obtained by an isoelectronic smoothing of available reliable experimental data, is good. The largest discrepancy (5%) occurs for B II and only for this ion does the predicted value lie outside the error bars derived

Table 1. Comparison of model-potential oscillator strengths with other values.

System	Transition	Oscillator strength			
		Model potential†		Other	Coulomb approximation
		(1)	(2)		
Li	2s ^{2}S - 2p ^{2}P^o	0.7536	0.7471	0.7416±0.0012[a], 0.7480[b]	0.763
Na	3s ^{3}S - 3p ^{3}P^o	0.9784	0.9572	0.9536±0.0016[a], 0.9714[b]	0.981
Li^+	2s ^{3}S - 2p ^{3}P^o	0.3091	0.3083	0.3080[c]	0.303
Li^+	2p ^{3}P^o - 3d ^{3}D	0.6258	0.6241	0.6247[d]	0.618
Be^{2+}	2s ^{3}S - 3p ^{3}P^o	0.2505	0.2517	0.2526[c]	0.248
C^{4+}	2p ^{3}P^o - 3s ^{3}S	0.06730	0.06789	0.06784[c]	0.0671
C^{4+}	2p ^{3}P^o - 4s ^{3}S	0.01377	0.01395	0.01396[c]	0.0144

†Column (1) is calculated with the dipole length operator **r**; column (2) includes a core polarisation correction (see equation (7) of text).
[a]Gaupp *et al* (1982); [b]Froese Fischer (1988); [c]Schiff *et al.* (1971) ; [d]Kono and Hattori (1984).

Table 2. Wavelengths and oscillator strengths for beryllium-like ions.

Ion	Transition	Wavelength (Å)	Oscillator strength	
			Model potential	Experiment
Be I	$2s^2$ ^{1}S – 2s2p ^{1}P^o	2349.3	1.372	1.341±0.047[a]
B II	$2s^2$ ^{1}S – 2s2p ^{1}P^o	1362.5	1.012	0.965±0.020[a]
C III	$2s^2$ ^{1}S – 2s2p ^{1}P^o	977.0	0.764	0.754±0.014[a]
	2s2p ^{1}P^o – 2s3s ^{1}S	690.5	0.021	0.022±0.002[b]
N IV	$2s^2$ ^{1}S – 2s2p ^{1}P^o	765.1	0.614	0.620±0.014[a]
	2s2p ^{3}P^o – 2s3d ^{3}D	283.5	0.625	0.602±0.060[c]
	2s3p ^{3}P^o – 2s3d ^{3}D	7117.0	0.143	0.127±0.041[c]
	2s2p ^{1}P^o – 2s3d ^{1}D	335.1	0.541	0.477±0.052[c]
	2s3s ^{3}S – 2s3p ^{3}P^o	3481.0	0.578	0.125±0.048[c]
O V	$2s^2$ ^{1}S – 2s2p ^{1}P^o	629.7	0.513	0.527±0.014[a]
	$2s^2$ ^{1}S – 2s3p ^{1}P^o	172.2	0.406	0.373±0.041[c]
	2s2p ^{3}P^o – 2s3d ^{3}D	192.9	0.657	0.576±0.075[c]
	2s3p ^{1}P^o – 2s3d ^{1}D	3144.7	0.227	0.469±0.122[c]
	2s2p ^{1}P^o – 2s3d ^{1}D	220.4	0.544	0.510±0.066[c]
	2s3s ^{1}S – 2s3p ^{1}P^o	5114.1	0.210	0.318±0.079[c]
Ne VII	2s3s ^{3}S – 2s3p ^{3}P^o	1987.0	0.380	0.781±0.063[c]

[a]Reistad and Martinson (1986); [b]Ishii *et al* (1985); [c]Lang *et al* (1987).

by Reistad and Martinson (1986). We observe that the model-potential and configuration-interaction (Hibbert (1974), Serrão (1986)) oscillator strengths for this transition are in harmony and are discrepant with Reistad and Martinson's value.

A comparison of our N IV, O V and Ne VII results with the experimental results of Lang *et al* (1987) reveals some puzzling features. For some transitions there is good agreement, whilst for others there are large discrepancies. The experimental method measured branching ratios and employed beam-foil lifetime measurements of the common upper level to deduce transition probabilities. Errors in the lifetime measurements would clearly lead to unreliable transition probabilities, and this may partly explain some of the discrepancies. However, there are situations where experimental and theoretical branching ratios differ significantly, for example, the experimental and theoretical branching ratios for the 2s3p ^{1}P°–2s3d ^{1}D and 2s2p ^{1}P°–2s3d ^{1}D transitions in O V are, respectively, $4.41.10^{-3}$ and $2.05.10^{-3}$. The discrepancy here does not arise from cancellation effects in the dipole matrix elements (neither oscillator strength is small) and, in fact, all recent theoretical calculations are in good accord.

Relative oscillator strengths for lines of neutral calcium absorbed from the 4s4p ^{1}P° level have recently been measured by Smith (1988) and in Table 3 we compare these with the model-potential values. The agreement between the two sets of results is, on the whole, reasonable. A large discrepancy occurs for the weak 4s4p ^{1}P°–4s6s ^{1}S transition which is severely affected by cancellation effects in the dipole matrix element. This transition has also been studied by Froese Fischer and Hansen (1985) and their oscillator strength, 0.001, does not agree with either of the values in Table 3, though it is intermediate between them.

Table 3. Absorption oscillator strengths from the level 4s4p ^{1}P° of neutral calcium.

	Oscillator strength	
Upper level	Model potential	Experiment[a]
4s5s ^{1}S	0.143	0.160
4s6s ^{1}S	0.0003	0.0089
4p^2 ^{1}S	0.113	0.115
4s7s ^{1}S	0.0152	0.0133
4s4d ^{1}D	0.254	0.207
4p^2 ^{1}D	0.594	0.580
4s5d ^{1}D	0.353	0.281

[a] Smith (1988).

QUARTET LEVELS OF LITHIUM-LIKE IONS

Core-excited 1s2s*nl* ^4L and 1s2p*nl* ^4L levels of 3-electron ions have been actively investigated by both experimental and theoretical groups in recent years. These levels are readily populated by foil excitation and, as they are metastable against Coulomb autoionisation, optical emission spectra can readily be observed and radiative lifetime measurements may be performed. Various theoretical approaches have been employed, including model-potential (see, for example, Laughlin (1988) and references therein). The quartet term system of N V has recently been investigated by beam-foil spectroscopy (Blanke *et al*, 1987; Garnir *et al*, 1988) and by charge exchange in a gas cell (Bouchama *et al*, 1988) but there is a paucity of theoretical data, so we now present some results in Table 4 for this system.

The identifications proposed by Blanke *et al* (1987), Garnir *et al* (1988) and Bouchama *et al* (1988) for wavelengths shorter than 230 Å are confirmed by the present model-potential calculations and the wavelength predictions of Chung (Baudinet-Robinet *et al*, 1986). Garnir *et al* (1988) observed a line at 633.18 Å which they assigned to the 1s2p3d ^{4}F°–1s2p4f ^{4}G transition in N V. However, our wavelength for this transition is 675.01 Å, and we would therefore propose that the observed line arises from 1s2p3p ^{4}D–1s2p4d ^{4}F°. Garnir *et al* (1988) also observed a line of medium intensity at 672.88 Å which they assigned to 1s2p3d ^{4}F°–1s2p4f ^{4}F, and a weak blended line at 673.90 Å which they assigned to 1s2s3d ^{4}D–1s2s4f ^{4}F°. Our results (Table 4) suggest that these assignments should be interchanged. If this suggestion is correct then it is puzzling that the 1s2p3d ^{4}F°–1s2p4f ^{4}G line has not been observed in the beam-foil spectrum. The model-potential transition probabilities indicate that the 445.60 Å line should probably be assigned to 1s2s3p ^{4}P°–1s2s5d ^{4}D, rather than to 1s2p3p ^{4}D–1s2p5d ^{4}D°.

FINE-STRUCTURE SPLITTINGS AND INTERCOMBINATION TRANSITIONS

We parameterise the spin-orbit interaction $V_{so}^{(1)}$ as

$$V_{so}^{(1)} = \tfrac{1}{2}\alpha^2 Z_f \frac{\boldsymbol{l}\cdot\boldsymbol{s}}{r^3}, \qquad (8)$$

where α is the fine-structure constant and Z_f is determined empirically so that $V_{so}^{(1)}$ reproduces the observed fine-structure splittings of the $j = l \pm \frac{1}{2}$ levels of the 1-electron ion. The effective nuclear charge Z_f depends on the angular momentum l but, for fixed l, it varies very little with the principal quantum number n (Weisheit and Dalgarno, 1971). For 2-valence-electron ions we also include the spin-own-orbit and spin-spin interactions (Bethe and Salpeter, 1971) in the fine-structure Hamiltonian H_1. For ions near the neutral end of an isoelectronic sequence, H_1 is small and may be treated as a perturbation. Some calculated and observed fine-structure splittings for triplet terms of 2-valence-electron ions are presented in Table 5. It may be observed that the errors

Table 4. Wavelengths and transition probabilities in the quartet spectrum of N V.

Transition	Wavelength (Å)					Transition probability (10^{-8} s^{-1})
	Model potential	Chung	Garnir *et al* (1988)	Blanke *et al* (1987)	Bouchama *et al* (1988)	
1s2s2p ^{4}P° – 1s2s4d ^{4}D	151.4	151.43	151.50	151.58	151.5	238.4
1s2p^2 ^{4}P – 1s2p4d ^{4}D°	160.0	159.84	159.84	159.82	159.7	293.8
1s2s2p ^{4}P° – 1s2s3d ^{4}D	193.4	193.52	193.54	193.50	193.6	760.9
1s2p^2 ^{4}P – 1s2p3d ^{4}P°	202.5	202.38	202.40	202.41	202.4	412.1
1s2s2p ^{4}P° – 1s2s3s ^{4}S	211.0	211.13	211.10	211.11	211.1	177.5
1s2p3p ^{4}D – 1s2p5d ^{4}D°	445.4		445.60			5.6
1s2s3p ^{4}P° – 1s2s5d ^{4}D	445.6					21.8
1s2s3s ^{4}S – 1s2s4p ^{4}P°	555.1				555.4	17.1
1s2p3s ^{4}P° – 1s2p4p ^{4}D	595.0		594.96			18.4
1s2s3p ^{4}P° – 1s2s4d ^{4}D	626.0	625.43	626.01			45.1
1s2p3p ^{4}D – 1s2p4d ^{4}F°	633.7					46.4
1s2s3d ^{4}D – 1s2s4f ^{4}F°	673.1	673.01	673.90			92.8
1s2p3d ^{4}F° – 1s2p4f ^{4}F	673.5	672.61	672.88			14.4
1s2p3d ^{4}F° – 1s2p4f ^{4}G	675.0		633.18			84.9

in the predicted values are usually less than 5%, thus validating our representation of H_1.

Table 5. Calculated (Δ^c) and observed (Δ^o) fine-structure splittings (cm^{-1}) for triplet terms of 2-valence-electron ions.

Ion	Term	0 — 1		1 — 2	
		Δ^c	Δ^o	Δ^c	Δ^o
C III	2p3s ^{3}P°	33.4	33.3	68.1	68.6
C III	2p3d ^{3}P°	−14.3	−14.5	−25.4	−26.3
O V	2p^2 ^{3}P	159.8	155.7	279.6	268.8
Mg I	3s3p ^{3}P°	20.3	20.1	41.3	40.7
Mg I	3s4p ^{3}P°	3.46	3.30	7.03	6.75
Si III	3s3p ^{3}P°	132.1	128.6	267.2	261.7
Si III	3p^2 ^{3}P	132.0	133.5	261.5	258.5
S V	3p^2 ^{3}P	383.0	362.0	775.0	767.0
Ca I	4s4p ^{3}P°	53.2	52.2	106.6	105.9
Ca I	4s4d ^{3}P°	4.14	3.67	6.24	5.58

Intercombination transitions, such as 3s^2 ^{1}S$_0$ – 3s3p ^{3}P$_1^o$ in magnesium-like ions, arise from the mixing of singlet and triplet levels, for example, 3s3p ^{3}P$_1^o$ with 3s3p ^{1}P$_1^o$ and 3s^2 ^{1}S$_0$ with 3p^2 ^{3}P$_0$, by the fine-structure Hamiltonian H_1. The model-potential results for 3s^2 ^{1}S$_0$ – 3s3p ^{3}P$_1^o$ transitions in selected ions of the magnesium sequence (Laughlin and Victor, 1979) are compared with recent theoretical and experimental values in Table 6.

Table 6. 3s^2 ^{1}S$_0$ – 3s3p ^{3}P$_1^o$ intercombination transition wavelengths (λ) and oscillator strengths (f) for magnesium sequence ions.

Ion	λ (Å)	f (10^{-5})		
		Model potential	Other theory	Experiment
Mg I	4572.4	0.211		0.206 ± 0.029[a]
Al II	2669.2	1.10	1.12[b]	1.07 ± 0.07[c]
Si III	1892.0	2.85	2.67[d]	2.67 ± 0.16[e]
S V	1204.4	10.6	11.1[f]	

[a] Kwong *et al* (1982); [b] Hibbert and Keenan (1987); [c] Johnson *et al* (1986); [d] Ojha *et al* (1988); [e] Kwong *et al* (1983); [f] Dufton *et al* (1986).

The agreement obtained is most satisfactory. For Si III,

the model-potential value lies just outside the experimental error bars of Kwong *et al* (1983). It has been pointed out by Ojha *et al* (1988) that our oscillator strength is probably too large by approximately 4.6% since we overestimate the fine-structure splitting in this case by about 2.3%. We have used experimental singlet-triplet energy separations in our perturbation calculations of $^3P_1^o - {}^1P_1^o$ and $^1S_0 - {}^3P_0$ mixings, but have preferred to use without modification the prescription given by equation (8) for $V_{so}^{(1)}$, with Z_f determined as described previously.

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