Simulation of atomic transition arrays for opacity calculations

J. Bauche, C. Bauche-Arnoult, and J.-F. Wyart
Laboratoire Aimé Cotton, Bâtiment 505, 91405 Orsay, France

P. Duffy
Lawrence Livermore National Laboratory, Livermore, California 94550

M. Klapisch
Lawrence Berkeley Laboratory, Berkeley, California 94720
(Received 25 June 1991)

A method is proposed for simulating resolved transition arrays of ionized atom spectra in full intermediate coupling. The wave number and intensity of each line in an array are picked at random from separated but correlated distributions. Even though each line is not exactly reproduced, this procedure yields the correct following characteristics of the supposedly symmetric array: total intensity; second and fourth moments of the distributions of unweighted wave numbers, of intensity-weighted wave numbers, and of transition amplitudes; numbers of lines and sums of intensities in consecutive narrow energy ranges. All the parameters of the distribution are obtained by means of compact formulas, or tabulated. Applications to the arrays $4d^4$-$4d^3 5p$ of Pd^{6+} and $4d^7 5s$-$4d^7 5p$ of Cd^{4+} are presented. Comparison with the explicit results of the Slater-Condon method shows good agreement. It is proposed to use this method for fast and reliable computation of Rosseland means and other opacity properties.

PACS number(s): 32.70.−n, 97.10.Ex, 52.25.−b

I. INTRODUCTION

The computation of bound-bound transition contributions to opacities in hot plasmas has long been recognized as a major problem in computations of radiation transfer and plasma equilibrium, for instance, for stellar atmospheres [1,2]. The problem is essentially computational. In principle, accurate and detailed calculations of relevant energy levels and transition probabilities are not impossible. However, for atomic ions of astrophysical interest in local thermodynamic equilibrium (LTE), the number of individual (level-to-level) transitions can amount to millions. Considerable computational and theoretical efforts [3–5] are invested in such calculations. Many involve some kind of approximation like an average atom model [6], pure *LS* coupling [7,8], or use of an experimental database [9]. It turns out that the results depend critically on the amount of details in the atomic model used in these computations. For instance, equilibrium properties of Cepheid stars are very sensitive to the way the opacities of Fe and Ni ions in the plasma are calculated [10].

For heavier ions in laboratory plasmas possessing open *d* or *f* subshells the number of levels is even greater, and detailed calculations of each energy level are plainly impractical, even with the most powerful computers available. Therefore it would be extremely useful to find an approximation which would circumvent the exact computation of energy levels and transition probabilities, but would keep the level of detail required for the opacity problem.

One approach would be to use the unresolved-transition-array (UTA) [11] model. Here, each configuration-to-configuration transition array is treated as a single broad unresolved feature. The first few moments in a Gram-Charlier–type expansion [12] of these features can be calculated very quickly by compact formulas, without resorting to the detailed calculations [13,14]. This model was successfully used for the interpretation of emission spectra [15–17], because, in that case, it is useful to compare the actual spectral features, even if partially resolved, to unresolved Gaussians. A low instrumental resolving power may actually improve the comparison between UTA theory and experiment. However it was shown previously [10,18] that neglecting the resolved character of the transition arrays could lead to serious discrepancies in the computation of the Rosseland mean because the latter is sensitive to the gaps between lines. An additional difference between emission and absorption is that, in the latter, there is no "instrumental" line broadening, as far as the radiative transfer is concerned. Thus, it turns out that, for the purpose of opacity calculation, the UTA model is not as useful as for emission spectroscopy.

The aim of the present work is to formulate an approximate description of resolved transition arrays which would hopefully help solving the problem of opacity calculations. The basic idea, which is actually not new (see Ref. [1], Chap. 7, and references therein), is quite simple: Since the Rosseland mean involves some integral of the quotient of a smooth, slowly varying function over the absorption coefficient, it should not really matter if the lines of the arrays are not at their exact places as long as the correct number of lines are there, with a "proper" distribution of intensities and wave numbers.

Thus, we shall look for a way of using random numbers to *simulate in a realistic way* the energies and intensities of the transitions in an array. These, of course, will not

be exact. It is required only that some characteristics of the array may be correctly reproduced: the average wave number, the total number of lines, the array skewness and kurtosis, etc. This simulation is proposed for obtaining easy and reliable evaluations of the Planck and Rosseland means. Other authors have used random numbers [19] for opacity calculations. Our approach is different because we apply statistical ideas to the transitions themselves, for which we find some physically meaningful distribution, not to some matrix elements of the Hamiltonian.

Previous implementations of the same ideas were already reported. For a superposition of many transition arrays, the distributions of line energies and of line intensities were correctly represented by separated statistical distributions [20]. But, for a single resolved transition array, it has been shown [21] that these distributions ought to be correlated for the array to be reproduced in a satisfactory way.

In the present paper, such a model of a joint distribution is derived from phenomenological results computed for an array in full intermediate coupling and discussed (Sec. II). Its parameters can be derived from compact formulas already published (Sec. III). The application to two different arrays is presented (Sec. IV). Then, the generalization to other types of arrays is discussed (Sec. V).

This paper is concerned with distributions of lines only. The lines are supposedly infinitely narrow. Actual results of Rosseland means computations with proper line profiles are published in the following paper [22]. For the sake of simplicity, we restrict the analysis in this paper to arrays that are symmetrical and for which the shift δE (Eq. 30 of Ref. [11]) is small.

Throughout the following, the energy E of a line stands for its wave number ν', according to $E=hc\nu'$. The intensity of a line αJ-$\alpha' J'$ is replaced by its strength S, which is the square of its amplitude:

$$a=(\alpha J\|\mathbf{D}^{(1)}\|\alpha' J')\ ,$$

$\mathbf{D}^{(1)}$ being the electric dipole moment of the atom. This replacement implies that the J levels of the initial configuration are supposed to be populated proportionally to their statistical weights $2J+1$, and that the energy dependence of the transition probability over the span of the array can be neglected.

The proposed simulation is tested by comparison with detailed line-by-line calculations, obtained through explicit diagonalizations of the Hamiltonian. In the following, such detailed results are referred to as *exact*.

II. CORRELATION BETWEEN LINE ENERGIES AND INTENSITIES

The correlation between the energies of the lines and their strengths is a conspicuous phenomenon which has been presented in a previous paper [21]. It is supported by general arguments and by many examples of detailed line-by-line calculations. It may be sufficient to recall here that the FWHM of the line energy distribution is smaller, or even much smaller, when these energies are weighted by their strengths than when they are not. Many numerical examples of that property can be obtained by means of the relevant analytical formulas [13,14].

In other words, the correlation is a trend for the stronger lines to lie at energies closer to the center (of gravity) of the array than the weaker lines. This qualitative fact has not yet been represented by a general analytical formula. However, it is possible to study it in examples of line-by-line calculations.

A. Choice of an example

We have chosen a case where the statistical methods are likely to be the most appropriate. Indeed, it has been shown in fundamental papers [23–25] that the basic statistical properties of the best-known mathematical model for random matrices, the Gaussian orthogonal ensemble [26], may be spoiled by the occurrence of approximate *symmetries* in the system. What is meant by approximate symmetry is the existence of a *good* quantum number for labeling the levels in addition to *rigorous* quantum numbers like J, the total angular momentum. Such good quantum numbers in the vicinity of the Russell-Saunders coupling are S, the total spin and L, the total orbital angular momentum. In the vicinity of jj coupling, the j quantum numbers of some electrons are good quantum numbers.

For this reason we consider here configurations where both major intra-atomic interactions, namely, the interelectronic electrostatic repulsion G and the spin-orbit interaction Λ, have the same order of magnitude. More precisely, the variances of the matrix elements of both interactions ought to have nearly the same value. The expansions of these variances in terms of the energy radial integrals can be found in Refs. [13] and [14]. It is clear that this condition may not be fulfilled simultaneously in the energy variances of both configurations of a given physical array. We shall assume, as a compromise, that it is fulfilled in the sum of these variances. This sum is used in Sec. III as a fair approximation for the unweighted variance v_u of the array line energies, i.e., with unity weight for each line.

Let us consider as a good example the $4d^4$-$4d^3 5p$ transition array in the Pd^{6+} spectrum. It has the additional advantage that it is quite symmetrical, and that δE is small. The values of the relevant energy radial integrals used here are listed in Table I. These are Hartree-Fock values, corrected by scaling factors (Ref. [27], p. 623) close to unity.

B. Functional shape of the correlation

To determine the shape of the correlation, one can apply the following procedure to the *exact* energy and amplitude values of the lines, obtained by means of the Slater-Condon method. The exact energies are distributed into consecutive ranges of equal widths on both sides of the average energy $E_{\rm av}$. Because this array is nearly symmetrical, with a skewness coefficient $\alpha_3=-0.50$, two ranges symmetrical with respect to $E_{\rm av}$ can be combined

TABLE I. Values of the parameters used for the diagonalization of the $4d^4$-$4d^3 5p$ array in the Pd^{6+} spectrum, in cm^{-1}.

	$4d^4$	$4d^3 5p$
$F^2(4d,4d)$	73 800	76 300
$F^4(4d,4d)$	50 500	52 700
$F^2(4d,5p)$		30 323
$G^1(4d,5p)$		10 000
$G^3(4d,5p)$		8 020
ζ_{4d}	2 200	2 390
ζ_{5p}		5 784

into one. Then, for each range, the variance v_a of the line amplitudes is computed.

It turns out that the closer the range to E_{av}, the larger the v_a value. The variation is nearly a decreasing exponential function of $|E-E_{av}|$, where E is the average of the range boundaries $E=(E_1+E_2)/2$:

$$\ln(v_a)=\alpha+\beta|E-E_{av}| \ . \tag{1}$$

For the Pd^{6+} $4d^4$-$4d^3 5p$ array, a least-squares fitting of α and β to the values of $\ln v_a$ for nine values of E yields $\alpha=2.07\pm0.20$ and $\beta=(-1.08\pm0.04)\times10^{-4}$ cm, which are the correlation parameters. This fitting is presented in Fig. 1. The same shape has already been found [21] in the $3d^4$-$3d^3 4p$ array of Fe^{4+} and is also observed in the $4d^7 5s$-$4d^7 5p$ array of Cd^{4+} (Sec. IV B).

In the following, we will assume that the correlation between energies and amplitudes is properly described by Eq. (1) for the cases of interest to this paper. We will show in Sec. III that once the functional form is assumed, the parameters α and β can be determined without using the *exact* results.

C. A joint distribution

Now that the correlation between the distributions of energies and of amplitudes is fixed, it is necessary to determine quantitatively one of these distributions. For that purpose, we use the numerical values of the *exact* centered moments of order n computed from the general formula

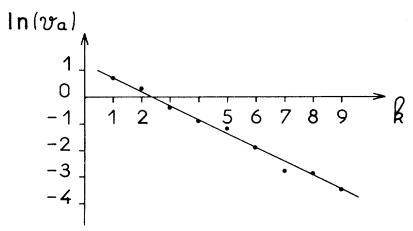

FIG. 1. Correlation between energies and strengths in the *exact* Pd^{6+} $4d^4$-$4d^3 5p$ array. The variance v_a of the amplitudes of the lines lying between $(k-1)\times10^4$ and $k\times10^4$ cm^{-1} from the array average wave number is a decreasing exponential function of k.

$$\mu_n(Q)=\frac{\sum_{i=1,L}(Q_i-Q_{av})^n w_i}{\sum_{i=1,L} w_i} \ , \tag{2}$$

where L is the total number of lines and Q_{av} is the average value of the generic quantity Q. We apply Eq. (2) for $n=2$ and 4, successively, to (i) $Q\equiv E$ with weights $w_i=1$ (unweighted moments), (ii) same as above with $Q\equiv a$, and (iii) $Q\equiv E$ and weights $w_i=S_i$, the strength of line i. This gives weighted moments.

All the values obtained for $\sigma=[\mu_2-(\mu_1)^2]^{1/2}$ and the kurtosis coefficient $\alpha_4=\mu_4/(\mu_2)^2$ are gathered in the left column of Table II. It appears that α_4 is close to 3, the value for a Gaussian distribution, in the case of the unweighted energy distribution only. Therefore we adopt a Gaussian distribution for the unweighted energies.

Based on this and the log-linear form for the strength-energy correlation [Eq. (1)], a joint distribution function of energies E and amplitudes a can be proposed:

$$D(\varepsilon,a)=\frac{L}{2\pi\sqrt{v_u}}\exp\left[-\frac{\varepsilon^2}{2v_u}\right]\times\exp\left[-\frac{a^2}{2}\exp(-\alpha-\beta|\varepsilon|)\right]\times\exp\left[-\frac{\alpha+\beta|\varepsilon|}{2}\right] , \tag{3}$$

where $\varepsilon=E-E_{av}$, v_u is the variance of the unweighted energies, α and β are the correlation parameters, and L is the total number of lines. $\sigma_u=(v_u)^{1/2}$ is given in the left column of Table II.

The following built-in properties can be checked by means of various integrations.

(i) $\int_{-\infty}^{\infty} d\varepsilon \int_{-\infty}^{\infty} D(\varepsilon,a)da=L$.

(ii) The variance of the amplitudes for a given energy value E is equal to v_a as defined in Eq. (1).

(iii) The variance of the energies is equal to v_u as can be seen after first integrating $D(\varepsilon,a)$ over $a=-\infty$ through $+\infty$.

The simulated array defined by Eq. (3) can be generated numerically as follows. First, one picks at random L energies in a Gaussian distribution with average value E_{av} and variance v_u. Second, to each random energy E one assigns an amplitude a picked at random in a Gaussian distribution with average value zero and variance v_a computed by means of Eq. (1).

D. Discussion

That the energy distribution in Eq. (3) is truly Gaussian (after integrating over a) is in fair agreement with the phenomenological result for α_4 (Table II). On the other hand, the amplitude distribution is only *assumed* to be Gaussian *at a given energy*. This is equivalent to assuming that the distribution is approximately Gaussian in each of the narrow energy ranges defined in Sec. II B.

Now, the adequacy of the joint distribution D [Eq. (3)] can be checked by comparing the exact and the simulated

TABLE II. Comparisons of various moments in the Pd^{6+} $4d^4$-$4d^3 5p$ and Cd^{4+} $4d^7 5s$-$4d^7 5p$ arrays.

	Pd^{6+} $4d^4$-$4d^3 5p$		Cd^{4+} $4d^7 5s$-$4d^7 5p$	
	Exact	Simulated	Exact	Simulated
rms deviation σ_u of the line energies[a]	29 068	26 470	24 869	23 869
rms deviation σ_w of the weighted line energies[a]	11 115	11 110	6 503	6 593
rms deviation σ_a of the line amplitudes[b]	1.31	1.31	4.92	4.92
Kurtosis α_4 of the line energies[c]	3.1	2.8	2.9	3.0
Kurtosis α_4 of the weighted line energies[c]	4.9	4.8	7.4	5.1
Kurtosis α_4 of the line amplitudes[c]	8.1	6.0	10.8	10.0
Largest line strength of the array[b]	53	34	1050	1569

[a]In cm^{-1}.
[b]Calibrated so that the total strengths of the arrays are 2940 and 50 400 in Pd^{6+} and Cd^{4+}, respectively.
[c]The kurtosis coefficient is equal to 3 for any Gaussian distribution.

values of the number of lines, and of their total strength, in each energy range. These comparisons are presented in Table III. The two columns under the heading N_i verify that N_i, the number of lines in the energy range i, has almost the same value in the exact and simulated arrays. The number of lines and the total strength in range i can be obtained from the distribution $D(\varepsilon,a)$ by integrating over adequate ranges (see Appendix). The exact array and one sample random simulation are plotted in Fig. 2. For the purpose of drawing, the lines were given a Voigt profile, with a full width at half maximum (FWHM) of 90 cm^{-1}.

Although not perfect, the agreement between the two arrays is quite good. This is satisfactory in view of the simplicity of the model. The amplitudes exhibit a more complicated behavior than the energies, but this could be anticipated from the results of many previous studies.

III. *AB INITIO* CALCULATIONS

An essential property of the distribution proposed in Eq. (3) is the possibility of deriving its various parameters without resorting to any detailed Slater-Condon procedure, unlike what has been done in Sec. II for the phenomenological study. This is shown more precisely in the following.

(i) The average energy E_{av} is the difference of the average energies of the corresponding configurations, which can be obtained by means of any *ab initio* code [28–33], to which δE, the shift for the l^{N+1}-$l^N l'$ arrays [Ref. [11], Eq. (30)] is added. Let us recall that in this work, we consider only cases where δE is small enough so that using the same E_{av} for the weighted and unweighted moments is acceptable.

(ii) The number of lines L is determined, within 2% of

TABLE III. Comparisons between the exact and simulated line distributions in the Pd^{6+} $4d^4$-$4d^3 5p$ array.

Energy range[a]	Number of lines N_i		Total strength[b]	
	Exact	Simulated[c]	Exact	Simulated[d]
1	479	518	1983	2047
2	420	447	757	657
3	308	332	146	182
4	215	213	38.1	43.3
5	150	118	13.6	8.9
6	77	56	1.7	1.6
7	30	23	0.1	0.2
8	25	8	0.1	0.0
9	11	2	0.0	0.0

[a]The lines in the range k lie between $(k-1)\times 10^4$ and $k\times 10^4$ cm^{-1} from the array average.
[b]Calibrated so that the total strength of the array is 2940.
[c]Equation (A1).
[d]Equation (A2).

accuracy, by a statistical formula [Ref. [34], Eq. (26)].

(iii) The variance v_u of the unweighted energies has not yet been evaluated in compact form. However, as indicated in Sec. II, it is approximately equal to the sum of the variances of the unweighted energies of the αJM states of both configurations [13,14]. Of course, this way of computing does not account for the electric dipolar selection rule on J. Its validity relies on two assumptions. First, it can be assumed that the energies of the lines forbidden by the selection rule on J are distributed in nearly the same way as the energies of the allowed lines. Second, the state-energy distribution is often nearly Gaussian [35,36] except in highly asymmetrical configurations (Ref. [27], p. 624). Then, the distribution of the line energies follows from the convolution of two Gaussian curves, resulting in the additivity of the variances.

There remains the problem of determining *ab initio* the values of the correlation parameters α and β. For that purpose, the *ab initio* value of v_w, an exact expansion in terms of squares and crossed products of energy radial integrals [13,14] can be used in the following way.

As mentioned in Sec. II, the correlation between energies and amplitudes is closely linked with the fact that the variance of the unweighted line energy distribution v_u is larger than v_w. The latter can be expressed in the form

$$v_w=\frac{\int_{-\infty}^{\infty}\varepsilon^2 d\varepsilon\int_{-\infty}^{\infty}D(\varepsilon,a)a^2da}{\int_{-\infty}^{\infty}d\varepsilon\int_{-\infty}^{\infty}D(\varepsilon,a)a^2da}$$

resulting in

$$v_w=v_u(1+\beta^2v_u)+\sqrt{2/\pi}\frac{\beta v_u^{3/2}\exp(-\beta^2v_u/2)}{\operatorname{erfc}(-\beta\sqrt{v_u/2})}\ , \tag{4}$$

where erfc is the complementary error function. It is noteworthy that the α parameter does not appear in Eq. (4).

Let us define $X=-\beta\sqrt{v_u}$. Then Eq. (4) can be rewritten

$$\left[X^2+1-\frac{v_w}{v_u}\right]\exp\left[\frac{X^2}{2}\right]\operatorname{erfc}\left[\frac{X}{\sqrt{2}}\right]=X\sqrt{2/\pi}\ . \tag{5}$$

TABLE IV. Solutions of Eq. (5) vs $\rho=v_w/v_u$.

ρ	X	ρ	X	ρ	X
0.005	6.841	0.08	4.520	0.30	1.714
0.010	6.794	0.10	3.939	0.32	1.608
0.015	6.771	0.12	3.503	0.34	1.510
0.020	6.738	0.14	3.158	0.36	1.419
0.025	6.707	0.16	2.876	0.38	1.335
0.030	6.651	0.18	2.638	0.40	1.256
0.035	6.586	0.20	2.434	0.42	1.182
0.040	6.477	0.22	2.255	0.44	1.113
0.045	6.252	0.24	2.098	0.46	1.047
0.050	5.935	0.26	1.957	0.48	0.985
0.055	5.627	0.28	1.827	0.50	0.926
0.060	5.354				

Equation (5) can be solved numerically for any value of the ratio v_w/v_u after the numerical values of the variances v_u and v_w have been calculated by means of the compact formulas [13,14]. For general use, solutions of Eq. (5) are tabulated in Table IV.

The value of β is immediately deduced from that of X. The value of α can be derived from the average value $S_{\rm av}$ of all the strengths in the array. $S_{\rm av}$ being the ratio of the total strength over L, it is reached through the computation of the double integral

$$\int_{-\infty}^{\infty}d\varepsilon\int_{-\infty}^{\infty}D(\varepsilon,a)a^2da\ .$$

Using Eq. (5), it then follows that

$$\alpha=\ln(S_{\rm av})+\ln\left[X^2+1-\frac{v_w}{v_u}\right]-\ln(X)+\tfrac{1}{2}\ln\left[\frac{\pi}{2}\right]\ . \tag{6}$$

For example, in the Pd case, using the values $v_u=(25\,820\ \mathrm{cm}^{-1})^2$ and $v_w=(11\,115\ \mathrm{cm}^{-1})^2$, one obtains $X=2.584$ by means of Table IV, then $\alpha=1.83$ and $\beta=-1.0\times10^{-4}$ cm.

The total strength of the array is an exact multiple of the square of the electric-dipolar radial integral [37]. All the needed values of atomic radial integrals can be evaluated, in general, by means of *ab initio* computer codes [28–33].

IV. NUMERICAL EXAMPLES

A. The Pd^{6+} $4d^4$-$4d^3 5p$ array

The tests and applications presented above only concern the $4d^4$-$4d^3 5p$ array in the spectrum of Pd^{6+}, which contains 1718 lines. That array has been chosen because, in both configurations, the matrix elements of the electrostatic interelectronic repulsion G and of the spin-orbit interaction Λ have the same order of magnitude. As discussed earlier, such an array looks best suited for testing the proposed statistical model. The comparisons with the detailed exact results, obtained by means of the Slater-Condon method with the same values of the radial integrals (Table I), are presented in the two columns on the left of Table II, in Tables III and V, and in Fig. 2. The agreement is good.

B. The Cd^{4+} $4d^7 5s$-$4d^7 5p$ array

The same model can be used for simulating another array where G and Λ have approximately equal magni-

TABLE V. Comparison between the fitted and calculated values of the correlation coefficients α and β.

	Pd^{6+}	Cd^{4+}
$\alpha_{\rm fit}$ [a]	2.07±0.20	4.42±0.31
$\alpha_{\rm calc}$ [b]	1.83	5.00
$\beta_{\rm fit}$ [a]	$-(1.08\pm0.04)\times10^{-4}$	$-(1.42\pm0.08)\times10^{-4}$
$\beta_{\rm calc}$ [b]	-1.00×10^{-4}	-1.97×10^{-4}

[a]From least-squares fit of Eq. (1). For Pd^{6+} see Fig. 1.
[b]Equations (5) and (6). β is in centimeters.

TABLE VI. Comparisons between the exact and simulated distributions in the Cd^{4+} $4d^75s$-$4d^75p$ array.

Energy range[a]	Number of lines N_i		Total strength[b]	
	Exact	Simulated[c]	Exact	Simulated[d]
1	677	678	45 404	44 486
2	554	570	4 366	5 330
3	365	402	466	536
4	239	239	132	45.3
5	137	119	28.4	3.2
6	77	50	2.6	0.2
7	32	18	0.3	0.0

[a]The lines in the range k lie between $(k-1)\times10^4$ and $k\times10^4$ cm^{-1} from the array average.
[b]Calibrated so that the total strength of the array is 50 400.
[c]Equation (A1).
[d]Equation (A2).

tudes: the $4d^75s$-$4d^75p$ array of Cd^{4+}, which contains 2082 lines. The relevant radial integrals have been determined by van Kleef and Joshi [38], who have classified the Cd^{4+} spectrum. From the exact array, the values $\alpha=4.42\pm0.31$ and $\beta=(-1.42\pm0.08)\times10^{-4}$ cm can be deduced, like in Sec. II B. Their small rms is a check of the fitness of the correlation shape.

The simulation can proceed as described in Sec. II C, using the constants derived from *ab initio* results like in Sec. III. The comparisons between the exact and simulated arrays are presented in the two columns on the right of Table II, in Tables V and VI, and in Fig. 3. The

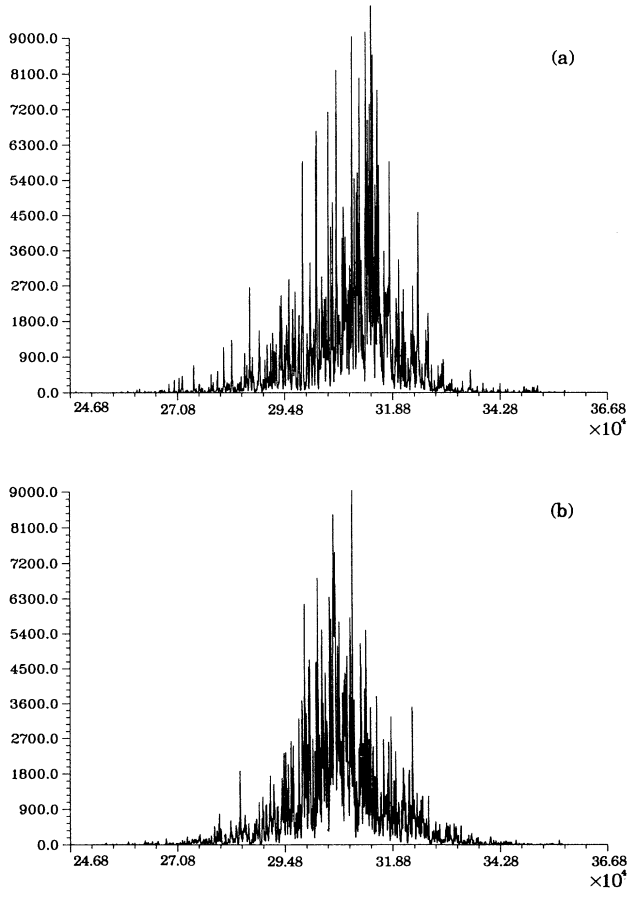

FIG. 2. Two calculated spectra of the Pd^{6+} $4d^4$-$4d^35p$ array. (a) Exact results of the Slater-Condon method. (b) Simulated spectrum (Sec. IV A). Abscissas in cm^{-1}, ordinates in the same arbitrary units in both plots.

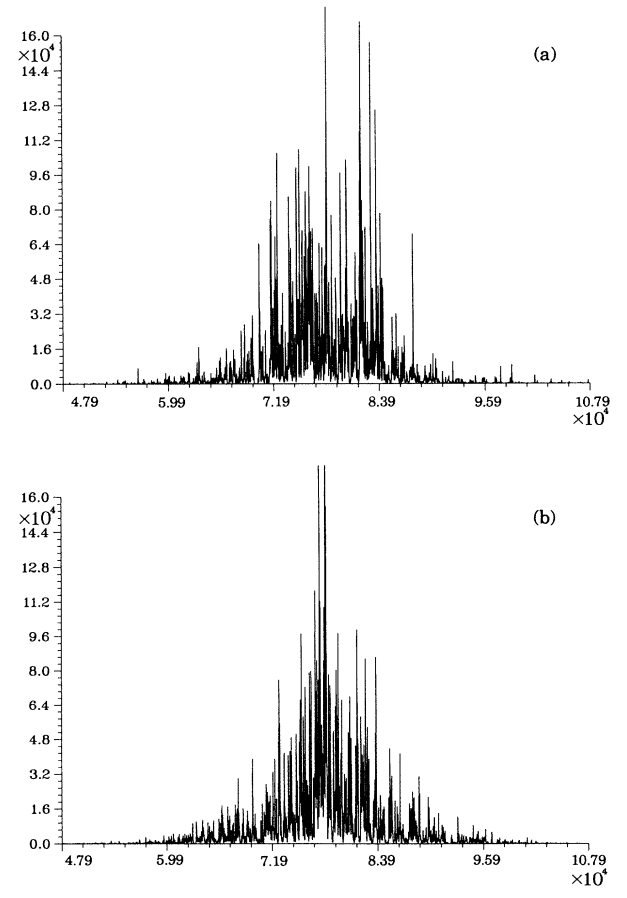

FIG. 3. Two calculated spectra of the Cd^{4+} $4d^75s$-$4d^75p$ array. (a) Exact results of the Slater-Condon method. (b) Simulated spectrum (Sec. IV B). Abscissas in cm^{-1}, ordinates in the same arbitrary units in both plots.

agreement is good. It can be stressed that the correlation between energies and amplitudes is very strong. In general, this occurs when the array is of the $l^N l'$-$l^N l''$ type, different from the l^{N+1}-$l^N l'$ type, which is that of the first example (Sec. IV A). Indeed, the $l^N l'$-$l^N l''$ type differs markedly from the latter by the existence of an electric-dipolar selection rule on the atomic core. This selection rule results in much smaller values of v_w/v_u and much stronger correlations.

V. CONCLUSION

A. Summary

In conclusion, the proposed simulation is very simple to apply. The different steps are the following:

(i) All the energy integrals relevant to the chosen array are calculated *ab initio,* together with the radial transition integral. Many relativistic Hartree-Fock or central-field codes are available for that purpose.

(ii) The weighted and unweighted energy variances of the array, the total number of lines L, and their average strength are derived by means of compact formulas.

(iii) One obtains the parameters for the strength-energy correlation from the value of a variable X [Eq. (5)] which can be deduced by interpolation between the numbers in Table IV.

(iv) A number L of energy values are chosen at random from a Gaussian distribution, and to each one a transition amplitude is assigned, chosen from another Gaussian distribution, which depends on the value of the energy.

The numbers obtained in this way for all the relevant arrays can be used as input for opacity codes. Calculations of the Rosseland mean over limited energy ranges, carried out for both exact and simulated arrays, have shown a good agreement, and are reported in the following paper [22].

B. Other cases and perspectives

The present model offers a wide range of applications, i.e., the numerous arrays in genuine intermediate coupling. In such cases, it appears that the correlation between energies and amplitudes is the crucial characteristic for a correct simulation.

However, it is not sufficient when the symmetry effects are large (Sec. II A). This happens essentially in two physical cases, i.e., where the electrostatic repulsion G largely predominates over the spin-orbit interaction Λ, and the opposite case.

In the former situation, the selection rules on the S and L quantum numbers are all the more efficient as the spin-orbit interactions are small. More precisely, the percentage of very weak lines is much larger than in the present model. Attempts have been made recently [21,22] for simulating the arrays Fe^{4+} $3d^4$-$3d^3 4p$ and Fe^{5+} $3d^3$-$3d^2 4p$. But no general approach is yet available. In some cases where exchange integrals are very large [39], the arrays can be very asymmetrical and δE quite large, and another correlation functional form could be needed.

For the latter situation, that of predominant spin-orbit interactions, the splitting of the array into subarrays [11] is clearly outside the range of application of the present work. Another model must be worked out.

In the future, the effects of configuration mixing ought also to be accounted for because they pervade the neutral and low-ionized atomic spectra, which are most interesting in astrophysics.

Despite the present limitations indicating a need for further study, we are confident that energy-amplitude correlated distributions can and will be useful for opacity calculations in hot plasmas, and will eventually make reliable models of plasma radiation equilibrium within reach. Preliminary encouraging results are planned to be published shortly.

ACKNOWLEDGMENT

Two of the authors (P.D. and M.K.) acknowledge the support of the U.S. Department of Energy through Lawrence Livermore National Laboratory, under Contract No. W-7405-Eng-48.

APPENDIX: ANALYTICAL FORMULAS FOR ARRAY PROPERTIES

From the definition of the joint distribution in Eq. (3), one can deduce analytical formulas for many characteristics of the array. Such formulas are useful for bypassing the statistical determination of these characteristics, i.e., their explicit calculation from the line energies and amplitudes picked at random (Sec. II C). The following examples are given.

(i) The number of lines in each of the "consecutive energy ranges" defined in Sec. II B is useful for detailed comparisons between the exact and simulated arrays (Tables III and VI). It is equal to

$$2\int_{\varepsilon_1}^{\varepsilon_2} d\varepsilon \int_{-\infty}^{\infty} D(\varepsilon,a)da = L\left[\operatorname{erf}\left[\frac{\varepsilon_2}{\sqrt{2v_u}}\right]-\operatorname{erf}\left[\frac{\varepsilon_1}{\sqrt{2v_u}}\right]\right] . \quad \text{(A1)}$$

(ii) The sum of the strengths of the lines in each energy range is useful in the same way. It reads

$$2\int_{\varepsilon_1}^{\varepsilon_2} d\varepsilon \int_{-\infty}^{\infty} D(\varepsilon,a)a^2 da = L\exp\left[\alpha+\frac{X^2}{2}\right]\left[\operatorname{erf}\left[\frac{X}{\sqrt{2}}+\frac{\varepsilon_2}{\sqrt{2v_u}}\right]-\operatorname{erf}\left[\frac{X}{\sqrt{2}}+\frac{\varepsilon_1}{\sqrt{2v_u}}\right]\right] \quad \text{(A2)}$$

with the values of α and X evaluated in Sec. III.

(iii) Moments of the whole array can also be derived. The fourth-order moment of the amplitude distribution reads

$$\mu_4(a)=\frac{1}{L}\int_{-\infty}^{\infty} d\varepsilon \int_{-\infty}^{\infty} D(\varepsilon,a)a^4 da .$$

From the result of the integrations, one deduces the kurtosis coefficient of the overall amplitude distribution:

$$\alpha_4 = 3\exp(X^2)\frac{\operatorname{erfc}(\sqrt{2X})}{[\operatorname{erfc}(X/\sqrt{2})]^2} . \quad \text{(A3)}$$

[1] D. Mihalas, *Stellar Atmospheres* (Freeman, San Francisco, 1978).
[2] D. Mihalas, in *Atomic Processes in Plasmas,* Proceedings of a Conference on Atomic Processes in Plasmas, Santa Fe, New Mexico, 1987, edited by A. Hauer and A. L. Merts, AIP Conf. Proc. No. 168 (AIP, New York, 1988).
[3] Y. Yu, in *Atomic Processes in Plasmas,* Proceedings of a Conference on Atomic Processes in Plasmas, Gaithersburg, Maryland, 1989, edited by Y. K. Kim and R. C. Elton, AIP Conf. Proc. No. 206 (AIP, New York, 1990).
[4] M. J. Seaton, J. Phys. B **20**, 6363 (1987).
[5] M. J. Seaton, J. Phys. B **23**, 3255 (1990).
[6] B. F. Rozsnyai, Astrophys. J. **341**, 414 (1989).
[7] F. J. Rogers, B. G. Wilson, and C. A. Iglesias, Phys. Rev. A **38**, 5007 (1988).
[8] F. J. Rogers, C. A. Iglesias, and B. G. Wilson, in *Atomic Processes in Plasmas,* Ref. [3].
[9] H. N. Magee, A. L. Merts, and W. F. Huebner, Astrophys. J **283**, 264 (1984).
[10] C. A. Iglesias, F. J. Rogers, and B. G. Wilson, Astrophys. J. **360**, 221 (1990).
[11] J. Bauche, C. Bauche-Arnoult, and M. Klapisch, Adv. At. Mol. Phys. **23**, 131 (1987).
[12] M. G. Kendall and A. Stuart, *The Advanced Theory of Statistics* (Griffin, London, 1963).
[13] C. Bauche-Arnoult, J. Bauche, and M. Klapisch, Phys. Rev. A **20**, 2424 (1979).
[14] C. Bauche-Arnoult, J. Bauche, and M. Klapisch, Phys. Rev. A **25**, 2641 (1982).
[15] M. Klapisch, P. Mandelbaum, A. Zigler, C. Bauche-Arnoult, and J. Bauche, Phys. Scri. **34**, 51 (1986).
[16] M. Klapisch, E. Meroz, P. Mandelbaum, A. Zigler, C. Bauche-Arnoult, and J. Bauche, Phys. Rev. A **25**, 2391 (1982).
[17] A. Zigler, M. Givon, E. Yarkoni, M. Kishinevsky, E. Goldberg, B. Arad, and M. Klapisch, Phys. Rev. A **35**, 280 (1987).
[18] A. Bar-Shalom, W. H. Goldstein, and J. Oreg, in *Sixth International Workshop on Radiative Properties of Hot Dense Matter, Sarasota, Florida, 1990,* edited by W. H. Goldstein, C. Hooper, and R. Lee (World Scientific, Singapore, in press).
[19] B. G. Wilson, F. J. Rogers, and C. A. Iglesias, Phys. Rev. A **37**, 2695 (1988).
[20] J.-C. Gauthier, J.-P. Geindre, C. Chenais-Popovics, M. Louis-Jacquet, J. Bruneau, D. Desenne, D. Naccache, C. Bauche-Arnoult, and J. Bauche, in *Sixth International Workshop on the Radiative Properties of Hot Dense Matter* (Ref. [18]).
[21] J. Bauche, C. Bauche-Arnoult, C. Chenais-Popovics, J.-C. Gauthier, and J.-P. Geindre, in *Sixth International Workshop on the Radiative Properties of Hot Dense Matter* (Ref. [18]).
[22] P. Duffy, M. Klapisch, J. Bauche, and C. Bauche-Arnoult, following paper, Phys. Rev. A **44**, 5715 (1991).
[23] T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. M. Wong, Rev. Mod. Phys. **53**, 385 (1981).
[24] J. P. Draayer, J. B. French, and S. S. M. Wong, Ann. Phys. (N.Y.) **106**, 472 (1977).
[25] J. P. Draayer, J. B. French, and S. S. M. Wong, Ann. Phys. (N.Y.) **106**, 503 (1977).
[26] M. L. Mehta, *Random Matrices and the Statistical Theory of Energy Levels* (Academic, New York, 1967).
[27] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
[28] R. D. Cowan, J. Opt. Soc. Am. **58**, 808 (1968).
[29] C. Froese-Fischer, Comput. Phys. Commun. **1**, 151 (1969).
[30] M. Klapisch, Comput. Phys. Commun. **2**, 239 (1971).
[31] E. Koenig, Physica **62**, 393 (1972).
[32] J.-P. Desclaux, Comput. Phys. Commun. **9**, 31 (1975).
[33] M. Klapisch, J. L. Schwob, B. S. Fraenkel, and J. Oreg, J. Opt. Soc. Am. **67**, 148 (1977).
[34] J. Bauche and C. Bauche-Arnoult, J. Phys. B **20**, 1659 (1987).
[35] M. Bancewicz and J. Karwowski, Acta Phys. Polon. A **65**, 279 (1984).
[36] N. Rosenzweig and C. E. Porter, Phys. Rev. **120**, 1698 (1960).
[37] J. Bauche, C. Bauche-Arnoult, E. Luc-Koenig, J. F. Wyart, and M. Klapisch, Phys. Rev. A **28**, 829 (1983).
[38] T. A. M. van Kleef and Y. N. Joshi, Physica **114C**, 117 (1982).
[39] J. Bauche and C. Bauche-Arnoult, Comput. Phys. Rep. **12**, 1 (1990).