Monte Carlo simulation of complex spectra for opacity calculations

P. Duffy
University of California, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550

M. Klapisch*
University of California, Lawrence Berkeley Laboratory, Berkeley, California 94720

J. Bauche and C. Bauche-Arnoult
Laboratoire Aimé Cotton, Bâtiment 505, 91405 Orsay, France
(Received 21 May 1991)

A Monte Carlo technique for modeling spectra with many resolved lines of ions in intermediate coupling was presented in the preceding paper [Phys. Rev. A **44**, 5707 (1991)]. We use the same concept here with a modification for the near-*LS*-coupling case. Rosseland and Planck means of transition arrays of Fe V and Fe VI are evaluated. Comparison with "exact" computations shows much better agreement than is found using the simple unresolved-transition-array approximation.

PACS number(s): 32.30.Rj, 52.25.Nr, 32.90.+a, 97.10.Ex

I. INTRODUCTION

Line-rich, partially resolved bound-bound atomic-transition arrays contribute significantly to opacities, but there is currently no totally satisfactory method for calculating that contribution. Although exact calculations of these spectra (and their opacities) are not hard in principle, the number of lines involved makes them time-consuming and often impractical. Opacities can also be calculated using the unresolved-transition array (UTA) approach [1] in which each transition array—all the lines between two specified electronic configurations—is treated as a single, broad, unresolved spectral feature, often approximated as a Gaussian. When the lines are unresolved, this is often a very good approximation. When spectra are wholly or partly resolved into lines, however, the UTA approach is not useful for calculating wavelength-averaged opacities, as we shall see below.

In a preceding paper [2], referred to below as I, we presented a concept for random simulation of line-rich partially resolved arrays, which allowed for much quicker computations than "exact" models without losing much precision. This model is based on the idea that wavelength-averaged opacities do not depend much on the strengths or positions of individual lines in a complex spectrum. That is, if there are enough lines in the spectrum, calculated opacities will be approximately right as long as certain *statistical* properties of the spectrum are correct. This approach allows opacities to be found very quickly because it does not require calculating real line strengths or energies.

There are other models which calculate both line energies and amplitudes randomly, although not from realistic distributions (see I for references and discussion). In the present paper, we apply the concept and we show results for Rosseland and Planck mean opacities for a case of astrophysical interest, namely, a near-*LS*-coupling spectrum of Fe V and Fe VI.

The idea in I is demonstrated with intermediate coupling spectra. The arrays are assumed to be symmetrical, and the correlation is found in the following way: the exact energies are distributed into consecutive ranges of equal widths on both sides of the average energy $e_{\rm av}$. The symmetrical arrays are then folded in such a way that two ranges symmetrical with respect to $e_{\rm av}$ can be combined into one for purposes of statistics. Then for each energy range, the variance v_a of the line amplitudes is computed for some typical examples.

It turns out that to a good approximation v_a is nearly a decreasing exponential function of $|e-e_{\rm av}|$, where e is the mean of the range boundaries $e=(e_1+e_2)/2$:

$$\ln v_a=\alpha+\beta|e-e_{\rm av}| \ . \tag{1}$$

This functional form is then assumed for any symmetrical array in intermediate coupling, and it was shown in I that the parameters α and β can be evaluated simply without knowing the exact transition energies and amplitudes. Several relevant statistical characteristics of the transition arrays $4d^4$-$4d^3 5p$ of Pd^{6+} and $4d^7 5s$-$4d^7 5p$ of Cd^{4+} were very well reproduced.

In the present work, on the other hand, since we wish to apply the concept to an astrophysically relevant *LS*-coupling spectrum, we introduce a different form for the energy-strength distribution. By the same token, this form will not be limited *by construction* to symmetrical arrays.

Our model is essentially a fast way of generating line strengths and energies, and does not try to do state-of-the-art calculations of line profiles, bound-free opacity, or free-free opacity. These are separate problems which must be addressed no matter how line strengths and energies are found; we approximate them simply here to allow our model to be tested against more detailed calculations and a UTA approach. Ultimately, we envision our model being used inside a large opacity code like OPAL [3] or

 ©1991 The American Physical Society

MONTE [4] to find line strengths and energies in spectra where transition arrays are highly resolved.

In Sec. II we explain the model in more detail. In Sec. III, we present preliminary results for a simple spectrum of iron where detailed atomic structure calculations are possible for comparison; we show that our model gives nearly the same Rosseland and Planck mean opacities as the relativistic parametric potential model RELAC [5], and much better opacities than the UTA approach. Section III also discusses work needed for the model to be further improved. Section IV gives our conclusions.

II. MODEL

The broad outline of how our model works is as follows. First, we assign a random energy and strength to each line, as described in detail below. The energy is chosen first, from an assumed distribution. Choosing the strength (i.e., the square of the amplitude) is more complicated because there is a correlation between line energies and strengths which must be modeled. After each line is assigned a strength and energy, it is given an assumed shape and added to a plot of the spectrum. This is done one transition array at a time. When all the lines in all the arrays are done, we add the continuum opacity to the spectrum and calculate the Rosseland and Planck means.

The part of the model that is new is the scheme for obtaining line energies and strengths. To get a line energy we assume the energies in each transition array obey a Gaussian distribution and generate a random number obeying this distribution. That is, the number of lines per unit energy dN/de, irrespective of the strength, is given by

$$\frac{dN}{de}=\frac{N}{\sqrt{2\pi v_u}}\exp\left[\frac{-(e-\bar{e}_u)^2}{2v_u}\right], \tag{2}$$

where N is the total number of lines in the array, e is the line energy $h\nu$, $\bar{e}_u$ is the mean line energy, i.e., the difference between the configuration average state energies, and v_u is the unweighted variance of the line energies. This distribution is significantly wider than that of the strength-weighted energies, which can also be closely approximated by a Gaussian in many cases. This shows that there is a correlation between the line energies and strengths, such that the average strength of lines in a given energy range decreases farther from the center of the array. This important part of our model is further discussed below.

The number N of lines and the mean line energy $\bar{e}_u$ in Eq. (2) are found using statistical approaches which have been shown to be quite accurate in a wide range of cases [6]. As in I, we find the variance v_u of the line energies by combining the energy ranges of the upper and lower configurations. Specifically, if $v_{\rm up}$ and $v_{\rm low}$ are the variances of the energies of the states in the upper and lower configurations, the variance of the transition energies is taken to be

$$v_u=v_{\rm up}+v_{\rm low}\ . \tag{3}$$

This approximation is equivalent physically to assuming that transitions occur between states whose energies completely span the ranges of their respective configurations. This is *not* true of the strong transitions, which occur predominantly between relatively narrow regions, called emissive zones, of the upper and/or lower configurations (Ref. [1], p. 166). It is, however, a reasonable approximation for the entire set of transitions, most of which violate LS-coupling selection rules and are very weak. Wilson [4] also makes this approximation. In the two arrays we use as examples, the $3d^4$-$3d^3 4p$ array of Fe V and the $3d^3$-$3d^2 4p$ array of Fe VI, this method gives unweighted variances of 4.2 and 3.1 eV, which are 87% and 78% of the actual variances of 4.8 and 4.0 eV, as calculated by the atomic-structure code RELAC.

After each line energy is found, its strength is found by choosing its amplitude from an assumed distribution and then squaring it. Unfortunately, the actual distribution is not known theoretically, and there is no simple way to model it accurately. Earlier papers showing that simple strength distributions work well model only some of the lines—those allowed in pure LS coupling. The other lines, those which violate LS coupling rules, are much more difficult to model and have a big effect on the opacity.

Another aspect of the strength-modeling scheme which opacities are sensitive to is the correlation between line strengths and energies alluded to earlier and discussed in I. This correlation means that the amplitude distribution varies as a function of the line energy. This strength-energy correlation is illustrated in Figs. 1(a) and 1(b), which are scatter plots of line energies and strengths in the $3d^4$-$3d^3 4p$ array of Fe V and the $3d^3$-$3d^2 4p$ transition array of Fe VI, as calculated by RELAC. These plots show two aspects of this correlation: first, that strong lines occupy a narrower range of energies than weak lines, and second, that there is a scarcity of weak lines near the centers of the arrays.

As mentioned earlier, we use in this work a different form for the strength-energy correlation from that used in I. The reason is that in I we focused on spectra in "full intermediate coupling," i.e., not near either the LS or the jj limits. The rationale is that the spectra in intermediate coupling should be more readily modeled by random simulation, since any approximate symmetry in the Hamiltonian will cause nonrandom structure in the spectra. This is the reason for the vertical "stripes" in Figs. 1(a) and 1(b). On the other hand, there are many spectra of astrophysical interest near LS coupling, for which opacity calculations are crucial. Also, in many cases the "shift" [Ref. [1], Eq. (30)] between the weighted and unweighted transition energies is not negligible and the arrays are not symmetric. For the cases considered in I, the present functional form does not give as good a fit as the log-linear formula of I [Eq. (1) here]; however, it has more potential flexibility for the nonsymmetric cases.

We model the strength-energy correlation by calculating the average line strength as a function of energy. (Let us recall that the strength being the square of the amplitude, the average strength is the variance of the amplitudes.) We now use two assumptions already discussed.

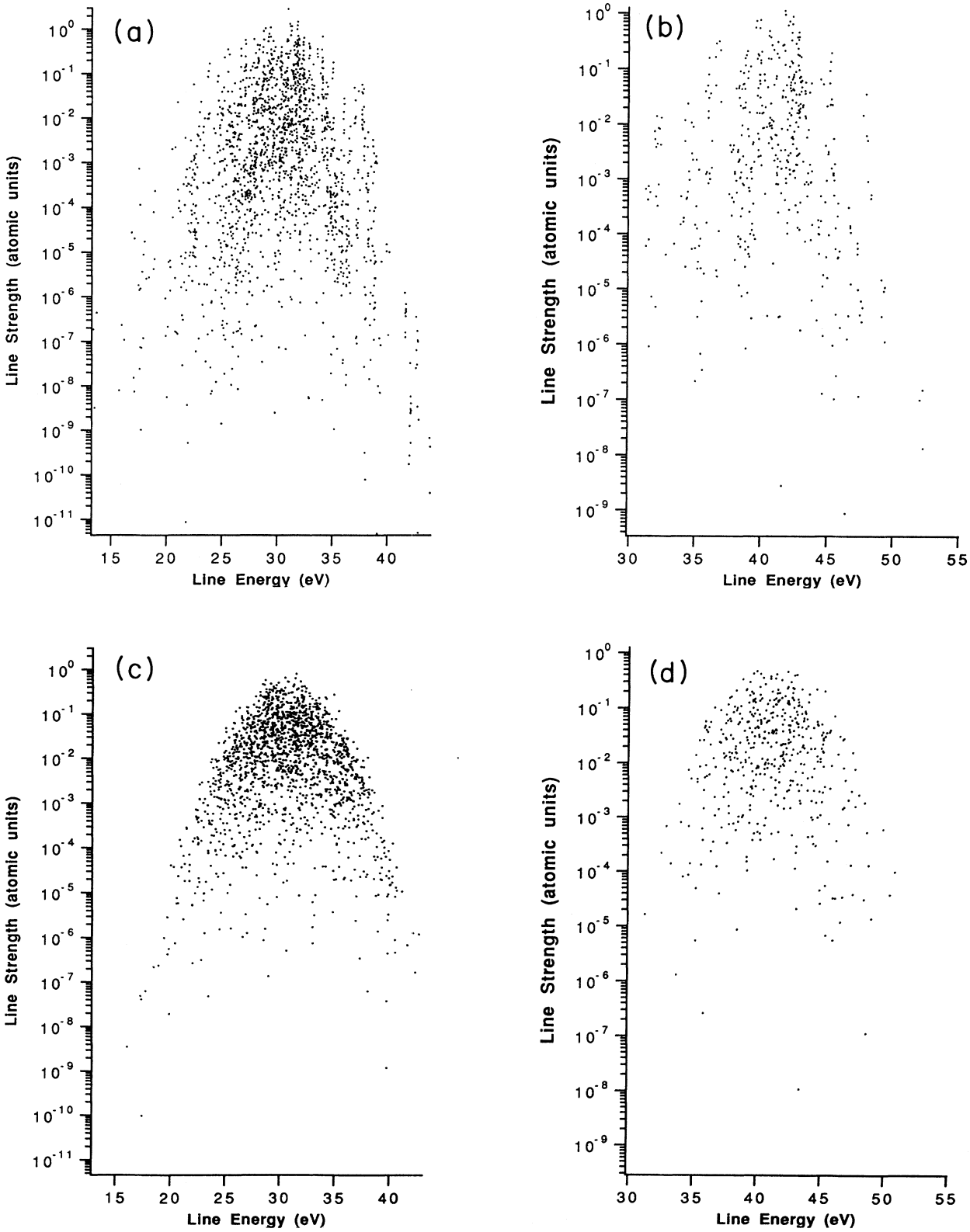

FIG. 1. Scatter plots of line energies and strengths in two transition arrays of iron, as calculated by the atomic structure code RELAC and by our Monte Carlo mode. Each line is represented by a point whose x value is the line's energy in eV and y value is the log of its strength in atomic units. (a) and (b) are RELAC calculations of the $3d^4$-$3d^3 4p$ array of Fe V and the $3d^3$-$3d^2 4p$ array of Fe VI, respectively. (c) and (d) are Monte Carlo calculations of the same arrays.

The first is that the number of lines per unit energy is given by a Gaussian with the unweighted variances, Eqs. (2) and (3). The second is none other than the UTA model (Ref. [1], p. 135). Ignoring the third- and higher-order moments, we treat the strength density distribution dS/de in each transition array as a Gaussian. Specifically, we assume that

$$\frac{dS}{de} = \frac{S_{\text{tot}}}{\sqrt{2\pi v_w}} \exp\left[\frac{-(e-\bar{e}_w)^2}{2v_w}\right] . \tag{4}$$

Here, S_{tot} is the total strength in the array, and the average weighted line energy $\bar{e}_w$ and the weighted variance v_w are defined as

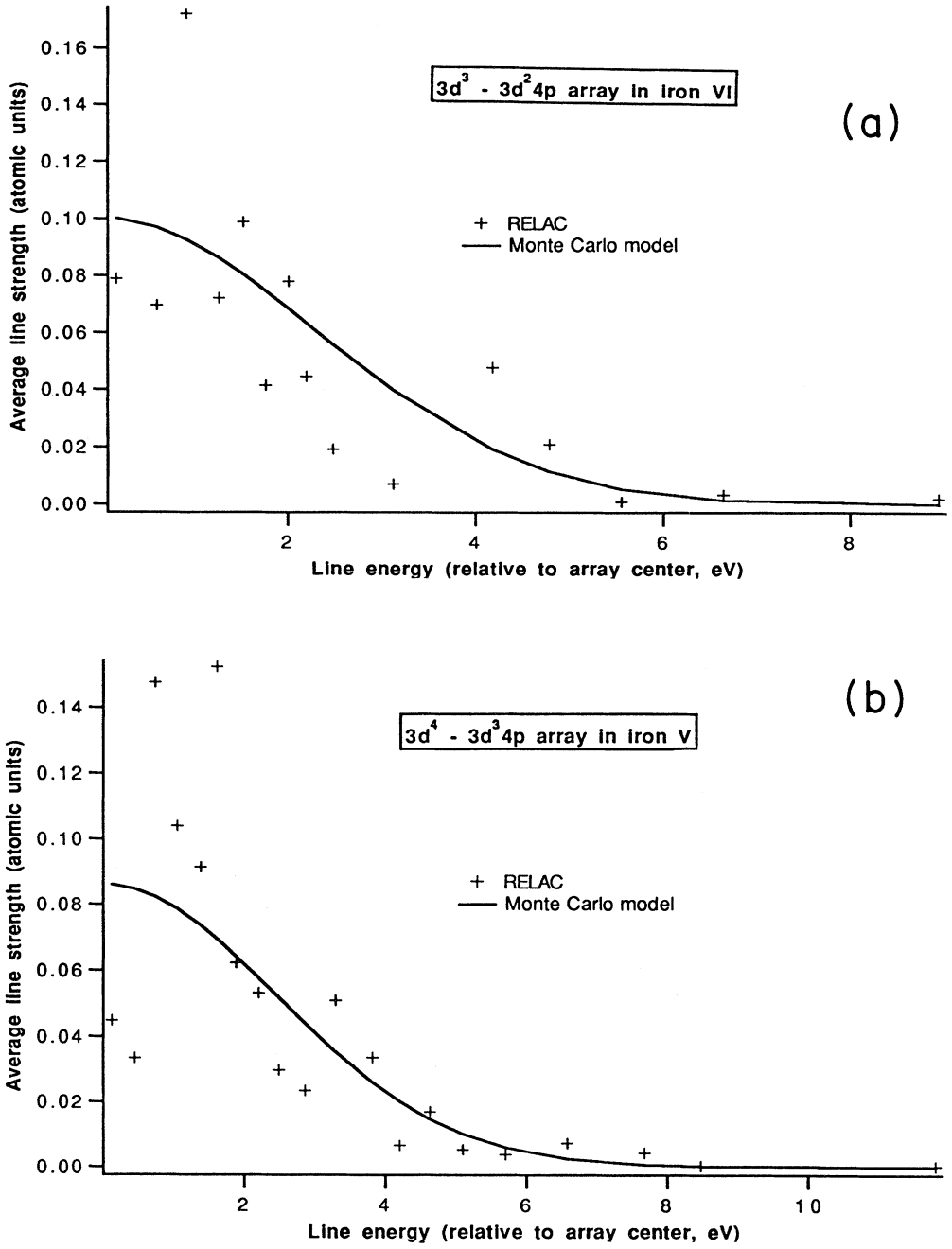

FIG. 2. Line strength as a function of line energy in the (a) $3d^3$-$3d^2 4p$ array of Fe VI and (b) $3d^4$-$3d^3 4p$ array of Fe V. The x axes are line energy, relative to the center of the array, in eV; the y axes are line strength in atomic units. The x and y values of each point are the average energy and strength, as calculated by RELAC, of the lines near that energy. The smooth curve shows the strength-energy correlation used in our model [Eq. (5)].

$$\bar{e}_w = \frac{\sum_{i=1}^{N} e_i s_i}{\sum_{i=1}^{N} s_i}$$

and

$$v_w = \frac{\sum_{i=1}^{N} (e_i - \bar{e}_w)^2 s_i}{\sum_{i=1}^{N} s_i} ,$$

where s_i is the strength of the ith line. The values of $S_{\rm tot}$, $\bar{e}_w$ and v_w are found using well-established procedures based on the statistical properties of transition arrays [1], i.e., without calculating the strengths and energies explicitly.

Thus the average strength, i.e., the variance of the amplitudes, of lines in a small range near energy e is the ratio of Eqs. (2) and (4):

$$\bar{S}(e) = \frac{dS/de}{dN/de} = \frac{S_{\rm tot}}{N} \left[\frac{v_u}{v_w} \right]^{1/2} \exp \left[\frac{(e-\bar{e}_u)^2}{2v_u} - \frac{(e-\bar{e}_w)^2}{2v_w} \right] . \quad (5)$$

Introducing now the "shift" [Ref. [2], Eq. (30)] such that $\bar{e}_w = \bar{e}_u + \delta e$, we have

$$\ln(v_a) = \ln \left[S_{\rm av} \left[\frac{v_u}{v_w} \right]^{1/2} \right] - \frac{\delta e^2}{2v_w} + \frac{\delta e}{v_w}(e-\bar{e}_u) + \frac{1}{2} \left[\frac{1}{v_u} - \frac{1}{v_w} \right] (e-\bar{e}_u)^2 ,$$

where we have used $S_{\rm av} = S_{\rm tot}/N$. For the sake of simplicity, in this work we shall apply (5) in cases where the shift δe is negligible. In principle, Eq. (4) can be regarded as the start of a Gram-Charlier expansion (Ref. [1]). However, the condition for refining Eq. (5) in that way is finding the corresponding expansion of Eq. (2), which is not known at this point.

We can now calculate individual line strengths. The scheme we use is simple and reproduces both the amplitude (or strength) distribution and the observed strength-energy correlation reasonably well. It has two steps, which are repeated for each line. First, we choose an amplitude randomly from a Gaussian distribution with a zero mean and a variance of 1; this is squared to produce a random strength obeying a χ^2 distribution with unit average strength. Next, this strength is normalized by multiplying it by an average strength obtained from the line's energy and Eq. (5). These two steps are equivalent to choosing a random strength from a χ^2 distribution with an average strength which depends on the line's energy as described by Eq. (5) (i.e., which decreases farther from the center of the array). As a result, the amplitude (strength) distribution of the lines in a narrow energy range is a Gaussian (χ^2 distribution) and the overall amplitude (strength) distribution is the sum of many Gaussians (χ^2 distributions).

Our model reproduces the observed correlation between line energies and strengths quite well. This can be seen from Figs. 1(c) and 1(d), which are scatter plots of line energies and strengths calculated with our Monte Carlo model for the same arrays shown in Figs. 1(a) and 1(b). Both the tendencies of strong lines to avoid the edges of the array and of weak lines to avoid the middle are reproduced. However, the nonrandom clumping of lines around certain energies is, of course, not reproduced. Another test of our strength-energy correlation is shown in Figs. 2(a) and 2(b), which display "actual" (calculated by RELAC) average strengths of lines in various energy bins, as well as our assumed average strength as a function of energy [Eq. (5)].

The rest of the model is straightforward. After each line is given an energy and strength, it is convolved with an assumed line shape and added to the plot of the spectrum. When all the lines are done, the free-free opacity is added using simple analytical models for inverse Bremstrahlung [7] and Compton scattering [8]. Finally, Rosseland and Planck means are calculated over a limited energy range, as explained below.

III. RESULTS

A. Rosseland and Planck mean opacities

We have tested our model on a relatively simple spectrum of iron where an "exact" atomic structure calculation can be made for comparison. The spectrum contains two transition arrays, the $3d^4$-$3d^3 4p$ array of Fe V and the $3d^3$-$3d^2 4p$ array of Fe VI, and a total of 2184 lines. We compare Rosseland and Planck mean opacities calculated by the relativistic parametric potential model RELAC, by our Monte Carlo model, and by an unresolved-transition-array approach. The opacities are averaged over a limited energy range which includes almost all the lines in the spectrum but little area where the opacity is dominated by the continuum contribution. Thus, what we call a Rosseland mean κ_R is actually defined by

$$\frac{1}{\kappa_R} = \frac{\int_{\nu_1}^{\nu_2} \frac{dB_\nu/dT}{\kappa_\nu} d\nu}{\int_{\nu_1}^{\nu^2} \frac{dB_\nu}{dT} d\nu} \quad (6)$$

and our "Planck means" κ_P are actually

$$\kappa_P = \frac{\int_{\nu_1}^{\nu_2} \kappa_\nu \frac{dB_\nu}{dT} d\nu}{\int_{\nu_1}^{\nu_2} \frac{dB_\nu}{dT} d\nu} .$$

Here, ν is photon frequency, B_ν is the Planck function, κ_ν is the frequency-dependent opacity, and T is temperature; the limits of integration are $h\nu_1 = 15.72$ eV and $h\nu_2 = 54.93$ eV. These are the same as the usual definitions except that there the limits of integration are zero and infinity. We use a limited energy range to em-

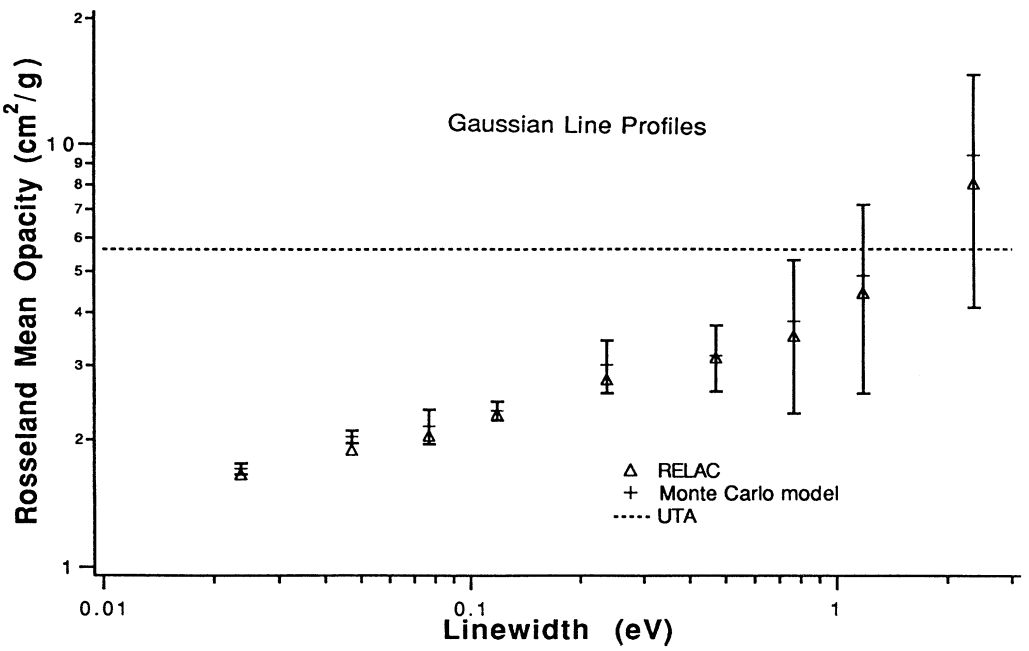

FIG. 3. Partial Rosseland mean opacities as a function of linewidth calculated by three different models. Line profiles are Gaussians. The averages are calculated over the energy range 15.72–54.93 eV [Eq. (6)]. The x axis is the Doppler width [fullwidth at half maximum, (FWHM)] in eV. Results for the Monte Carlo model are the average of ten independent runs; error bars indicate statistical fluctuations. The dashed line is UTA opacity, which by definition is independent of linewidth.

phasize differences between the models. Averaging over a wider range would make the models seem to agree better because the results would be more heavily influenced by the continuum opacity, which is the same in all three models.

The Rosseland mean opacity is much harder to model than the Planck mean because it is extremely sensitive to the presence or absence of even a few gaps in the spectrum. Even so, our Rosseland means are quite close to RELAC's. This is shown in Figs. 3 and 4, which plot

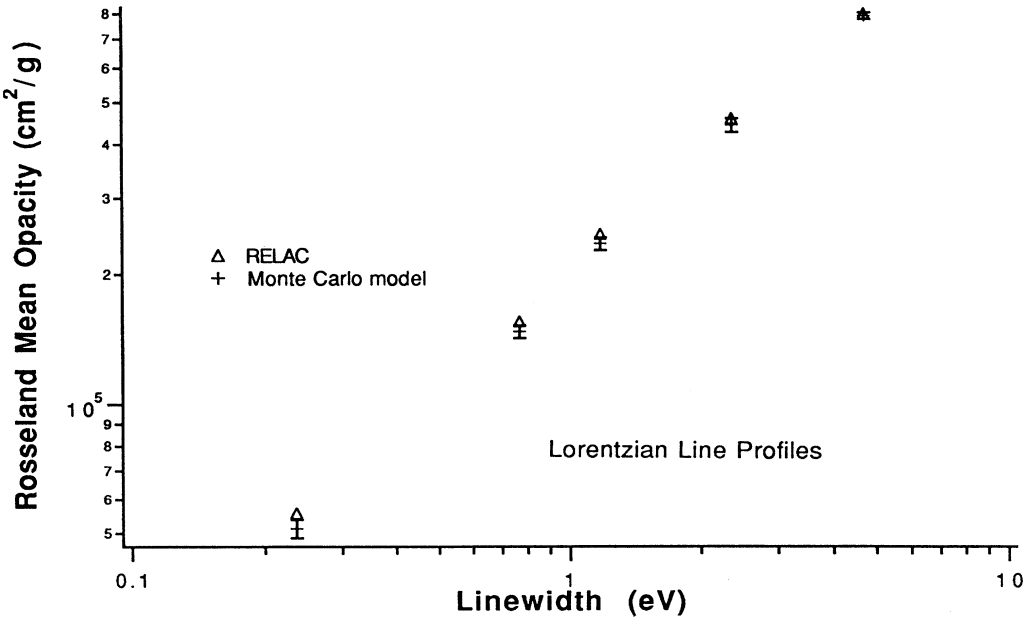

FIG. 4. Partial Rosseland mean opacities as a function of linewidth calculated by two different models. Line profiles are Lorentzians. The averages are calculated over the energy range 15.72–54.93 eV, as indicated in Eq. (6). The x axis is scaled so that points in Figs. 3 and 4 with the same x values have the same FWHM. Results for the Monte Carlo model are the average and standard error of ten independent runs; error bars thus indicate statistical fluctuations.

TABLE I. Partial Planck mean opacities (in cm^2/g) calculated by our Monte Carlo model and by an "exact" model (RELAC). The averages are calculated over the energy range 15.72–54.93 eV, as indicated in Eq. 7; the uncertainties shown are one standard deviation of 10 independent runs. The UTA value (not shown) is $2.63 \cdot 10^6$.

Model \ Linewidth	Gaussian line profiles 0.01 eV	0.1 eV	1.0 eV
RELAC	2.62×10^6	2.66×10^6	2.63×10^6
Monte Carlo	$(2.63 \pm 0.13) \times 10^6$	$(2.61 \pm 0.17) \times 10^6$	$(2.60 \pm 0.16) \times 10^6$
	Lorentzian line profiles 0.1 eV	0.3 eV	1.0 eV
RELAC	2.61×10^6	2.58×10^6	2.47×10^6
Monte Carlo	$(2.67 \pm 0.12) \times 10^6$	$(2.59 \pm 0.18) \times 10^6$	$(2.47 \pm 0.16) \times 10^6$

Rosseland means calculated by our model and by RELAC as a function of assumed linewidth; UTA opacities, which do not depend on line width, are also plotted. We show results for both Gaussian (Fig. 3) and Lorentzian (Fig. 4) line profiles. Of course, any number of other line shapes are also possible; we use these because, besides being simple, they typify two extremes of possible shapes in that the Lorentzian has long "wings" or "tails" and the Gaussian does not. (As the figures show, long wings can dramatically increase the Rosseland mean, because they fill in low places in the spectrum. In this case that occurs mainly outside the arrays, and the difference between the Rosseland and Planck means would be much smaller if the limits of integration were narrower.) Thus testing our model on these two simple line shapes gives us confidence that it would work well with others, too.

As expected, both our Monte Carlo opacities and RELAC's are less than the UTA opacity for small linewidths, when the spectrum is highly resolved, and increase as the lines get wider and the spectrum becomes unresolved. When the width of each line approaches UTA width (about 2 eV for both arrays), the Monte Carlo and RELAC opacities actually exceed the UTA value.

Our Planck means agree virtually perfectly with RELAC's, for both types of line shape and a wide range of linewidths. These results are shown in Table I. The Planck mean is much easier to model than the Rosseland mean because it is defined [Eq. (7)] with the κ_ν factor in the numerator, not the denominator. This means that the Planck mean is sensitive mainly to the total strength in the spectrum and not to gaps between the lines, as the Rosseland mean is. Because of this, the Planck means are virtually independent of the assumed linewidth and line shape and are the same in RELAC and the Monte Carlo model (as well as in the UTA approach).

B. Spectra

Our model's spectra appear similar to RELAC's except that the strongest lines are too weak, especially when the lines are highly resolved (Fig. 5). This happens because the strongest lines in our spectra are about three times too weak in the Fe V array and two times too weak in the Fe VI array. This is due to an inadequacy in the strength distribution. The variance of the amplitudes near the center of the array is too small, or perhaps a Gaussian representation of these amplitudes is inaccurate. Another way of describing this question is the following: we ignore the fact that there are two distinct types of lines in these arrays—those allowed in pure LS coupling and those which violate LS-coupling rules. The LS-allowed lines contain almost all the strength (of order 90%) but fewer than half the lines (about $\frac{1}{3}$ in the Fe V array and $\frac{1}{2}$ in the Fe VI array); hence, in these two arrays the average strength of the LS-allowed lines is 2 or 3 times the overall average. In our model, however, essentially the same amount of strength is split among all the lines, thus our maximum strengths are too small by the same factors (3 in the Fe V array and 2 in the Fe VI array). This makes our spectra too short when the lines are highly resolved; when the linewidth approaches the width of the whole array, the height of the spectra are determined mainly by the total strength in the array (not individual line strengths), so our model does a better job.

Although we have not done any formal tests of the speed of our model, we are confident that it is inherently much faster than exact methods. A Monte Carlo simulation of the 2184 lines and energies in the test spectrum shown here takes about 10 s on a MacIntosh II personal computer; a RELAC calculation of the same spectrum on similar machines takes roughly 10 min. (Neither time includes calculating line shapes or opacities, or plotting.)

C. Discussion

The opacities we calculate here agree very closely with RELAC's—within 5% on the average. This level of agreement is not needed for the model to be useful. We say this because the other uncertainties, e.g., those involving line shapes, in most current calculations of Rosseland means are at least this large. Also, most applications of the Rosseland mean involve making the "diffusion approximation" [9] which often involves uncertainties as large as the discrepancies shown here.

Despite these good agreements, there are at least two aspects of our model we would like to improve. The first is the distribution of line strengths, whose inadequacies we have already discussed. Improving the strength distribution would require a better theoretical understanding of actual distribution. By experimenting with various *ad hoc* strength distributions, we estimate that a better one would probably increase our Rosseland means by 10% or so.

The second problem with our model, which was also mentioned earlier, involves the line energies. It explains why our Rosseland means tend to be higher than RELAC's for Gaussian line profiles and not for Lorentzians. (This effect is small now, but as just mentioned, would probably be larger with a better strength distribution). The problem is a tendency in real arrays for line energies to "clump" together nonrandomly, an effect we cannot model by a random distribution. We believe this occurs

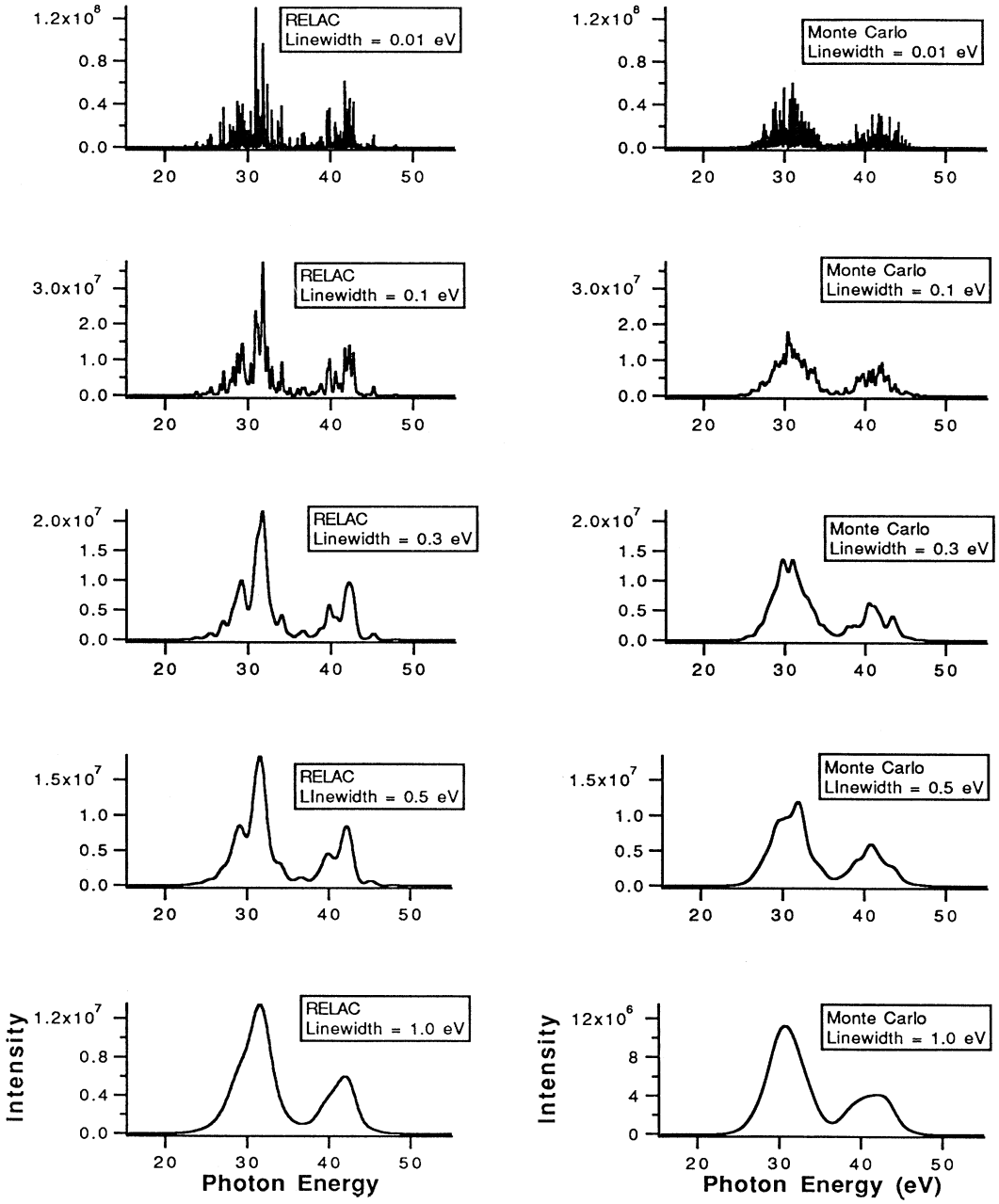

FIG. 5. Plots of the test spectrum of iron as calculated by our Monte Carlo model (right) and the "exact" model RELAC (left). Each pair of plots assumes a different Gaussian linewidth, as indicated. Also, each Monte Carlo spectrum is from a different run of the code, so the line energies and strengths are slightly different. The spectrum contains two arrays, the $3d^4$-$3d^3 4p$ array of iron V, centered at 30.61 eV, and the $3d^3$-$3d^2 4p$ array of iron VI, centered at 41.08 eV.

because levels with the same *LS* designations have almost the same energies this close to pure *LS* coupling. The effect can be seen in Figs. 1(a) and 1(b) as a tendency for the points to form vertical stripes. The same effect is seen in Figs. 6(a) and 6(b), histograms of the number of lines per unit energy in the Monte Carlo and RELAC calculations. In the Monte Carlo model the energy distribution is Gaussian, and the deviation from the Gaussian in each bin is roughly the square root of the number of points in the bin, as expected. In the RELAC model, on the other hand, the broad outline of the energy distribution is nearly Gaussian but the individual bins deviate much more from this than in the Monte Carlo model. Also, unlike in the Monte Carlo model, the deviations do not vary much as the number of points in the bin changes. In short the actual distribution of line energies is quite nonrandom.

This nonrandomness of the line energies decreases the Rosseland mean because it results in energy ranges with relatively few lines, which tends to open up gaps in the spectrum. Since we do not model this effect, our Rosseland means are consistently too high, especially with Gaussian line profiles, whose short tails emphasize gaps

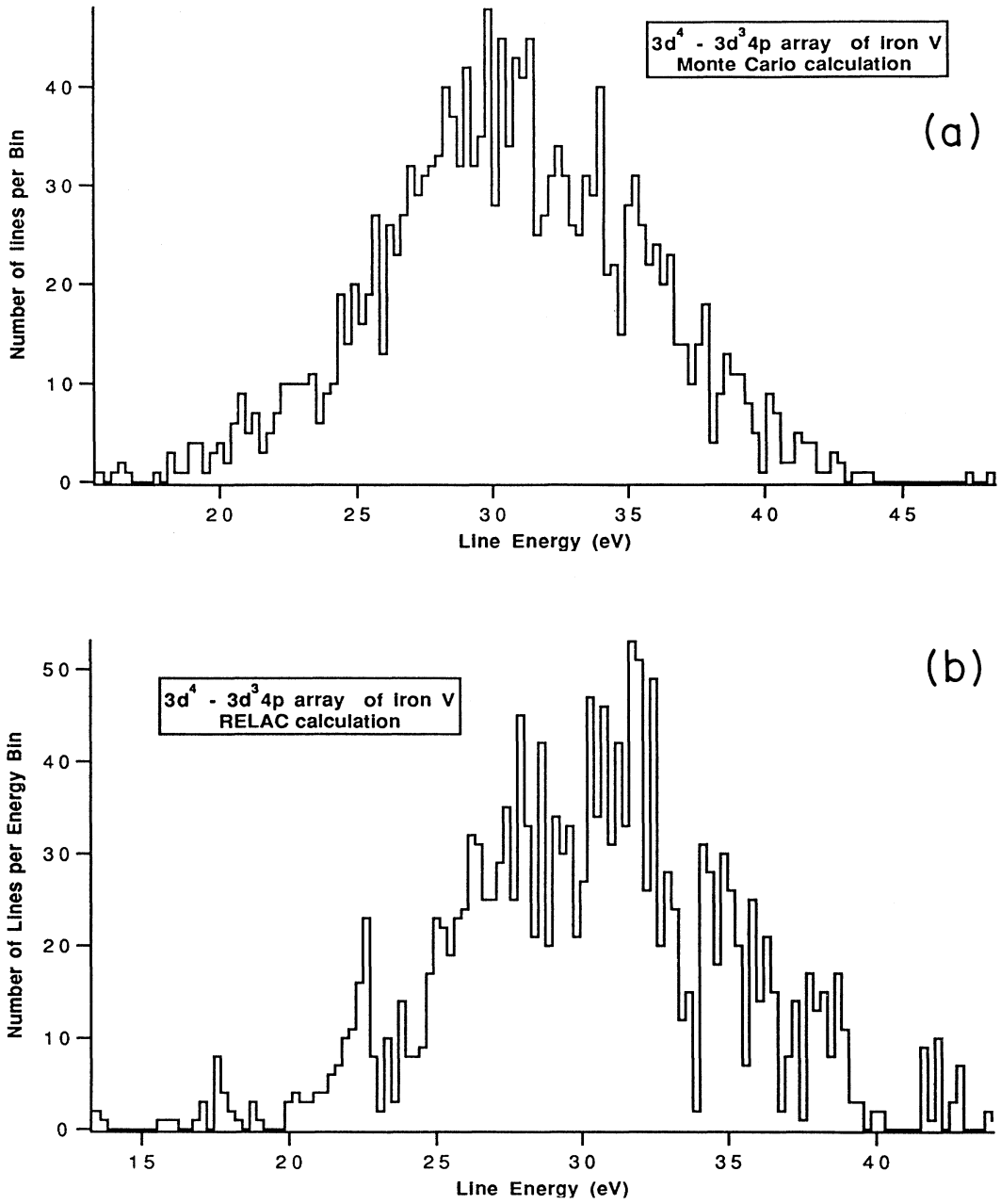

FIG. 6. Histograms of the distribution of line energies in our Monte Carlo model and in the "exact" model RELAC. The horizontal axis is line energy in eV and the vertical axis is number of points per energy bin.

in the spectrum. To prove that this is the reason, we did a simple test in which we substituted RELAC's line energies for the random energies in our model without changing anything else. The resulting Rosseland means were much closer to RELAC's. With Lorentzian line profiles, however, the long wings of the lines largely fill in any gaps between the lines, making the clustering of line energies much less important. Hence our model, which neglects this effect, works better.

VI. CONCLUSIONS AND FUTURE WORK

We have described a fast Monte Carlo method for calculating opacities of transition arrays where individual lines are resolved. In tests on a simple spectrum of iron it gives Rosseland and Planck mean opacities within 10% of those from a detailed atomic structure calculation; this holds for both Gaussian and Lorentzian line profiles and a wide range of linewidths. The method has been applied only to cases near *LS* coupling and would probably need modifications to work elsewhere. In addition, it has at least two known shortcomings, discussed above.

If the model can be made to work quite generally, it could be included in a large opacity code like MONTE or OPAL as a fast way of calculating bound-bound opacities in highly resolved spectra.

ACKNOWLEDGMENTS

It is a pleasure to thank Brian Wilson and William Goldstein for helpful discussions. This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

[1] J. Bauche, C. Bauche-Arnoult, and M. Klapisch, Adv A. Mol. Phys. **23**, 131 (1987), and references therein.
[2] J. Bauche, C. Bauche-Arnoult, J. F. Wyart, P. B. Duffy, and M. Klapisch, preceding paper, Phys. Rev. A **44**, 5707 (1991).
[3] C. Iglesias, F. Rogers, and B. Wilson, Astrophys. J. **360**, 221 (1990).
[4] B. J. Wilson (unpublished).
[5] M. Klapisch, J. L. Schwob, B. S. Fraenkel, and J. Oreg, J. Opt. Soc. Am. **67**, 148 (1977).
[6] J. Bauche and C. Bauche-Arnoult, Comput. Phys. Rep. **12**, 1 (1990).
[7] Dimitri Mihalas, *Stellar Atmospheres* (Freeman, San Francisco, 1978), p. 102; Kenneth R. Lang, *Astrophysical Formulae* (Springer-Verlag, Berlin, 1980), p. 46.
[8] Kenneth R. Lang, *Astrophysical Formulae* (Ref. [7]), p. 69.
[9] Dimitri Mihalas, *Stellar Atmospheres* (Ref. [7]), pp. 49–52.