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SAMPLING METHODS

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RESUMEN. El gran aumento en la capacidad computacional nos ha permitido resolver la ecuación de transporte radiativo en varios miles de puntos de frecuencia en la solución iterativa del modelo atmosférico clásico, y construir un muestreo más detallado y realístico de la opacidad que en modelos anteriores. Mientras que la media armónica y la media recta permiten un cálculo muy rápido de la estructura del modelo, los errores de estos tratamientos tan simples de la opacidad pueden ser mayores que todos los errores que resultarían si se excluyeran del cómputo del modelo atmosférico de estrellas frías todos los avances físicos de los últimos 25 años! Sin embargo, el método más simple de muestreo basado en la media armónica—la media de Rosseland—todavía se utiliza para calcular las condiciones de frontera en los modelos de evolución de las estrellas frías. La transformación estadística en líneas individuales de los coeficientes de absorción media recta que se miden, seguido de un muestreo cuidadoso, es una mejora considerable sobre el uso corriente del coeficiente de absorción media recta en la construcción de modelos atmosféricos.

ABSTRACT. A tremendous increase in computing capacity has allowed us to solve the radiative transfer equation at several thousand frequency points during the iterative solution of the classic model atmosphere problem, and to construct a much more detailed and realistic sampling of the opacity than in earlier models. Whereas the harmonic mean and straight mean enable a very fast computation of the model structure, the errors in such simple opacity treatments may be bigger than the errors due to neglect of all improvements in the physics included in computations of model atmospheres of cool stars during the last 25 years! Yet the most simple harmonic mean sampling method—the Rosseland mean—is often still used to compute boundary conditions for evolutionary models of cool stars. Statistical transformation of measured straight mean absorption coefficients into individual lines, followed by careful sampling, has been a considerable improvement over the direct use of the straight mean absorption coefficient in the construction of model atmospheres.

Key words: OPACITIES – STARS: ATMOSPHERES

I. INTRODUCTION

In the very early models, before the use of electronic computers, the absorption coefficient was an average over the whole spectrum; e.g. the Rosseland mean opacity that is valid where the diffusion approximation applies and can also be a reasonable first approximation in a limited group of model atmospheres. However, when the absorption coefficient is a very irregular function of frequencies, for example where molecules are dominant, models based on the Rosseland mean are too far from a realistic solution to be used even as a trivial value for starting the iterations, and it is surprising to see that the method is still in use to compute boundary conditions to interior evolutionary models. In the earliest model atmospheres computed on electronic computers, the opacity was treated as a simple mean for the number of spectral intervals that could be handled by the computer, typically up to 100 intervals throughout the spectrum. Through trial and error, and a tremendous increase in computer capacity, a picture has slowly emerged on how accurate we need to sample the monochromatic opacity in order to converge a good flux-constant model, in the sense that more detailed sampling would not increase the accuracy of the computed atmosphere. Other recent reviews that describe

aspects of sampling methods include those of Carbon (1984) and Johnson (1986). We will here describe the methods that are presently in use and illustrate, with some examples, the size of the errors that are introduced when excessively approximate sampling methods are used.

II. STRAIGHT MEAN AND HARMONIC MEAN

The two simplest mean-based methods in use approximate the monochromatic absorption coefficient, χ_ν, by either a harmonic mean, χ^i_H, or a straight mean, χ^i_{SM}, absorption coefficient,

$$(\chi^i_H)^{-1} = \int_{\nu_i}^{\nu_{i+1}} \chi_\nu^{-1}\, d\nu/(\nu_{i+1}-\nu_i) \approx \sum_{j_i=1}^{n_i} \chi_\nu^{-1}(j_i)/n_i \tag{1}$$

$$\chi^i_{SM} = \int_{\nu_i}^{\nu_{i+1}} \chi_\nu\, d\nu/(\nu_{i+1}-\nu_i) \approx \sum_{j_i=1}^{n_i} \chi_\nu(j_i)/n_i \tag{2}$$

where $\chi_\nu(j_i)$ is computed or measured in n_i points in each interval i from ν_i to ν_{i+1}. Since 1 divided by a number close to zero is a big number, the integral to determine χ^i_H is dominated by χ_ν in the frequency intervals where $\chi_\nu \to 0$. In contrast, the integral that determines χ^i_{SM} is dominated by χ_ν in the intervals where χ_ν is big. If $\chi_\nu(j_i) = 0$ in one frequency point, j_i, χ^i_H will be zero for the whole interval, i, and if $\chi_\nu(j_i)$ is very big compared to the average in that interval, $\chi^i_{SM} \approx \chi_\nu(j_i)/n_i$. We see that the harmonic mean will over-emphasize the effect of continuum points, and the straight mean will over-emphasize the effect of the strongest spectral lines. The more χ_ν fluctuates, the more unrealistic is the mean-based description; and either the spectrum interval of the average must be chosen smaller or another sampling method must be introduced. In fact $\chi_\nu(j_i)$ will itself always be a straight mean, for numerical or instrumental reasons, but with a very small step length, $\Delta\nu_i = (\nu_{i+1}-\nu_i)/n_i$. Because the stellar spectrum is a non-linear function of the absorption coefficient, the spectral flux calculated from the average of the monochromatic absorption coefficient will be very different from the average of the spectral flux calculated from the monochromatic absorption coefficient. The latter is of course the correct, but most tedious, way to calculate a synthetic spectrum. Fig. 1 illustrates this problem. In the upper panel it is shown a piece of a spectrum (of C_2 and CN) calculated by use of the high-resolution monochromatic absorption coefficient. The next panel shows the same spectrum but folded to a resolution of 1 Å. The third panel shows the corresponding spectrum computed from the harmonic mean absorption coefficient averaged over intervals of 1 Å, and the last panel shows the same spectrum but now computed from the straight mean absorption coefficient. Since the radiative transfer through the model atmosphere is calculated exactly as the radiative transfer giving rise to the spectrum, Fig. 1 also illustrates the effect we might expect on the model structure by using the two different average procedures. The straight mean is seen to block the light excessively, and therefore the underlying layers must be heated where energy is hindered from escaping such that the atmosphere thermodynamically expands, which will lead to a cooling of the surface layers. Conversely, the harmonic mean will make the atmosphere contract because the energy escapes too easily.

Auman (1967) was the first to include the large number of lines necessary for the description of a molecule. He used the measurements of 41 bands of the water molecule to establish the approximate line strength of $2.3 \cdot 10^6$ vibrational-rotational lines, and calculated from those both the harmonic and the straight mean absorption coefficients averaged for each 100 cm^{-1} in the interval 0.8 to 12.5 μm. The strength of the hot bands of the measured bands was estimated in the harmonic approximation, and difference bands were included with the same strength as that of the corresponding summation bands. Values up to J=41 were considered, and the line profile was considered to be a rectangular box with a width equal to twice the Doppler half-width. The error in the calculated line position varied from a few cm^{-1} for well-observed states up to several hundred cm^{-1} for some of the weak lines coming from transitions between highly excited states. From this absorption coefficient he computed a grid of model atmospheres (Auman 1969), based on 60 frequency points and 50 optical depth points. Continuum opacity sources, metals and molecular opacity from H_2O (only) were included. Most models were calculated with the H_2O opacity treated in the harmonic mean approximation, but a few models with straight mean opacities were tested as well. For a SM and a HM model, calculated for $T_{\rm eff} = 3000$ K and $\log(g) = 1$, the difference in the surface temperature between the two models was 600 K,

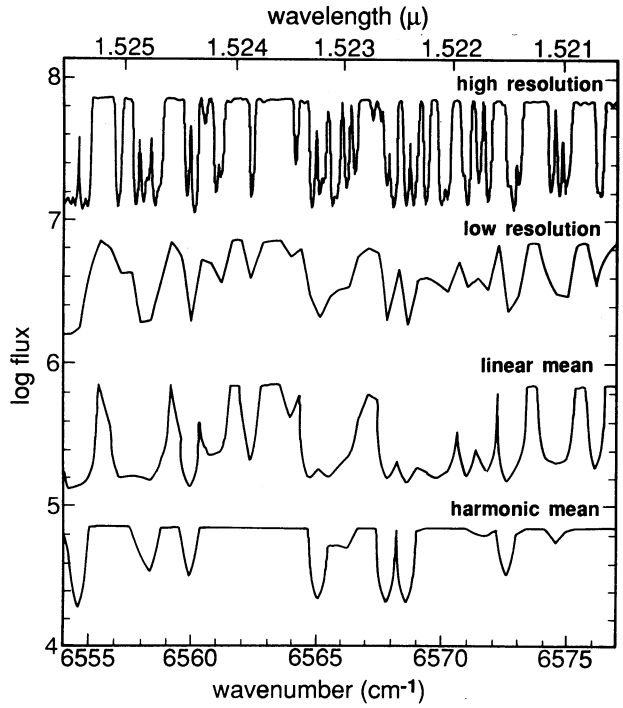

Figure 1: Interval of 50 Å in the spectrum of CN and C_2 in a cool red giant. Panel one (top) shows a spectrum computed from the detailed absorption coefficient, and panel two shows this spectrum averaged to a resolution of 1 Å. Panels three and four show the same spectrum, but computed with the absorption coefficient averaged to a resolution of 1 Å before the spectrum was computed, and by use of respectively the straight mean and the harmonic mean methods.

which has an enormous effect on the synthetic spectrum. Unfortunately, a comparison between observed and computed bands was never published (which would have shown the SM-bands to be far too strong), but the huge difference between the two models clearly demonstrates the enormous importance of sampling the opacity carefully.

III. POA, JOLA and VAEBM

Tsuji (1966) introduced the concept of the "partly overlapping lines" approximation (POA) where it is assumed that the molecular bands can be described as piecewise continuous absorbers. The basic number in each spectral interval, i, is the *smearing out* parameter, $\delta_i = 2\Delta\lambda_i/d_i$, where $\Delta\lambda_i$ is the spectral line half width and $d_i = (\lambda_{i,begin} - \lambda_{i,end}) \,/\, n_i$ is the average distance between each line in the *ith* interval from $\lambda_{i,begin}$ to $\lambda_{i,end}$, n_i being the number of lines in the same interval. If $\delta_i \leq 1$ the total absorption is assumed to be due to lines and true continuum sources in a (continuous) fraction δ_i of the *ith* interval, whereas the absorption is assumed to be due to only continuous sources in the other part of the interval. This has the advantage, compared to both harmonic and straight mean absorption coefficients, that the correct ratio (at least in principle) between line absorption and interline "holes" in the spectrum is considered. In practice n_i is not well defined since it depends on the lower limit chosen in line strength. The method is in some sense a straight mean where the average absorption coefficient is distributed over only a fraction of each interval considered. Throughout this fraction the absorption is considered constant, and the transport equation needs therefore only to be solved a maximum of twice the number of intervals selected. In 1966 the maximum possible spectral frequencies in which it would be affordable to solve the transfer equation was of the order 100, and 42 spectral intervals were therefore chosen. If $\delta_i \geq 1$ in all intervals the method is called "just overlapping lines approximation" (JOLA)

or "complete overlapping approximation". In the computation of the absorption coefficient, measured bands and estimates of their hot bands from the harmonic approximation are summarized, but unmeasured bands are not considered.

Brett (1990) used the JOLA technique to re-compute the opacity of water in 200 frequency points in the interval 0.3 to 9 μm, based on the band strengths listed by Auman (1967). The opacities obtained were used to construct model atmospheres (Brett, 1989) with 50 optical depth points for red giants of solar metallicity and with T_{eff} in the interval 2250 to 3500 K. The opacity of OH, CO, CN, TiO, and VO were also considered (in the JOLA). Particularly, the TiO ϵ and the VO A-X and B-X systems were introduced for the first time from "astrophysical band strength" estimates (Brett 1990). Bessell et al. (1989; BBSW) used the new set of opacities to study sphericity effects in models of red giants.

Tsuji (1976) introduced, instead of the measured f-values of individual bands from H_2O, the measured straight mean absorption coefficient, χ^i_{SM}, and mean line separation, d_i, from the work of Ludwig et al. (1973; L73). In the Voigt-analogue-Elsasser band model (VAEBM) used, the lines are assumed to be Voigt profiles that overlap, in the sense that the absorption coefficient in each interval can be expressed as a Fourier expansion times the straight mean absorption coefficient of the same interval. The basis for this analytical description is the assumption that all lines are equally spaced, with the spacing d_i, and have the same strength, S_i, such that the line strengths can be expressed as $S_i = \chi^i_{SM}/d_i$. This method has the advantage compared to the POA that the line profiles are treated more elaborately, but still the choice of the number of lines per interval, $n_i = 1/d_i$, is not well defined and the assumption that all lines have the same strength is also clearly undesirable. Possibly the most important advantage of the VAEBM compared to POA, and to the straight mean as well as the harmonic mean, is that it is able to use the temperature dependent observed low-resolution data instead of single-band f-values. The two sets of data are only equal if all bands were assigned an f-value and if a perfect description of the temperature dependence (including knowledge of the ratio between the intensity of the lowest level bands and their corresponding hot bands) was available; neither of which is fulfilled for any molecule. Of the two observational approaches described for water, the low-resolution, temperature dependent data of L73 are the most complete.

IV. ODF and OS

Today, the two most accurate and commonly used sampling methods of extensive molecular and atomic line data are the Opacity Distribution Function (ODF) technique and the Opacity Sampling (OS) technique. Both methods are based on the use of a detailed monochromatic absorption coefficient that is assumed to be well known in a sufficient number of frequency points such that, for example, a full synthetic spectrum (showing at least in principle the detailed line profile of all relevant lines) can be computed from it. The difference between the two methods is in the way they use the data in solving the transfer equation in the iterative process of producing a model atmosphere, but they seem to give rise to an almost identical model atmosphere; and therefore their respective advantages and disadvantages are only concerned with computational speed, flexibility to variation of model parameters, etc. The two methods have been extensively described and compared by, for example, Querci et al. (1974), Johnson and Krupp (1976), Carbon (1979, 1984), and Ekberg et al. (1986).

The basic principle of the ODF method is to rearrange the monochromatic absorption coefficient within a number of spectral intervals. In each such ODF-interval all frequency points with a large absorption coefficient are shifted toward one end of the interval, and frequency points with successively smaller values of the absorption coefficient are shifted successively further toward the other end of each interval. In this way the correct length of the spectrum occupied by lines with a certain strength is preserved by the ODF, only the exact frequency is changed. The accuracy of the ODF to represent the monochromatic absorption coefficient from which it is constructed can therefore be increased by decreasing the length of the ODF intervals. Inside each interval, the absorption coefficient is picked in a limited number of frequency points along the ODF, and these values are used for solving the transfer equation during the model atmosphere computation. The accuracy of this step can therefore be increased to the desired accuracy by increasing the number of pickets, and the accuracy can also be increased by reversing the direction toward which the strong lines are shifted in some of the intervals. During each iteration in the model atmosphere computation, the opacity of a given species (an atom or a molecule) at each depth in the atmosphere will be obtained by multiplying its ODFs by the

relevant partial pressure. The total opacity is then obtained by adding the opacity for all species considered. For cool stars, where molecules dominate the opacity, it is often convenient to collect the total opacity from all the atoms in a set of pre-calculated tables. Each table represents one ODF frequency and gives the combined atomic opacity for a grid of temperatures and electron pressures. The total atomic ODFs are then obtained by a simple interpolation in these tables, but such ODFs are of course restricted to a pre-specified relative abundance (which could be the solar value) of all the atoms. Typically 50 ODFs of 10 pickets will be a good description of the absorption coefficient, and hence the whole set of ODFs can be stored in core memory during calculation of the model atmosphere, which obviously is a great advantage for saving computer time. If more than one species (e.g. two different molecules) is contributing to the opacity, the ODF technique has the disadvantage that, for example, the strongest lines of all the species will be arranged at the same spectral frequency (which can partly be compensated for by reversing the ODF for some of the molecules), and the sum of the ODFs will therefore no longer be identical to the ODF of the sum of the monochromatic absorption coefficients (which, after multiplication with the relevant partial pressures, would be the correct opacity to use). In principle ODFs of the summarized monochromatic absorption coefficient could be calculated and tabulated as a function of temperature, pressure, and chemical composition, and this was in fact how the first ODFs were stored (e.g. Querci et al. 1974). Even though the ODFs computed in this way have the advantage of speed and theoretical correctness, they have the disadvantage of low flexibility; the whole grid of ODFs has to be re-computed each time a new microturbulence, isotopic ratio, or chemical composition is to be studied. Instead, most recent computations have been based on individual (molecular) ODFs that depend only on temperature (if Doppler profiles are assumed for the lines), and the individual ODFs have (after multiplication with the relevant partial pressures) been added during the model computations in the way prescribed by Saxner and Gustafsson (1984).

The basic principle of the OS technique is to pick the value of the monochromatic absorption coefficient in a sufficiently large number of frequency points, such that the statistical character of the variation of a complex absorption coefficient is well represented inside regions where the source function does not vary too much. This number is easily found from numerical experiments, because choosing a bigger and bigger number of points in the OS eventually will lead to convergence of the model structure toward a specific model, which supposedly is the same model that would had been obtained if the transfer equation had been solved for an infinite number of frequencies. The necessary number of points in an OS has been estimated by various authors to values between 1 000 and 10 000. Presumably the first few iterations of a model can even be performed with only 100 points (Johnson and Krupp 1976). If 10 000 points are picked, the solution of the radiative transfer equation will be 10 times slower in an OS model than in an ODF model with 100 ODFs and 10 pickets. Since the spectral lines of the contributing atoms and molecules have not been rearranged to construct OSs, the theoretical correct total opacity will be a simple arithmetic addition (after multiplication with the relevant partial pressures) of the OSs of each contributing species. Since this addition is fast, compared to the more cumbersome addition of the ODFs, the total CPU time required per iteration in the model construction from ODFs will exceed that from OSs as soon as more than about 5 or 6 different species are considered in the total opacity. Since the addition of OSs is so fast, it is often convenient to store an OS for each isotope of each molecule, which makes it easier to experiment with the effect of varying isotopic composition of the models; and if the molecular data are in the form of a line list, even the microturbulence can in principle be a variable in model construction, and the theoretical correct behavior of the opacity in, for example, an atmosphere with a velocity field different from zero can be described, which is not the case in the ODF approximation. For species of very discrete spectral nature (e.g. single, strong metal lines or widely spaced strong molecular lines like those of CO) the OS method may not assure the picking of the few strong lines that govern the energy balance in the optically thin parts of the atmosphere, and this problem is sometimes solved by treating the strong lines separately. The ODF approximation faces the same problem if the picking in the strongest end of the ODF intervals is not very dense where such lines occur.

V. COMPARISON OF THE METHODS

Johnson et al. (1980; JBK) extended their earlier treatment of molecular species to include CO, CN, C_2, TiO, and H_2O, and a small number of lines from CH, NH, MgH, OH. The most important revision compared to their earlier models was that the opacity was now considered in the OS approximation, except for water which

was still treated in SM over 100 cm^{-1} as in the work of Auman (1969). The increased computer capacity was reflected in the fact that the transfer equation now was solved in more than 1 000 frequency points (for 60 optical depths). Gustafsson et al. (1975 and particularly later unpublished models; GBEN) computed models based on ODFs prepared from an extensive line list for the diatomic molecules C_2, CO, and CN compiled by Querci et al. (1974), atomic lines from the work of Kurucz and Peytreman (1975), and a smaller number of lines from CH, MgH, OH, and NH from unpublished work. Johnson and Krupp (1976) compared the models from GBEN with models from JBK (the two grids are based on independent codes and quite different opacities), and the agreement for the $T-P_g$ structure was found to be very good (within 30 K at all P_g for a T_{eff} = 4000 K, log(g) = 2.25 model). In contrast an SM model (computed with the JBK code) with T_{eff} = 3500 K and log(g) = 0 was about 800 K cooler than the corresponding OS model in the surface layers (JBK). Comparison with a model of T_{eff} = 3600 K and log(g)=0 from Tsuji's (1976) grid (that included basically the same molecules as JBK but treated in the VAEBM approximation) showed a cooling of $\approx$ 30 K in the inner layers ($\tau_{ross} \approx -1.5$), and a corresponding heating of $\approx$ 200 K in the surface layers ($\tau_{ross} \approx -4$) compared to the corresponding JBK model. Seemingly the VAEBM method hereby proved to be an improvement over the SM method, but the ODF and the OS approximations generally include fewer approximations than the VAEBM and must therefore be considered more accurate, although a strict comparison involving observed spectra has not been performed to prove this statement.

Alexander et al. (1989; AAJ) introduced a new statistical treatment of the same laboratory data for water (L73) that had earlier been treated statistically by Tsuji (1976) in constructing a VAEBM absorption coefficient. In the method introduced by AAJ all the lines were, in contrast to the approximations used in the VAEBM, allowed to have different line strengths. Since L73 gives a measure for the average line separation, $d_i = (\nu_{i+1} - \nu_i)/n_i$, in each spectral interval, ν_i to ν_{i+1}, the line positions (and number of lines, n_i) could be computed by stepping through the spectrum and selecting one line in each interval of the length d_i. Inside each such interval the line position was selected randomly. AAJ further considered the line strengths, S, of 34 000 lines measured in the laboratory to construct a probability distribution function, $P(S) = S_0^{-1} \exp(-S/S_0)$, of line strengths. S_0 was determined from the data of L73 at 3000 K as $S_0 = d_i \chi^i_{SM}$. Finally the lower excitation levels of the lines were determined from a random generator with a tailed exponential distribution determined from the same 34 000 laboratory lines. To check the accuracy of this method, the final absorption coefficient was computed for several temperatures and compared with the measured straight mean absorption coefficient of L73. The coefficient at 3000 K was obviously in closest agreement with the data of L73, but also the data for T = 2000 K and T = 2500 K were equal to L73's measured results to within a factor of two throughout the spectrum, and, for example, in the region of the strongest fundamental band ($\approx$ 6.3 μm) the agreement was appreciably better. Since the lines in the study of AAJ cannot be assigned a quantum number, there is no possibility to compare with f-values for individual bands, but the straight mean absorption coefficient should reflect the areas with weak and strong bands through the selection of $S_0 = S_0(\nu)$. Since Auman's (1967) data only include individual measured bands, whereas AAJ's data in principle include all absorption measurable at 3000 K, one would expect the SM by AAJ to be bigger than the one of Auman. In the long wavelength region ($\approx$ 1 000 cm^{-1}) this is also the case, since Auman's straight mean value is less or $\approx$ half of the AAJ value. At 2000 K, Auman's data in two spectral regions of strong absorption is about 50% above AAJ's data. Since Auman's data are based on band strengths measured in the 1960s, a comparison with more up-to-date values should definitely be interesting. Yet, agreement of the straight mean absorption coefficient is far from a guarantee for the data to have an identical effect on the atmospheric structure, since the ratio between the number of strong and weak lines is also important and hidden in the SM comparison. A good way of comparing absorption coefficients is by their ODFs, since these show the ratio between strong and weak lines. An even better way is obviously to compare the model atmospheres they produce or the computed spectra. The best is, nevertheless, to compare computed spectral features from atoms or molecules that do not themselves contribute to the opacity, since one is then avoiding feed-back effects between changes in opacity and the model structure, which can have a tendency to hide possible errors in the opacity. The most important improvement in distributing the measured straight mean into individual lines is that this permits a more accurate sampling, and Brown et al. (1989; BJACS) constructed OS data from the line list of AAJ on the basis of which they constructed model atmospheres by solving the transfer equation in $\approx$ 1000 frequency points (compared to Auman's 60).

Plez et al. (1991; PBN) constructed a line list for the water molecule in a way very similar to the one prescribed by AAJ, and an OS produced from that list was then used in more than 10 000 frequency

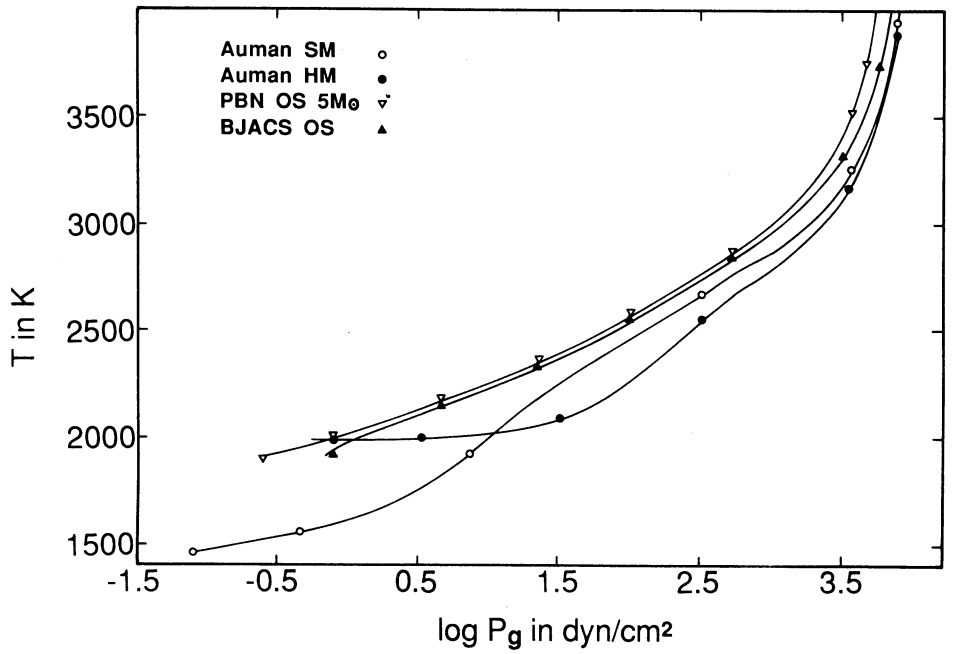

Figure 2: Four computed model atmospheres for an M-type giant of T_{eff} = 3000 K, log(g) = 1.0 and Z = $Z_\odot$. The two most recent computations are marked with open (BJACS) and filled (PBN) triangles, respectively. Symbols indicate $\log(\tau_R) = -5, -4, -3, -2, -1, 0$, and 0.2. Two older models due to Auman (1969) are marked with open circles where the straight mean absorption coefficient was used, and filled circles where the harmonic mean was used. Symbols indicate $\log(\tau_{std}) = -4.3, -3, -2, -1, 0$, and 0.6.

points to construct spherical model atmospheres with 62 depth points. The average line strengths, S_0, in each interval of the spectrum, were computed from the data of L73, as $S_0 = \chi^i_{SM}/n_i = \chi^i_{SM}\, d_i/(\nu_{i+1} - \nu_i)$. The line strengths, S, of individual lines were then computed from S_0 as $S = S_0 \ln(u)$, where u is a random number uniformly distributed in the interval $0 < u \leq 1$. PBN noticed that d_i was a decreasing function of temperature in the L73 data, which they interpreted as being due to the fact that a bigger number of high-excitation lines will be observed at high temperatures than at low temperatures. AAJ avoided this problem by using (from the measurements of L73) only the data at 3000 K, then assigning the lower excitation level statistically, and finally computing the absorption coefficient at other temperatures from these data. PBN tried to compensate for the measured temperature dependence of n_i by forcing agreement to the temperature dependence of the measured SM opacity by introducing weak and strong lines. The strong lines were defined as those actually seen in the measurement of n_i at a given temperature, whereas weak lines were given a strength that was 0.001 times the strength of the strong lines and assumed to be present in a number $n_i^{weak}(T) = n_i(T{=}3000) - n_i^{strong}(T)$. The absorption coefficient obtained in this way was never compared to the one obtained by AAJ, but in Fig. 2 we compare a model from each of the grids, both with T_{eff} = 3000 K, $\log(g) = 1$ and $Z = Z_\odot$. The agreement is found to be very good, which is stimulating since the two codes are independent. Because the molecular opacity when excluding water is rather different in the two grids, it indicates that H_2O must be very dominant at least for temperatures below 3000 K. That the effect of H_2O is similar in the two computations may, of course, just reflect that they are computed in an almost identical manner in the two grids, and an independent line-by-line computation without the statistical treatment that includes the somewhat weak assumption of pre-specified values of n_i and d_i would be desirable. Also shown in Fig. 2 are the two models described in paragraph II (with identical T_{eff}, $\log(g)$, and Z, and due to Auman's 1967 calculations) that were based on the water opacity computed with harmonic and straight mean samplings, respectively. The fascinating thing about this comparison is that the difference between Auman's two models (e.g. measured as the difference in the surface temperature) is bigger than the difference between any of the other models. In other words, at least as to what concerns the computations of the upper model layers, ***a correct sampling of the water opacity has been of greater importance to the model structure of M stars than the combined effect of all the other improvements***

that have been introduced in model computations during the last 25 years! A somewhat similar illustration was done by PBN in comparing their models with the models of BBSW. The latter, described in paragraph III, were computed with line data very similar to those used by PBN, but with the sampling being the JOLA (straight mean) method. The most pronounced difference was a heating in the PBN models of up to 1000 K for $\tau_{Ross} \leq 10^{-2}$ compared to the BBSW models; the difference being due to the artificial blocking by the SM H_2O opacities in the BBSW models. A comparison of computed synthetic spectra with observed spectra of M star giants finally proved that the models computed with the OS sampling of the opacity were in appreciably better agreement with observations than those computed on the basis of the SM (JOLA) absorption coefficient.

VI. CONCLUSIONS

We have described the various sampling methods that are in use, and results from models calculated with different samplings have been compared. The ODF and the OS techniques are equally capable of representing the monochromatic absorption coefficient, but each has its strengths and weaknesses in terms of speed, flexibility, and range of applicability. Methods to transform straight mean absorption coefficients into line opacities have been discussed, and it has been shown that the two methods in use give similar results and that both are significant improvements compared to direct use of the straight mean.

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