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CROSS SECTIONS FROM COMPUTER EXPERIMENTS

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ABSTRACT

The use of the width fluctuation corrected Hauser-Feshbach formula is summarized and recent evidence which supports it as compared to other proposed formulas is reviewed. A new formula for the channel fluctuation degree of freedom parameter is given, and other recent developments are summarized.

The Hauser-Feshbach formula is the basic tool for the calculation of average compound nucleus reaction cross sections initiated by neutrons. It was first derived some 43 years ago in Bethe's 1937 review of nuclear physics,[1] and was given wider applicability with the appearance of the optical model of Feshbach, Porter, and Weisskopf.[2] The practical use of this formula was clarified in papers by Wolfenstein[3] and by Hauser and Feshbach[4] and its accuracy was sharpened by the introduction of the width fluctuation correction factor by Dresner[5] and by Lane and Lynn.[6] However in all these years no satisfactory generally applicable derivation of the formula has been found. Only in the weak absorption limit (small transmission factors) is Bethe's old derivation applicable. Because of its widespread use, both in applications and in basic physics, there has been a great effort in recent years by a number of groups[7-12] to derive a formula that is applicable also for strong absoption cases. These efforts have been at most partially successful. It has not been possible so far, to average the extremely complicated expression for the cross section which is obtained when one includes the required constraints of unitarity and causality.

One way of circumventing these theoretical difficulties has been to produce numerical averages of computer generated cross sections which satisfy all required conditions and constraints. Such calculations have been done principally at Argonne[11-15] and in Heidelberg.[16-18]

I want to describe the results of recent calculations of this kind. They seek to answer the following questions. What kind of formula best describes average compound cross sections, how do the parameters in such a formula depend on the dynamics of the reaction (e.g. numbers of channels and their transmission factors), and finally, how sensitive are these results to the statistical assumptions that are made.

The method used is to draw R-matrix parameters[7,19] at random from appropriate statistical distributions (e.g. normally distributed level amplitudes $\gamma_{\mu c}$ and level spacings having the Wigner distributions,) and to construct from them R-matrices and from these numerical cross sections which can then be averaged. I shall refer to these as computer experiments.

Several forms for the average cross section formula from partial wave channel a to partial wave channel b have been suggested.[7-12] The width fluctuation corrected Hauser-Feshbach formula[11] is of the form

$$\bar{\sigma}^{fl}_{ab} = \frac{\pi}{k_a^2}\left\langle \frac{t^a_\mu\, t^b_\mu}{t_\mu} \right\rangle_\mu \tag{1}$$

where the average is over the index μ and the positive quantitives t^a_μ and t^b_μ are distributed independently in μ, and $t_\mu = \Sigma_c\, t^c_\mu$ is the sum over competing channels. For all channels c

$$\left\langle t^c_\mu \right\rangle_\mu = T_c \tag{2}$$

where T_c is the transmission factor for channel c. The distributions of the t^c_μ are usually taken to be one of the family of chi-squared distributions with frequency functions

$$f_\nu(x) = \left(\frac{\nu}{2}\right)^{\frac{\nu}{2}} x^{\left(\frac{\nu}{2} - 1\right)} e^{\left(-\frac{\nu}{2} x\right)} \Big/ \Gamma\left(\frac{\nu}{2}\right) \tag{3}$$

so that with each channel c is associated the positive degree of freedom ν_c of the distribution function of the t^c_μ. Then the average cross section (1) can be written

$$\bar{\sigma}^{fl}_{ab} = \frac{\pi}{k_a^2}\, \frac{T_a\, T_b}{\Sigma_c\, T_c}\, G_{ab}\, C_{ab} \tag{4}$$

where the width fluctuation correction is given by the product of the two factors

$$G_{ab} = \left\langle \frac{t^a_\mu\, t^b_\mu}{t_\mu} \right\rangle \Big/ \frac{\left\langle t^a_\mu\, t^b_\mu \right\rangle}{\left\langle t_\mu \right\rangle} \;, \tag{5}$$

$$C_{ab} = \frac{\left\langle t^a_\mu\, t^b_\mu \right\rangle}{\left\langle t^a_\mu \right\rangle \left\langle t^b_\mu \right\rangle} = 1 + \delta_{ab} 2/\nu_b \quad . \tag{6}$$

The correlation enhancement factor C_{ab} has been evaluated in Eq. (6) for the assumption that t_μ^a and t_μ^b are uncorrelated for $a \neq b$. It ordinarily causes an enhancement of the elastic cross section $\bar{\sigma}_{aa}^{fl}$ by a factor of $W_a = 1 + 2/\nu_a$ and a corresponding reduction in all cross sections due to G_{ab} which keeps the total flux $\Sigma_b\, \bar{\sigma}_{ab}^{fl} = \pi T_a/k_a^2$ the same. As a result the net elastic enhancement due to $G_{aa}\, C_{aa}$ is less than W_a. The values of ν_a vary from unity in the weak absorption limit to a value of up to 2 for strong absorption, as we shall see later. Therefore elastic enhancements vary from between factors of 3 and 2. The value of ν for lumped channels is a weighted sum of the ν's for the component channels and so for lumped gamma ray channels ν_γ may be quite large. Similarly, if a fission channel is taken to include two or more fission modes, ν_f may be greater than 2.

It is, however, also possible for the factor G_{ab} to yield an enhancement. This occurs if there are only a few strong channels competing so that the distribution of the total t_μ is given by small ν_t, but channels a and b are weak, so that t_μ^a and t_μ^b contribute little to t_μ and are thus only weakly correlated with t_μ.[14] Then G_{ab} can approach the value of

$$G_{ab} \sim \left\langle t_\mu^{-1} \right\rangle \left\langle t_\mu \right\rangle = \begin{cases} \infty \text{ for } \nu_t < 2 \\ \left(1 - \frac{2}{\nu_t}\right)^{-1} \text{ for } \nu_t > 2 \end{cases} \quad . \tag{7}$$

We see that in such cases the enhancements of both elastic and inelastic cross sections can become arbitrarily large. That this is indeed so can be seen from Fig. 1 where the cross section enhancements obtained from computer experiments are compared with the predictions of Eq. (4).[14]

The importance of these results lies in part in the practical possibility of such large enhancements, and in part because these computer experiments discriminate effectively against competing cross section formulas[8,9,16] all of which include an elastic enhancement but do not envisage large enhancements of nonelastic cross sections. For this reason we prefer Eq. (4) for which there exists also some detailed theoretical support.[11]

The next questions is then, what are the values of the channel degree of freedom parameters ν_c. In the low energy weak absorption limit the result is well known. There the t_μ^c are equal to $2\pi\, \bar{\Gamma}_\mu^c/D$, where the Γ_μ^c are the familiar partial resonance widths which have a Porter-Thomas distribution for which $\nu_c = 1$. D is the resonance level spacing. For weak absorption ($T \lesssim 0.2$) the formulas derived in Ref. (11) work well. Many arguments have been given[7-10] why ν_c should vary from 1 to a value of 2 as the strong absorption limit ($T_c = 1$) is approached. These arguments are based on applications of the central limit theorem but they do not take into account the severe constraints which the unitarity condition imposes on cross sections. Recently systematic computer experiments were undertaken to study the behavior of ν_a.[15] The results are shown in Fig. 2, where ν_a is plotted against the sum of all competing channel transmission coefficients and different symbols are used for different values of T_c. A least square fit to a three-parameter formula which incorporates the qualitative features of these results yields

$$\nu_c = 1.78 + \left(T_c^{1.212} - 0.78\right) e^{-0.228 \Sigma_c T_c} \quad . \tag{8}$$

These values are then to be used to evaluate Eqs. (5) and (6) using the integral expression.[7,11]

$$G_{ab} = \int_0^{\infty} dt \prod_f \left(1 + \frac{2t\nu_f^{-1} T_f}{\Sigma_g T_g}\right)^{-\left(\frac{1}{2}\nu_f + \delta_{fa} + \delta_{fb}\right)} \quad , \tag{9}$$

which can be evaluated satisfactorily by a twenty point Gauss-Laguerre quadrature. It is interesting to note that contrary to naive expectations ν does not go to 2 in the strong absorption limit. This indicates that the unitarity effects are strong enough to spoil the statistical central limit theorem arguments. In the many channel limit ν appears to approach a value of about 1.8 regardless of channel transmission factors.

In addition to these results, the dependence of ν_a upon the R-matrix statistics were studied for the case of strong absorption (T = .99.) Results were obtained by modifying the normal distribution of R-matrix pole amplitudes $\gamma_{\mu a}$ (having a fourth central moment $\mu_4 = 3.0$) so that μ_4 took on values of 2.77 and 3.26. The surprisingly large effect displayed in Fig. 3 again contradicts the central limit theorem argument which is independent of starting statistics. Perhaps even more surprising is the large dependence of ν upon the R-matrix level spacing distribution which is also displayed in Fig. 3. In addition to the Wigner distribution of level spacings, with standard deviation $\sigma_D = 0.523$, calculations were performed with uniformly spaced levels with $\sigma_D = 0.0$, and with uncorrelated level position, that is an exponential spacing distribution with $\sigma_D = 1.0$. These results tend to explain the difference of the present results (Eq. (8)) from those of the Heidelberg group[16-18] which obtained the expected value of $\nu = 2$ in the strong absorption limit with similar computer experiments. However, their R-matrix level spacing distributions are generated from biased random number samples which do not generate a Wigner distribution.[17] Their actual spacing distribution has a $\sigma_D = 0.475$, which, by interpolation should yield the dotted curve in Fig. 3, and thus, in consideration of statistical errors, is consistent with $\nu = 2$ for all T = .99 cases which they considered.

Another question of recent interest has been what the effect of competing direct reactions is upon average compound nucleus cross sections. The method for dealing with this problem has been developed by Engelbrecht and Weidermüller[20], who showed that the problem can be transformed to one without direct reactions by means of a unitary transformation of the matrix of average reaction amplitudes. As a result of this, average compound nucleus cross sections that compete with direct reactions can acquire a share of the elastic enhancement. However, as shown in Ref. (12), this will be of practical significance in only very special situations which are characterized by few directly coupled channels and an average S-matrix that is very close to a limiting condition imposed by the causality requirement.

In summary, the best presently available method for the evaluation of average compound nucleus cross sections is given by the width fluctuation corrected Hauser Feshbach formula of Eqs. (4)-(6), (9) with the channel degree of freedom parameters ν_c determined by Eq. (8). The optical model is used to obtain the transmission factors T_c for the neutron channels. For non-optical mode channels, such as fission and gamma ray emission, the T_c are evaluated from $2\pi\ \Gamma_c/D$. Angular distributions are calculated as described in Ref. (64), Section C. where $\Theta_{\mu c}$ is the same as t_μ^c.

Because of the great sensitivity of strong absorption average cross sections to statistical assumptions, as shown in Fig. 3, it remains to be investigated whether the R-matrix parameter statistics are in fact the same for all absorption strengths, as has been assumed here as reasonable because the R-matrix itself is not affected by channel properties, such as transmission factors.

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REFERENCES

1. H. A. BETHE, Revs. Mod. Phys., 9, 69 (1937).

2. H. FESHBACH, C. E. PORTER and V. F. WEISSKOPF, Phys. Rev., 96, 448 (1954).

3. L. WOLFENSTEIN, Phys. Rev., 82, 690 (1951).

4. W. HAUSER and H. FESHBACH, Phys. Rev., 87, 366 (1952).

5. L. DRESNER, CU-175, p. 71 (1957).

6. A. M. LANE and J. E. LYNN, Proc. Phys. Soc., (London) A70, 557 (1957).

7. P. A. MOLDAUER, Phys. Rev., 135, B642 (1964).

8. M. KAWAI, A. K. KERMAN and K. W. McVOY, Ann. Phys. N.Y. 75, 156 (1973).

9. D. AGASSI, H. A. WEIDENMÜLLER and G. MANTZOURANIS, Phys. Lett. C 22, 145 (1975).

10. P. A. MELLO, Phys. Lett. B 81, 103 (1979). P. A. MELLO and T.H. Seligman to be published.

11. P. A. MOLDAUER, Phys. Rev., C 11, 426 (1975).

12. P. A. MOLDAUER, Phys. Rev., C 12, 744 (1975).

13. P. A. MOLDAUER, Phys. Rev., 171, 1164 (1968).

14. P. A. MOLDAUER, Phys. Rev., C 14, 764 (1976).

15. P. A. MOLDAUER, Nucl. Phys., to be published.

16. J. W. TEPEL, H. M. HOFMANN and H. A. WEIDENMÜLLER, Phys. Lett. B 49, 1 (1974).

17. H. M. HOFMANN, J. RICHERT, J. W. TEPEL, and H. A. WEIDENMÜLLER, Ann. Phys. N.Y. 90, 403 (1975).

18. H. M. HOFMANN, J. RICHERT, J. W. TEPEL, Ann. Phys. N.Y. 90, 391 (1975).

19. A. M. LANE and R. G. THOMAS, Revs. Mod. Phys., 30, 257 (1958).

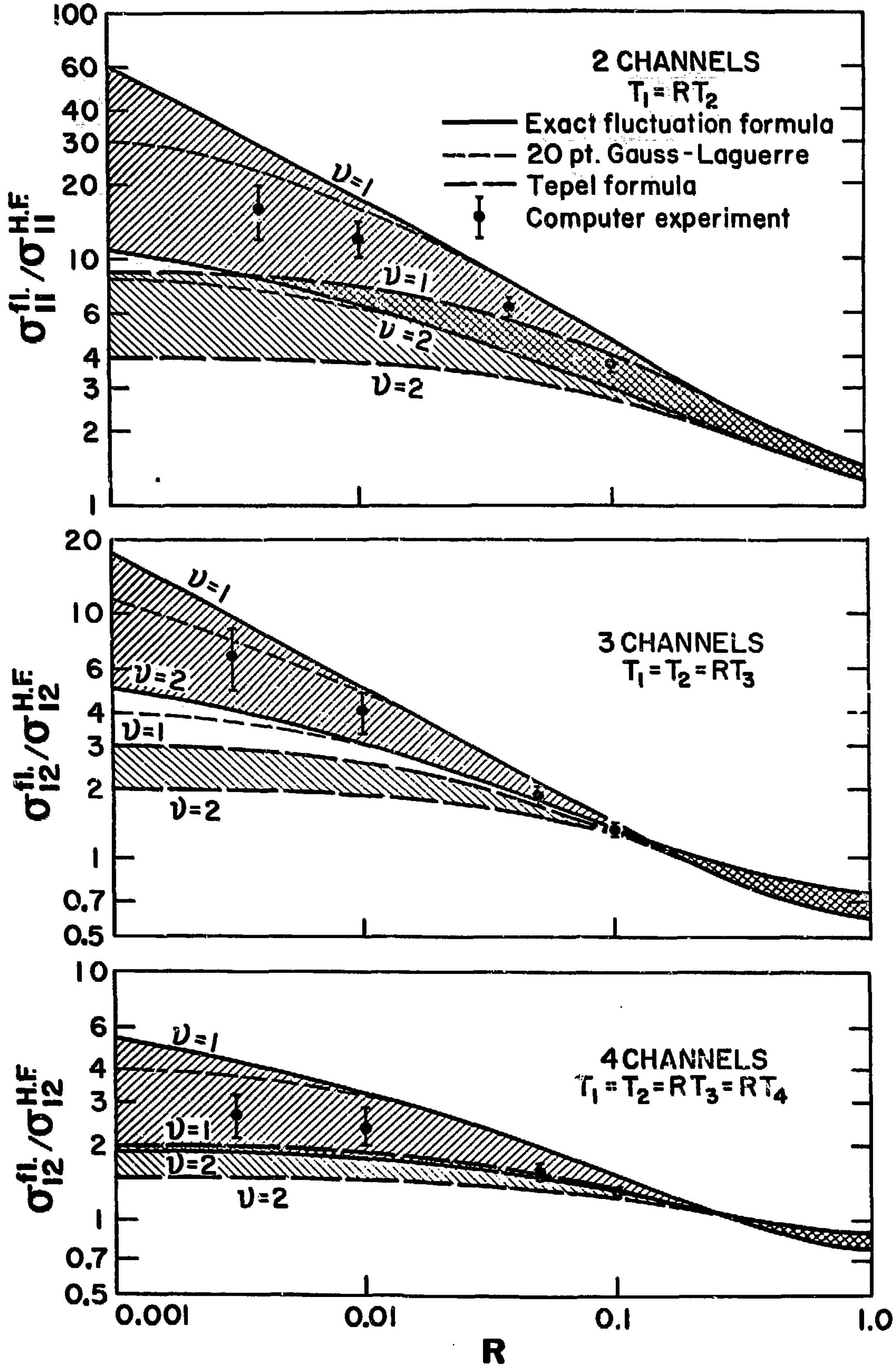
20. C. A. ENGELBRECHT and H. A. WEIDENMÜLLER, Phys. Rev. C 8, 859 (1973).

FIGURE CAPTIONS

Fig. 1. Enhancements, compared to Hauser-Feshbach, of small compound cross sections for a variety of two, three and four channel cases. The predictions of each of two theories lie within the shaded regions bounded by the curves for $\nu = 1$ (all channels) above and $\nu = 2$ (all channels) below. In each case the upper shaded region corresponds to the width fluctuation effect in Eq. (4); the lower region corresponds to the formula of Refs. 16 and 17. The points show the average results and variances of computer experiments with T(large) = 0.91 (two channel cases) and T(large) = 0.84 (three and four channel cases).

Fig. 2. Channel degree of freedom parameters ν vs. the transmission coefficient sum ΣT as calculated numerically with standard statistics for various channel transmission factors T. The solid lines give the results obtained from the formula of Eq. (8).

Fig. 3. Strong absorption dependence of the channel degree of freedom parameters ν upon R-matrix pole statistics as discussed in the text. All channels have transmission coefficients T = 0.99. The solid line is computed from Eq. (8) with standard statistics. The dashed lines indicate the trend of the results with non-standard statistics.



2 CHANNELS
$T_1 = RT_2$
Exact fluctuation formula
20 pt. Gauss-Laguerre
Tepel formula
Computer experiment
$\nu=1$
$\nu=2$
3 CHANNELS
$T_1 = T_2 = RT_3$
4 CHANNELS
$T_1 = T_2 = RT_3 = RT_4$
$\sigma_{11}^{fl.}/\sigma_{11}^{H.F}$
$\sigma_{12}^{fl.}/\sigma_{12}^{H.F}$
0.001
0.01
0.1
1.0
R

Figure 1

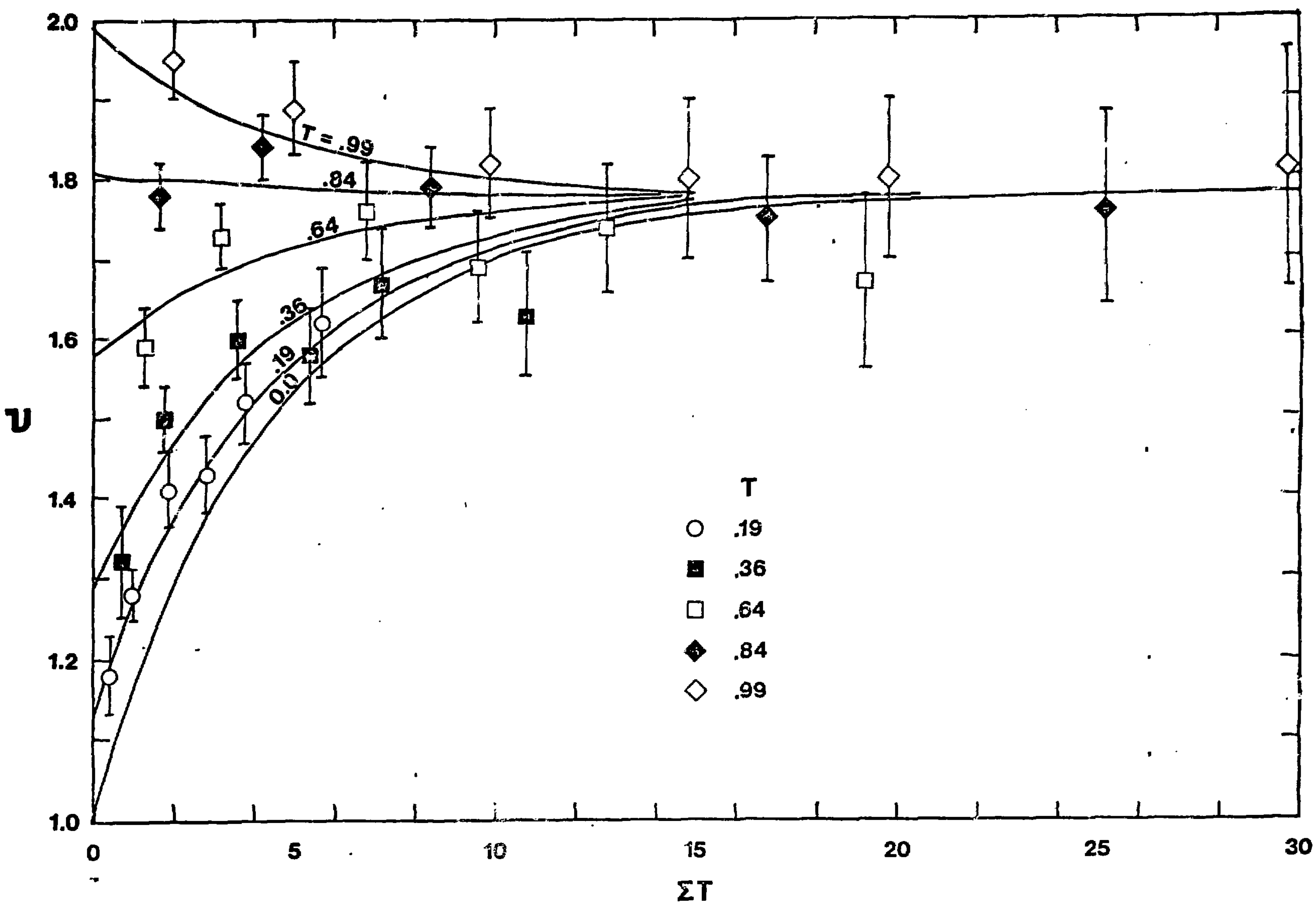
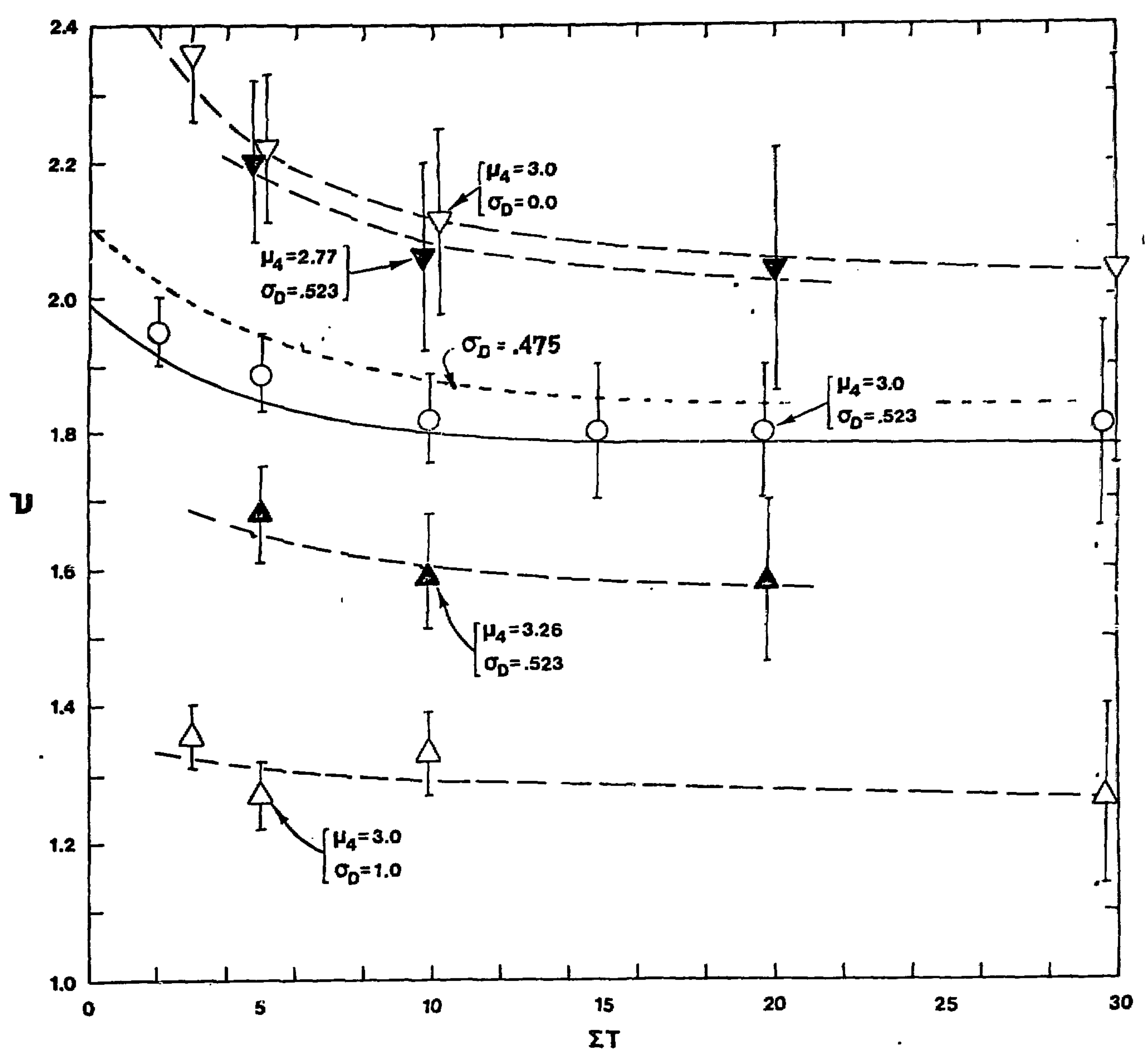

2.0
1.8
1.6
1.4
1.2
1.0
υ
0
5
10
15
20
25
30
ΣT
T = .99
.84
.64
.36
.19
0.0
T
.19
.36
.64
.84
.99

Figure 2



2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ν
0
5
10
15
20
25
30
ΣT
μ4=3.0
σD=0.0
μ4=2.77
σD=.523
σD = .475
μ4=3.0
σD=.523
μ4=3.26
σD=.523
μ4=3.0
σD=1.0

Figure 3