Improved analysis of parity violation at neutron p-wave resonances of ²³⁸U based on resonance spin assignments

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We have measured the spins of p-wave resonances in the reaction of low energy neutrons with 238 U nuclei and used them to reanalyze the parity violation experiment of the TRIPLE Collaboration carried out with this nucleus. The estimate of the root-mean-square matrix element of the parity violation interaction, M, including a bias correction, is found to be $\hat{M} = 0.62^{+0.33}_{-0.20}(68\% \text{ C.L.})^{+0.88}_{-0.33}(95\% \text{ C.L.})$ meV. The spin assignments of the resonances improved the analysis.

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In this journal the TRIPLE Collaboration published its first result on parity violation (PV) at p-wave resonances of ²³⁸U in a transmission experiment with polarized low energy (10-300 eV) neutrons using a neutron time-of-flight beam from the LANSCE facility [1]. In this work PV could be studied at many, that is 16, p-wave resonances. This experiment is therefore a considerable improvement with respect to pioneering experiments of this kind at Dubna in which PV has been studied at one or two resonances per isotope below 20 eV [2]. In the zero-spin nucleus 238 U the $1/2^-$ p-wave resonances can be admixed with the $1/2^+$ s-wave resonances due to PV weak nuclear interactions, and thus, may show PV effects. Strong enhancements of these PV effects occur due to (i) the proximity of s and p resonances, and (ii) by admixing a (strong) s-wave resonance or several s-wave resonances into a weak p-wave resonance $(\Gamma_n^s \gg \Gamma_n^p)$. Although one might expect parity mixing between 3/2 and 3/2 compound nuclear levels of ²³⁹U, there are no 3/2⁺ neutron resonances in the reaction of low energy neutrons with ²³⁸U to make parity violation manifest at the 3/2 p-wave resonances. The weak p-wave resonances can be distinguished easily from the strong s-wave resonances in the considered low energy range of the $^{238}\text{U}+n$ reaction; however, their spins (1/2 and 3/2) are not known without further informa-

The TRIPLE results made it possible for the first time to analyze PV data in a statistical manner under the assumption that the PV matrix elements of one isotope are from a Gaussian distribution with zero mean and variance M^2 ; that is, M, is a parameter, which can be identified with the root-meansquare of these matrix elements if the above assumed distribution is correct. M is related to the strength of the weak nuclear PV force. It is therefore an important quantity to know [1,3]. The 63.5 eV resonance in the $^{238}\text{U}+n$ reaction shows a PV effect ≈ 6 times its standard deviation (σ), and hence, this must be a 1/2 resonance to a very high degree of reliability. There are three p-wave resonances with PV ef-

An experimental program has been started at the GELINA facility in Geel (Belgium) to determine spins of p-wave resonances on the basis of neutron capture γ spectroscopy for the following reasons: (i) to see whether the spin assignments of ²³⁸U correlate with the PV effects or not, (ii) to check the 10.2 eV resonance spin assignment proposed by Wasson et al., and (iii) to improve the estimate \hat{M} [7–9]. Since the number of PV data is still relatively small the possibility that a bias in estimating M may occur is considered. Because of the different interpretations of the results by TRIPLE and by Bunakov some of the expressions used in the analysis will be discussed in the Bayes approach first.

There are two conditional probabilities involved in this problem: (i) the conditional probability $P(\{X_i\}^N|M)$ of a set of N measured values $\{X_i\}^N = X_1, X_2, ..., X_N$ depending on the parameter M according to a specific theory or model, and (ii) the posterior probability $P(M|\{X_i\}^N)$ of M with the experimental results available. The question is now to determine an expression for $P(M|\{X_i\}^N)$ and use this to estimate M on the basis of the set of experimental data $\{X_i\}^N$. The relation between these two conditional probabilities is given by Bayes theorem [10,11]:

$$P(M|\{X_i\}^N) = \frac{P(\{X_i\}^N|M) \cdot P(M)}{P(\{X_i\}^N)},$$
 (1)

in which P(M) is the probability distribution of M describ-

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fects slightly above 2σ . However, one of them (at 10.2 eV) has been assigned by Wasson et al. as 3/2 [4]; thus, it should not show a PV effect. Either this spin assignment is wrong, or the deduced PV effect is zero with a small probability assuming that the measurement is correct. There are four other p-wave resonances with PV effects between 1σ and 2σ . The remaining eight p-wave resonances do not show PV effects within the quoted errors. TRIPLE analyzed these PV data on the basis of a maximum likelihood method without knowing the spins of these p-wave resonances and derived the estimate $\hat{M} = 0.56^{+0.41}_{-0.20}$ meV (68% confidence limit) of the parameter M [1]. Bunakov challenged the TRIPLE analysis stating that at most an upper limit of ≈1.5 meV (99% confidence limit) of the estimate can be achieved [5,6].

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ing prior information about this parameter, and $P(\{X_i\}^N)$ $=\int P(\lbrace X_i \rbrace^N | M) P(M) dM$ is the unconditional probability of $\{X_i\}^N$. This factor normalizes $P(M|\{X_i\}^N)$. Consider a set of N resonances, which are taken at random from a "nuclear box" in which the $1/2^-$ resonances occur with a fraction p and the $3/2^-$ resonances with fraction q = 1 - p. The probability of picking n of these $1/2^-$ resonances and N-n of the $3/2^-$ resonances without considering the order is $p^n q^{N-n}$. For each combination of n and N-n there are N!/n!(N-n)!possible sequences, which will be denoted as S_n^N , to order the spins over the resonances. These sequences have the same probability as long as no other information is taken into account. Consider the "reduced" PV asymmetries, denoted as Q_i in Ref. [1], as our set of experimental data $\{X_i\}^N$ at p-wave resonances i and assume that the measurements depend in a known way on the parameter M which can have different values for the different resonance spins. The conditional probability of this set of measured values, given M, can be expected as:

$$P(\{X_i\}^N|M) = \sum_{n=0}^N p^n q^{N-n} \sum_{S_n^N} P(\{X_i\}^N|S_n^N, M), \quad (2)$$

where $P(\{X_i\}^N|S_n^N,M)$ is the conditional probability of $\{X_i\}^N$ given a spin sequence S_n^N and M. For independent measurements this can be written as:

$$P(\{x_i\}^N | S_n^N, M)$$

$$= [P(X_1 | j_1, M) \cdot P(X_2 | j_2, M) \cdots P(X_N | j_N, M)]_{S_n^N}, \quad (3)$$

in which $j_1, j_2, ..., j_N$ are the resonance spins of a chosen spin sequence. The spin sequences can be paired in such a way, that one resonance (e.g., No. 1) can be factorized out in Eq. (2). That is:

$$P(\{X_i\}^N|M) = [pP(X_1|\frac{1}{2},M) + qP(X_1|\frac{3}{2},M)] \cdot P(\{X_i'\}^{N-1}|M), \quad (4)$$

in which $P(\{X_i'\}^{N-1}|M)$ is the same expression as Eq. (1) but with one measurement (No. 1) less, that is $\{X_i'\}^{N-1} = X_2, ..., X_N$. Carrying out this procedure for all resonances gives the expression:

$$P(\{X_i\}^N|M) = \prod_{i=1}^N \{pP(X_i|\frac{1}{2},M) + qP(X_i|\frac{3}{2},M)\}.$$
 (5)

Equation (5) gives the probability of a set of N measured values $\{X_i\}^N$ for a given M. However, one would like to reverse the procedure and try to get an estimate \hat{M} on the basis of these measurements. Using Bayes theorem, given by Eq. (1), the following equation for the posterior probability function is obtained:

$$P(M|\{X_i\}^N) = \left[\frac{P(M)}{P(\{X_i\}^N)}\right] \prod_{i=1}^N \{pP(X_i|\frac{1}{2}, M) + qP(X_i|\frac{3}{2}, M)\},$$
(6)

in which

$$P(\{X_i\}^N) = \int P(M)dM \prod_{i=1}^N \left\{ (pP(X_i|\frac{1}{2}, M) + qP(X_i|\frac{3}{2}, M) \right\}$$
(7)

takes care of the normalization of this function. In the Bayesian approach Eq. (6) is the posterior probability distribution of M based on the experimental data $\{X_i\}^N$ and prior knowledge of M expressed by P(M). In order to avoid subjectivity in the Bayesian approach one has to be careful about the prior knowledge of M which one wants to accept. In the current problem of parity violation with the assumed Gaussian distribution of the PV matrix elements one knows for sure that $M \ge 0$. Since at this point all values of $M \ge 0$ can be considered as equally probable, P(M) can formally be replaced by the unit step function U(M) = 1 for $0 \le M \le \infty$. Of course also a distribution P(M), which makes large values of M unlikely, can be introduced. However, this will not be pursued in this paper.

At this point a connection with the maximum likelihood method can be made. Equation (3) can be considered as the joint probability density function (PDF) of the set of independent measurements $\{X_i\}^N$ and Eq. (6) can be identified as the likelihood function L(M). The maximum value of L(M), or of $\ln L(M)$, gives the value of M which is the most likely. This is called the "estimate" and is indicated by \hat{M} .

In the TRIPLE experiment many runs, in which the neutrons have alternatingly positive and negative helicities, have been carried out to obtain the transmission asymmetries at a series of resonances simultaneously. For each resonance i a Gaussian fit of the histogram of the transmission asymmetry was made from which the mean value X_i with error e_i of the reduced PV asymmetries were derived [1]. We do not elaborate on the details how reduced PV asymmetries are obtained, but refer to the original papers [1]. X_i and e_i are expressed in meV. As mentioned before, the PV matrix elements are assumed to have a Gaussian distribution with zero mean and variance M^2 for the $1/2^-$ resonances. The probability density function is the convolution of two Gaussian functions, which again is a Gaussian function. For the $1/2^-$ resonances the PDF's can be written as:

$$f(x_i, M) = \frac{1}{\sqrt{2\pi(M^2 + e_i^2)}} \exp\left\{\frac{-x_i^2}{2(M^2 + e_i^2)}\right\}.$$
 (8)

These can be identified with the conditional probabilities $P(X_i|\frac{1}{2},M)=f(X_i,M)$ for the $1/2^-$ resonances in the Bayesian approach. For the $3/2^-$ resonances the PDF's are independent of M and the prior probabilities of these resonances can be written as:

$$P(X_i|\frac{3}{2},M) = \frac{1}{\sqrt{2\pi e_i^2}} \exp\left\{\frac{-X_i^2}{2e_i^2}\right\}.$$
 (9)

Combining Eqs. (6) to (9) gives the following expression for the likelihood function:

$$L(M) = \frac{1}{C} \prod_{i=1}^{N} \left[p \cdot \frac{1}{\sqrt{2\pi(M^2 + e_i^2)}} \exp\left\{ \frac{-X_i^2}{2(M^2 + e_i^2)} \right\} + q \cdot \frac{1}{\sqrt{2\pi e_i^2}} \exp\left\{ \frac{-X_i^2}{2e_i^2} \right\} \right]$$
(10)

in which 1/C denotes the normalization factor. This factor poses a problem since with the second (constant) terms in the factors of Eq. (10) the integral in C goes to infinity which means that Eq. (10) is not normalizable. Because of this problem TRIPLE introduced an upper limit of 10 meV in order to be able to normalize the likelihood function. In a way this is introducing prior knowledge about M, which is believed to be considerably below this accepted upper limit. In the TRIPLE publications [1] the values of p and q were taken to be 1/3 and 2/3. These values were justified on the basis of the assumed (2j+1) spin dependence near the neutron binding energy. If the better spin dependence function $(2j+1)\exp\{-(j+1/2)^2/2\sigma^2\}$ is used, with $\sigma \approx 3$ as lowest spin cutoff parameter for ²³⁸U conceivable with Ref. [12], the value of p becomes ≈ 0.38 . A change of p from 1/3 to 0.38 has very little effect on the estimate of M. Hence, we will stick to the original value of p. Reanalyzing the PV data of the 16 resonances of ²³⁸U with Eq. (10), that is without knowledge of the spins, we obtain the estimate \hat{M} =0.57 $^{+0.40}_{-0.21}$ (68% C.L.) $^{+1.18}_{-0.33}$ (95% C.L.) meV with the 68%, respectively, the 95% confidence limits indicated, a result in accordance with the earlier quoted value obtained by TRIPLE. With the 68% confidence limits there is still the possibility of 32% that the true value of M is outside this range. Therefore, we include 95% confidence limits.

Bunakov [5,6] used also Eq. (2) as a start to derive his likelihood function for the PV experiments. He considered in each spin sequence S_n^N first the subgroups of $n \ 1/2^-$ resonances and calculated their product (prior) probabilities using the PDF's given by Eq. (8). Thereafter, he applied Bayes theorem, Eq. (1), to obtain the posterior probabilities of the subgroups of 1/2 resonances; thus each having its own normalization factor. The same thing was done for the subgroups with m(=N-n) 3/2 resonances using the PDF's of Eq. (9) but multiplied by the delta function $\delta(M) = 1$ at M=0. Applying Bayes theorem to these subgroups again separately the $\exp\{-X_i^2/2e_i^2\}$ dependences are lost. Due to this procedure, spin sequences in which, e.g., the 63.5 eV resonance is assumed to be 3/2 get much larger probabilities than experimentally justified. For each spin sequence the normalized probabilities of the two subgroups were summed and subsequently all spin sequences were combined except the spin sequence with n=0, which was left out since it cannot produce PV. The likelihood function obtained in this way requires the calculation of $2^{N}-1$ integrals for normalization which makes the analysis very time consuming. It is not surprising that with Bunakov's likelihood function only an upper limit of M is obtained due to the introduction of the delta function and separate normalizations of the spin subgroups. By accepting an upper limit, Bunakov includes M=0. However, already on the basis of the PV effect of the 63.5 eV resonance alone M=0 is excluded.

The analysis simplifies if the resonance spins are known from another experiment making it possible to select on the

basis of physical information the 1/2 resonances for a maximum likelihood analysis. At the GELINA neutron facility in Geel (Belgium) spins of p-wave resonances of ²³⁸U have been determined on the basis of resonance neutron-capture γ-ray spectroscopy using high resolution Ge detectors and a neutron time-of-flight setup. Intensity ratios of low energy γ transitions as well as intensities of primary γ transitions to levels with known spins, made it possible to determine the spins of 19 p-wave resonances. These include the 16 p-wave resonances used in the TRIPLE experiment [7–9]. Seven of them turned out to have spin 1/2. Three of the four resonances showing PV effects larger than twice their standard deviation are within this group. The other nine resonances of the TRIPLE experiment were found to have spin 3/2, among them the 10.2 eV resonance for which a PV effect of slightly larger than two standard deviations has been quoted [1]. Something might be wrong with the deduced PV effect of this resonance. On the whole there is a reasonable correlation between the TRIPLE parity violation experiment and the Geel spin assignments. The fraction of 1/2 resonances of the set of assigned 19 resonances is 0.37 in agreement with the expected value of p based on Ref. [12].

The likelihood function for resonances with known assignments $1/2^-$ is given by:

$$L(M) = \frac{1}{C} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi(M^2 + e_i^2)}} \exp\left\{\frac{-X_i^2}{2(M^2 + e_i^2)}\right\}. \quad (11)$$

With more than one measurement this likelihood function is normalizable and thus it is not necessary to assume an upper limit for M in this case. The maximum of Eq. (11) can be obtained from $d \ln L(M)/dM = 0$, which leads to the likelihood equation:

$$\sum_{i=1}^{n} \frac{(M^2 + e_i^2 - X_i^2)}{(M^2 + e_i^2)^2} = 0.$$
 (12)

The root of this equation is the estimate \hat{M} . With unequal values of e_i Eq. (12) can only be solved numerically. With the PV data of the seven known $1/2^-$ resonances we obtain:

$$\hat{M} = 0.58^{+0.33}_{-0.20} (68\% \text{ C.L.})^{+0.88}_{-0.32} (95\% \text{ C.L.}) \text{ meV}$$

with the 68% and 95% confidence limits indicated. This estimate is close to the value obtained without knowing the spins; however, the 68% and 95% confidence intervals are smaller; 0.53 versus 0.61 meV, respectively, 1.20 versus 1.51 meV for the 68% and 95% intervals. The ratio of the 95% and 68% intervals is 2.26 with spins assigned and 2.48 without knowing the spins. Thus in our analysis the likelihood function resembles somewhat more closely a Gaussian function.

The Cramér-Rao lower bound which depends on $E\{d^2\ln L(M)/dM^2\}$, the expectation of the second derivative of the likelihood function at its maximum, gives an estimate of the smallest possible value of the variance of \hat{M} . For an unbiased estimator it is given by:

$$\operatorname{Var}(\hat{M}) \ge \frac{-1}{E\{d^2 \ln L(M)/dM^2\}} = \frac{1}{\sum_{i=1}^{n} \left[2M^2/(M^2 + e_i^2)^2\right]},$$
(13)

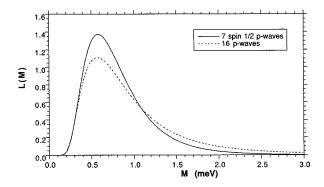
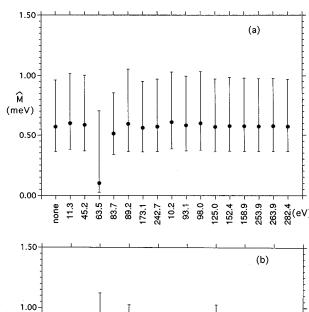


FIG. 1. Two likelihood curves; the dashed line relates to the 16 resonances of 238 U with the resonance spins not known, and the full line concerns the seven assigned $1/2^-$ resonances out of these 16 resonances.

in which the expectation values $E\{x_i^2\} = M^2 + e_i^2$ of the PDF's for the n $1/2^-$ resonances are used. Equation (13) gives the error estimate $\sigma_M = [\operatorname{var}(\hat{M})]^{1/2} \geqslant 0.23$ in fair agreement with the 68% confidence interval. However, the confidence limits obtained with the likelihood function are asymmetric due to its shape.

Figure 1 shows the likelihood function for the seven $1/2^-$ resonances compared with the likelihood function of all 16 resonances but with spins unknown. For the second curve p=1/3 is used. The likelihood function for the seven known $1/2^-$ resonances is sharper compared to the likelihood function for unknown spins which falls off more slowly at larger M values probably due to the additional resonances with small X_i values and larger errors. That both estimates \hat{M} are so close is likely related to the influence of the single strong PV effect of the 63.5 eV resonance and the fact that the observation of a PV effect with small error indicates spin 1/2. Mathematically this preference is automatically implemented in the analysis without knowledge of the spins by the $\exp\{-X_i^2/e_i^2\}$ terms in the likelihood function, Eq. (10), used by TRIPLE.

One may wonder how large the contribution of each resonance is to the estimate \hat{M} . This can be studied by removing all resonances once from the analysis and recalculating \hat{M} N (or n) times. Figures 2(a) and 2(b) show what happens in the case of the 16 resonances with spins unknown, respectively, in the case of the seven assigned $1/2^-$ resonances. In the first case removing the 63.5 eV resonance has a dramatic effect, while in the second case the effect of removing this resonance is considerably smaller and more in balance with the



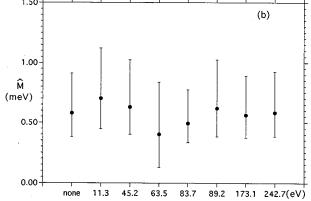


FIG. 2. Effect on the estimate \hat{M} when each resonance (indicated) is removed from the analysis one at a time; (a) for the 16 resonances without knowing the spins, and (b) for the seven assigned $1/2^-$ resonances. At the beginning of each plot the estimates \hat{M} without removing a resonance are given.

other six resonances. This suggests that by assigning spins to the resonances a more reliable analysis is achieved.

Parameter estimates obtained with small numbers of data should be looked at carefully for possible biases [10,11]. The estimator of M given by Eq. (12) is consistent; that is, it is unbiased in the limit of large number of data: $\lim_{n\to\infty} \hat{M} = M_{\rm true}$. However, with a small number of data points there might be a bias. This is already evident from a theoretical approach. Following the procedures given in Refs. [10] and [13] the bias $b_n(\hat{M}) = \hat{M} - M_{\rm true}$ can to first order approximation in 1/N be expressed as:

$$b_n(\hat{M}) \approx \frac{E\{d^3 \ln L(M)/dM^3\} + 2E\{[d \ln L(M)/dM] \cdot [d^2 \ln L(M)/dM^2]\}}{2E\{d^2 \ln L(M)/dM^2\}^2} = -\left\{4\hat{M}^3 \sum_{i=1}^n \left[1/(\hat{M}^2 + e_i^2)^2\right]\right\}^{-1}, \quad (14)$$

in which the right-hand part is based on expectations calculated with $E\{x_i^2\} = M^2 + e_i^2$ and $E\{x_i^4\} = 3(M^2 + e_i^2)^2$ using the PDF's given by Eq. (8). Assuming $\hat{M}^2 \gg e_i^2$ Eq. (14) reduces to $b_n(\hat{M}) = -\hat{M}/4n$, which gives $b_n \approx -0.021$ meV. Calculating the expectations with the experimental uncertainties e_i gives $b_n \approx -0.046$ meV.

Another method to get information about the bias is based on Monte Carlo simulations. We have carried out simulations with n values of X_i taken randomly from a normal (Gaussian) distribution $N(0,M^2)$ with errors from the normal distribution $N(0,\Sigma^2)$ in which Σ represents the averaged spread in the variances of x_i and taking $M_{\text{true}} = 1$ meV. For Σ we used 0, 0.5, 1, and 2. In all cases the average $\langle \hat{M} \rangle$ is systematically below M_{true} , but M_{true} is approached for increasing n. The bias observed in this simulation is fitted with:

$$b_n = \sum_r a_r / n^r \tag{15}$$

for r=1, and for r=1; 2. Accepting $\Sigma=0.5$ (roughly representing 238 U) and n=7 the bias, after scaling to $\hat{M}=0.58$ meV, is found to be -0.028 meV with only the r=1 term, and -0.031 meV with r=1 and 2.

An ingenious method to correct for the bias has been developed by Quenouille and is known as the jackknife method [14,15]. The method works as follows: if the estimate of a parameter from n data points is t_n , then by taking out each of the data points one by one, n other estimates t_{n-1} are obtained. With the bias in first order proportional to 1/n, the bias is given by $b_n \approx (n-1)\{t_n - \langle t_{n-1} \rangle\}$. The remaining bias is of order $1/n^2$. In this way we found $b_n \approx -0.064$ meV

Another Monte Carlo simulation has been carried out by Bowman and Sharapov [16] to test the likelihood function for unknown and known spins. They took values for the reduced matrix elements and their errors randomly from distributions closely resembling ²³²Th PV data [17]. The average $\langle \hat{M} \rangle$ obtained from 1000 pseudo random data sets is very close to $M_{\rm true}$ (spins not known) or equal to $M_{\rm true}$ (spins known). From their published histogram (number of events

against M) it can be concluded that the highest probability occurs for an estimate of M, which is several percent below $M_{\rm true}$ (the histogram is slightly asymmetric). Since the experiment can only be carried out with a limited number of resonances in $^{238}{\rm U}$ the probability of finding a value of \hat{M} slightly below the mean value ($M_{\rm true}$) is fairly large. Of course by improving the accuracy of \hat{M} the bias will be lowered, but will reach a limit of about a few percent when n remains small. It will be difficult to decrease the bias by increasing the number of studied $1/2^-$ resonances.

On the basis of the above considerations about the bias we accept $b_n \approx -0.04$ meV. As shown by Quenouille and other authors the variance of the estimate increases only slightly in this process of bias removal [14,15,18]. By combining the bias quadratically with the 68% confidence limits and $2.26b_n$ quadratically with the 95% confidence limits we arrive at the following final estimate:

$$\hat{M} = 0.62^{+0.33}_{-0.20} (68\% \text{ C.L.})^{+0.88}_{-0.33} (95\% \text{ C.L.}) \text{ meV}.$$

As conclusions we like to make the following statements: (i) The spin assignments of the 238 U p-wave resonances and the PV effects correlate well except for one resonance. (ii) The uncorrected estimates \hat{M} for both analyses (unknown versus known spins) are very close, however, the 68%, and especially the 95% confidence intervals are reduced with known spins. The analysis appears to be more reliable with assigned spins. (iii) A first order bias correction related to the small number of data points shifts \hat{M} by about +7%. (iv) If the spins are not known, the TRIPLE likelihood function is an excellent alternative.

One of us (H.P.) likes to acknowledge interesting discussions with J. David Bowman.

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