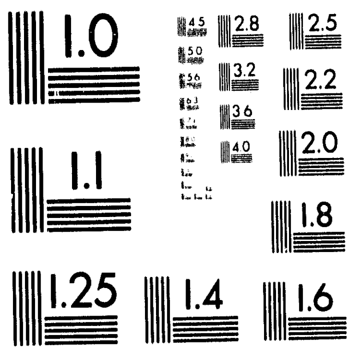
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Title: Likelihood Analysis of Parity Violation in the Compound Nucleus

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Likelihood Analysis of Parity Violation in the Compound Nucleus

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Abstract:

We discuss the determination of the root mean-squared matrix element of the parity-violating interaction between compound-nuclear states using likelihood analysis. We briefly review the relevant features of the statistical model of the compound nucleus and the formalism of likelihood analysis. We then discuss the application of likelihood analysis to data on parity-violating longitudinal asymmetries. The reliability of the extracted value of the matrix element and errors assigned to the matrix element is stressed. We treat the situations where the spins of the p-wave resonances are not known and known using experimental data and Monte Carlo techniques. We conclude that likelihood analysis provides a reliable way to determine M and its confidence interval. We briefly discuss some problems associated with the normalization of the likelihood function.

We consider the analysis of a set of measurements of parity-violating, PV, asymmetries of compound-nuclear, CN, states, $P_i = \dfrac{\sigma_+ - \sigma_-}{\sigma_+ + \sigma_-}$, where σ_+ and σ_- are the resonance cross sections for the i^{th} p-wave resonance for the neutron spin parallel or anti-parallel to the neutron momentum. Such data, for the spin-zero nucleus ^{238}U, were first published by the TRIPLE collaboration [1] and a value of M, the root mean-squared parity-violating matrix element between CN states, was extracted using likelihood analysis. The analysis was made difficult because the spins of the levels were not known. In this conference Corvi *et al.* [2] report a determination of the spins and apply the likelihood method to determine a more strict value of M. We discuss the particular problems of likelihood analysis of PV data. We expand the derivation given in Bowman *et al.* [1].

First we briefly review the formalism of PV in the CN and the statistical model of the CN. The PV asymmetry for the i^{th} level, P_i, may be written as a perturbation series [3, 4, 5]:

$$P_i = 2\sum_j \frac{V_{ij}}{E_i - E_j} \frac{g_j}{g_i}, \qquad 1.$$

where E_i and E_j are the energies of the p-wave resonance and the admixed s-wave resonances, V_{ij} is the matrix element of the PV interaction between states i and j, and g_i^2 and g_j^2 are their neutron widths. M can be extracted from a set of measurements of P_i by applying likelihood analysis. The treatment given here applies to spin-zero targets. Bunakov, Davis, and Weidenmüller [6] have extended the approach to non-zero target spins.

First, Equation 1. can be rewritten as:

$$P_i = \sum_j A_{ij} V_{ij}, \qquad 2.$$

where $A_{ij} = \frac{2}{E_i - E_j} \frac{g_i}{g_j}$. The squares of the A_{ij} are known since E_i and E_j and the neutron widths of the states, g_i^2 and g_j^2, are known experimentally. We assume that the V_{ij} are independent Gaussian random variables with a common variance, M^2, and mean zero. [A] The quantity, $Q_i = P_i / B_i$, where $B_i^2 = \sum_j A_{ij}^2$, can be written as:

$$Q_i = \frac{1}{B_i} \sum_j A_{ij} V_{ij} \text{ and} \qquad 3.$$

[A] This assumption follows from the statistical model of the CN. The wave functions of the states i and j are superpositions of large numbers of basis states. The statistical model of the CN assumes that the expansion coefficients of the states i and j in terms of the basis states l and m, a_l^i and b_m^j, are independent random variables with zero means. The matrix element $V_{ij} = \sum_l a_l^i \sum_m b_m^j \langle l|V_{PV}|m\rangle$ is then a sum of a large number of independent random variables. The Gaussian distribution of V_{ij} follows from the central limit theorem. V_{ij} has mean zero since each of the expansion coefficients is assumed to have mean zero.

$$\sum_j \left(\frac{A_{ij}}{B_i} \right)^2 = 1 .$$

Since Q_i is a sum of identically distributed Gaussian random variables (the V_{ij}) each with mean zero and the sum of the squares of the coefficients (the A_{ij}/B_i) is unity, Q_i itself has a Gaussian distribution with variance M^2 and mean zero. If many measurements of P_i with small errors and for p-wave resonances whose spins are known to be 1/2 are available, M^2 can be determined as the average of Q_i^2. (We demonstrate below that this assertion follows from likelihood analysis.) The situations where experimental errors are present and/or the spins of the p-wave resonances are not known can be treated using likelihood analysis.

Likelihood analysis is discussed in a number of standard references; the most familiar to experimental physicists is Eadie *et al.* [7]. The object of likelihood analysis is to determine the parameters of a theoretical model from a set of experimental data. Likelihood analysis also provides estimates of the errors in the parameters. We follow the Bayesian approach, as discussed in Eadie *et al.* [7], and assume the following: Let $\{x_i\}$ be a set of data with known experimental errors, $\{\sigma_i\}$. Let the outcomes of the experiments be given by a theoretical model having parameters $\{t_k\}$. Let $U(x_i, \sigma_i : t_k)$ be the joint probability density of the experimental outcome $\{x_i\}$, given model parameter values $\{t_k\}$. The likelihood function is defined as $L(t_k) = U(q_i, \sigma_i : t_k)$, where $\{q_i\}$ is a particular set of experimental data. The likelihood function may be considered to represent the probability density function of the model parameters, given the experimental outcome $\{q_i\}$. While $U(x_i, \sigma_i : t_k)$ is normalized when integrated over the x_i, $L(t_k)$ is not necessarily normalized when integrated over the t_k. The maximum-likelihood estimate, MLE, of the parameters $\{t_k\}$ are the values that maximize $L(t_k)$. The confidence region having confidence level α is the most compact region, Ω, such that $\int_\Omega L(t_i) d^n t_k = \alpha \int L(t_i) d^n t_k$. The range of integration for the right side is the full space available to the parameters t_k. We apply these ideas to the extraction of M when the spins of the levels are not known and when they are known.

When neutrons scatter from ^{238}U resonances in the CN ^{239}U are formed. p-1/2 resonances, which mix with nearby s-1/2 resonances, can have large PV longitudinal asymmetries; p-3/2 resonances cannot. If the spins of the p-wave resonances are not known, the spins of the p-wave levels must be considered to be unknown discrete theoretical parameters. The likelihood function, $L_j(M, j_i)$, will depend on the level spins as well as M. For a single level,

$$L_j(M,j) = \frac{1}{3}\delta\left(j,\frac{1}{2}\right)\frac{1}{\sqrt{2\pi\left(M^2+\sigma^2\right)}}\exp\left(-\frac{1}{2}\frac{Q^2}{\sigma^2+M^2}\right) + \frac{2}{3}\delta\left(j,\frac{3}{2}\right)\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{1}{2}\frac{Q^2}{\sigma^2}\right) = \frac{1}{3}\delta\left(j,\frac{1}{2}\right)R(Q,\sigma,M) + \frac{2}{3}\delta\left(j,\frac{3}{2}\right)S(Q,\sigma). \qquad 4.$$

The function $\delta(j, j')$ is unity if $j = j'$ and zero if $j \neq j'$. The factors 2/3 and 1/3 are taken as the *a priori* probabilities that a given resonance is p-3/2 or p-1/2. The term $R(Q,\sigma,M)$ is the probability density function of Q for j=1/2. $S(Q,\sigma)$ is the probability density of Q for j=3/2. The likelihood function for many levels is the product of the individual likelihood functions.

Recall that, the likelihood function is obtained by considering the dependence of a probability density function on a model parameter. R does depend on M. (If $Q^2 > \sigma^2$, R attains its maximum at $M = \sqrt{Q^2 - \sigma^2}$.) S does not depend on M. This contrast between the R and S terms in L(M) corresponds to an intuitive idea; while we can learn something about the value of M from the asymmetry for a p-1/2 resonance, no information on M can be obtained from a p-3/2 resonance; a p-3/2 resonance is expected to have an asymmetry value consistent with zero no matter what the value of M.

The likelihood function for M alone is obtained by averaging over all possible combinations of level spins. After evaluating the δ functions for each combination of level spins, there are 2^N terms in the sum. The sum can be expressed as a product:

$$L(M) = \prod_{i=1}^{N}\frac{1}{3}R(Q_i,\sigma_i,M) + \frac{2}{3}S(Q_i,\sigma_i). \qquad 5.$$

The likelihood function, L(M), is not normalizable since the term in the product that contains only S's does not depend on M. Bowman *et al.* [1] made the assumption that M could not be larger than an upper limit M_{max} and restricted the range of integration for the normalization of L(M) to [0, M_{max}]. This procedure is justified if results obtained are insensitive to the value of M_{max}.

The MLE for M is the value of M that maximizes L(M). Using the experimental data for ^{238}U [1] yields M = 0.57. A confidence interval for M, $M_1 < M < M_2$, analogous to the standard deviation of a Gaussian random variable can be obtained by minimizing M_2-M_1 subject to the constraint: [B] [C]

$$\int_{-1}^{+1} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx = .68 = \int_{M_1}^{M_2} L(M)\,dM \bigg/ \int_{0}^{M_{max}} L(M)\,dM \qquad 6.$$

The result is that with 68% confidence, $M = 0.57^{+0.55}_{-0.25}$.

Corvi *et al.* [2] measured the spins of the levels in the CN ^{239}U and applied likelihood analysis to make an improved determination of M. If the spins are known, then only the p-1/2 levels enter into the known-spin likelihood function;

$$K(M) = \prod_{i=1}^{N_{1/2}} R\left(Q_i^2, \sigma_i, M\right). \qquad 7.$$

[B] If $0 < M_1 < M_2 < M_{max}$, $L(M_1) = L(M_2)$. If $M_1 = 0$, $L(M_1) \neq L(M_2)$. This can be seen as follows: Find the most compact region Ω for which $\int_\Omega d^n t = \alpha \int L d^n t$ by minimizing $\int_\Omega d^n t$ with respect to the region Ω subject to the constraint that $\int_\Omega d^n t = \alpha \int L d^n t$ by introducing a Lagrange multiplier λ and minimizing $W = \int_\Omega L d^n t + \lambda\left(\int_\Omega d^n t - \alpha \int L d^n t = 0\right)$. W must be stable with respect to changing Ω by adding any infinitesimal region $\delta\Omega$. Therefore, $\int_{\delta\Omega} d^n t = \lambda \int_{\delta\Omega} L d^n t$ or $1 = \lambda L$ or L is constant for interior points of the region available to the parameters t_k. The interior points of the space available to M are $0 < M < \infty$. QED.

[C] An alternative approach to assigning errors is to find the values of M for which L(M) is reduced from its maximum value by a factor of $\exp\left(-\frac{1}{2}\right)$. This approach leads to $M = 0.57^{+0.39}_{-0.21}$ for the spins unknown and $M = 0.58^{+0.33}_{-0.20}$ for spins known. Corvi *et al.* [2] obtained $0.58^{+0.32}_{-0.20}$ using slightly different values than published in Zhu *et al.* [1] This approach has the advantage that it is not necessary to normalize L(M) in order to determine a confidence interval. The errors are smaller than for the approach in the text.

Since there is no M-independent term, K(M) is normalizable. [D] We obtain $M = 0.58^{+0.40}_{-0.22}$ using Equation 7. to determine the 68% confidence interval. The unknown-spin and known-spin results for M agree very well. The confidence interval obtained when the spins are known is slightly smaller. The fact that it is not much smaller can be understood. If a level exhibits a large PV asymmetry then its spin must be 1/2. Therefore adding spin information for such levels is to a large extent redundant and produces no great effect.

The MLE for M can be found explicitly when the spins are known. We introduce the log likelihood function;

$$k(M) = \ln(K(M)) = \sum_{i=1}^{N_{1/2}} \ln\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{1}{2}\ln\left(M^2 + \sigma_i^2\right) - \frac{1}{2}\frac{Q_i^2}{M^2 + \sigma_i^2} . \qquad 8.$$

Maximizing K(M) by setting $\frac{d}{dM}k(M) = 0$ yields;

$$\sum_{i=1}^{N_{1/2}} \frac{M}{M^2 + \sigma_i^2} = \sum_{i=1}^{N_{1/2}} \frac{M Q_i^2}{\left(M^2 + \sigma_i^2\right)^2} . \qquad 9.$$

In the case that all $\sigma_i^2 << M^2$, Equation 9. reduces to: [E]

$$M^2 = \frac{1}{N_{1/2}} \sum_{i=1}^{N_{1/2}} Q_i^2 . \qquad 10.$$

[D] Strictly speaking, while the probability that a level is p-3/2 is considerably reduced by spin-assignment measurements, there remains a non-zero probability that the each level is p-3/2. Therefore, while the coefficients of the M-independent terms, $S(Q_i,\sigma_i)$, are much reduced, they remain non-zero. This means that K(M) is not normalizable. Practically speaking, the use of Equation 7 for K(M) is fully justified.

The function K(M) is not normalizable if only one resonance is observed since $\int_0^\infty \frac{1}{\sqrt{2\pi(M^2+\sigma^2)}} \exp\left(-\frac{Q^2}{2(M^2+\sigma^2)}\right) dM$ diverges. In the text more than one resonance is involved; K(M) is normalizable.

[E] The next term in the expansion is:

$$M^2 = \frac{1}{N_{1/2}} \sum_{i=1}^{N_{1/2}} Q_i^2 + \sigma_i^2 - 2 \sum_{i=1}^{N_{1/2}} Q_i^2\sigma_i^2 \Big/ \sum_{i=1}^{N_{1/2}} Q_i^2 + \sigma_i^2 \sim \frac{1}{N_{1/2}} \sum_{i=1}^{N_{1/2}} Q_i^2 - \sigma_i^2$$

This demonstrates that the MLE of M^2 for the spins known and the errors in Q_i^2 small, is the average of the Q_i^2 as asserted above. Equation 10 can be used to estimate the error in M, ΔM, expected from a likelihood analysis of a set of data for which all $\sigma_i^2 << M^2$. The result is:

$$\frac{\Delta M}{M} = \frac{1}{2}\frac{\Delta M^2}{M^2} = \frac{1}{\sqrt{2N}} \qquad 11.$$

In order to assess the reliability of the application of the likelihood method to the determination of M we carried out a Monte Carlo simulation. We generated one thousand data sets with M=1 meV. Each data set represented the measurement of the Q values for a number of CN levels. The simulated data sets were similar to the data reported by Frankle *et al.* [8] for ^{232}Th. The errors in Q ranged from 0.03 to 1.0 meV. Each data set contained seven values of Q that differed from zero by more than 2.5 times its error. Each of the one thousand pseudo-random data sets was generated as follows: The j of each resonance was chosen randomly with the probability of j = 1/2 being 1/3 and j =3/2 being 2/3. The error in Q for each resonance, σ_i, was then chosen randomly according to the distribution of errors for the ^{232}Th experimental data. The value of Q for each resonance, Q_i , was generated as a Gaussian with mean zero and variance σ_i^2 for j = 3/2 and variance $\sigma_i^2 + M^2$ for j = 1/2. This process was continued until seven resonances with $Q_i > 2.5\ \sigma_i$ were generated. Likelihood analyses assuming the spins to be known and unknown were carried out for each of these thousand data sets. Figure 1 displays the results for known spins.

Figure 1. Monte Carlo Data

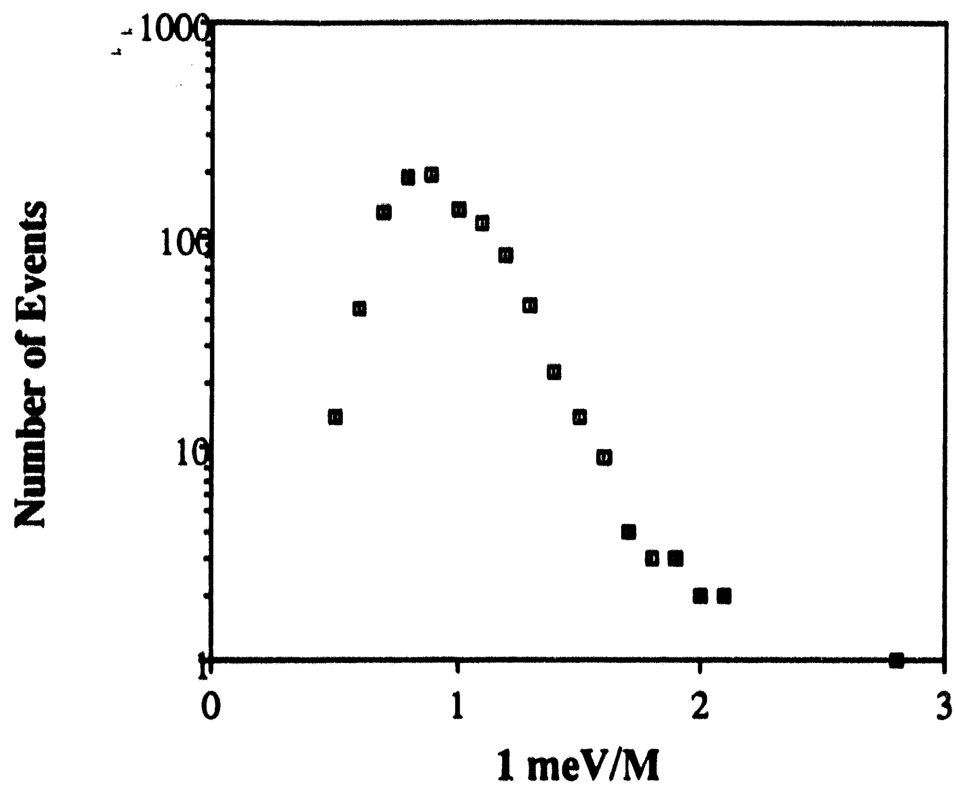

Figure 1. Results for the MLE's of M for one thousand pseudo-random data sets. The likelihood function was for known spins. The quantity 1 meV/M is the ratio of the true value of M (1.0 meV) to the MLE of M. Note that, the histogram of 1/M has a pronounced tail towards high values of 1/M just as the likelihood functions themselves. (See references 1, 2, and 8). This similarity supports the interpretation of L(M) as the probability density for the model parameter M.

With a known value of M we were able to investigate the bias of the MLE of M, the standard deviation of the MLE of M, the fraction of data sets for which the true value of M was contained in the 68% confidence interval about the MLE of M, and the average length of the 68% confidence interval. These results are summarized in Table 1.

Table 1. Summary of Monte Carlo Results

Spins	Average M	Standard Deviation M	Fraction in 68% Interval	Average 68% Interval
Not Known	0.96	0.22	0.76	0.56
Known	1.00	0.22	0.78	0.55

Table 1. Results of a Monte Carlo simulation of experimental data. The true value of M was 1.0 meV. One thousand data sets were generated as described in the text and the likelihood method applied assuming the spins to be known and unknown. Average M and Sigma M give the average and standard deviations of the MLE for M for the one thousand data sets. The bias of the MLE, the difference between the average of the MLE of M and the true value of M, is small compared to the standard deviation of M. Fraction in 68% Interval gives the fraction of data sets for which the 68% confidence interval about the MLE of M contained the true value of M. The fact that more than 68% of the data sets have the true value of M within the 68% confidence interval means that the confidence interval is too large. Average 68% Interval gives the average value of the length of the 68% confidence interval. The fact that one half the average value of the 68% confidence interval (0.28 for spins known or unknown) is larger than the standard deviation of M (0.22 for spins known or unknown) also indicates that the 68% confidence interval given by the likelihood method is somewhat too large.

We conclude that the likelihood method, using the forms of the likelihood functions given above, provides a trustworthy procedure for determining values of M from experimental asymmetry data. This conclusion is supported by the agreement of values of M and confidence intervals from experimental asymmetry data with and without the use of spin information. A Monte Carlo simulation lends additional support: The maximum-likelihood estimate of M has a small bias and the confidence intervals determined by the likelihood method are conservative.

One of us, JDB, thanks Gerry Garvey for suggesting Monte Carlo simulation as a means to establish the reliability of likelihood analysis.

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