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I. THE METHOD OF MOMENTS IN QUANTUM MECHANICS
II. THE π-MESIC DISINTEGRATION OF THE DEUTERON

Francis R. Halpern

(Thesis)

March 18, 1957

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I. THE METHOD OF MOMENTS IN QUANTUM MECHANICS

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ABSTRACT

The classical moment techniques of Tchebycheff, Markov, and Stieltjes have been applied to the problem of diagonalizing the Hamiltonian operator. These techniques lead in a natural way to an extension of the Rayleigh-Ritz principle and a series solution for the time-dependent Schrödinger equation. The application of these procedures to several simple problems is considered.

I. THE METHOD OF MOMENTS IN QUANTUM MECHANICS

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March 18, 1957

INTRODUCTION

The standard problem in quantum mechanics is the diagonalization of a Hermitian operator, the Hamiltonian. Usually the Hamiltonian consists of two parts; one can be diagonalized easily and the other cannot be diagonalized. Perturbation methods make use of the expansion of an eigenfunction of the total Hamiltonian in terms of the eigenfunctions of the diagonal portion of the Hamiltonian. The coefficients in this expansion are themselves power series in some parameter that characterizes the magnitude of the nondiagonal portion. Other techniques are also based on the possibility of expanding an eigenfunction of the total Hamiltonian in terms of eigenfunctions of the diagonal part.

By considering the inverse problem one is led to a class of methods for diagonalizing the Hamiltonian that may be called the method of moments. In principle it is always possible to expand the eigenfunctions of the noninteracting (diagonalizable) portion of the Hamiltonian in terms of the eigenfunctions of the total Hamiltonian. The coefficients and eigenfunctions in this expansion are of course unknown. The problem is now to remove all but one of the terms in the expansion by operating on the known eigenfunction of the diagonalizable portion. What remains is then an eigenfunction of the total Hamiltonian. A very simple example of this method is used to diagonalize finite matrices. If A is a finite matrix and ϕ is any vector, then we have

$$\lim_{n \to \infty} \frac{(\phi \,|\, A^{2n+1} \,|\, \phi)}{(\phi \,|\, A^{2n} \,|\, \phi)} = a_{max} \quad . \tag{1}$$

The vector ϕ is assumed to have an expansion of the form

$$\phi = \Sigma \alpha_i \psi(a_i) ,$$

where the $\psi(a_i)$ are the normalized eigenfunctions of A and belong to the eigenvalues a_i. The largest eigenvalue in the expansion is a_{max}. The quotient in Eq. (1) can be easily evaluated by use of the above expansion:

$$\frac{(\phi \left| A^{2n+1} \right| \phi)}{(\phi \left| A^{2n} \right| \phi)} = \frac{\Sigma \left| \alpha_i \right|^2 a_i^{2n+1}}{\Sigma \left| \alpha_i \right|^2 a_i^{2n}} .$$

As n tends to infinity, it is clear that the above expression tends to a_{max}.

The quantities $(\phi \left| A^n \right| \phi)$ will be denoted by A_n and are called the moments of the operator A, whether A is a finite matrix or not. It will be shown that they are also the moments of a probability distribution function $F_\phi(a)$. The method of moments consists of using the moments in as efficient a way as possible to find approximate eigenvalues and eigenfunctions and to solve the time-dependent Schrödinger equation. The precision of any calculation will of course depend on the number of moments employed. The principal advantage of the method of moments is that no separation is made of the Hamiltonian into perturbed and unperturbed portions, and the application of moment techniques does not depend on the size of the interactions (coupling constants) involved. It is necessary, however, to find initial-state vectors such that all the moments of the Hamiltonian under consideration are finite. This makes difficult the immediate application of these methods to problems having nonanalytic potentials and to problems in field theory that do not have a cutoff. The infinities encountered in field theory are no different from those found in perturbation theory, and are probably removable by appropriate renormalizations.

NOTATION

The operator under consideration is the Hamiltonian H. An initial state ϕ is assumed such that all the moments $(\phi \left| H^n \right| \phi)$, of the Hamiltonian in the state ϕ are finite. The eigenfunctions of H are $\psi(E_i, a_j)$, and they satisfy the equations

$$H\,\psi(E_i, d_j) = E_i, a_j),$$

$$A\,\psi(E_i, a_j) = a_j\,\psi(E_i, a_j),$$

and

$$\left[H, A\right] = 0.$$

The A's are one or more auxiliary variables that commute with the Hamiltonian and are necessary for the complete specification of the states of the system. In general it is possible to choose the initial state ϕ to be an eigenfunction of the auxiliary variables A, and they are then numbers during the course of a calculation. The system is also assumed to be contained in a box, so that the eigenvalues are discrete and the eigenfunctions are normalizable to unity.

The expansion of the state ϕ in terms of the eigenfunctions $\psi(E_i, a_j)$ is

$$\phi = \Sigma_i\, \alpha_i\, \psi(E_i) \quad .$$

Since ϕ is assumed to be an eigenfunction of the auxiliary variables A, only one eigenfunction of the Hamiltonian appears for each eigenvalue of the Hamiltonian, namely the one that belongs to the same set of values of the auxiliary variables as ϕ. Further reference to the auxiliary variables is suppressed. The moments of the Hamiltonian in the state ϕ can now be expressed in terms of the α's,

$$H_n = (\phi \left| H^n \right| \phi) = \sum_{i,j} (\alpha_i\, \psi(E_i) \left| H^n \right| \alpha_j\, \psi(E_j)) = \sum_i \left| \alpha_i \right|^2 E_i^{\,n} \quad .$$

It is convenient to introduce a function $F_\phi(E)$, the energy-distribution function of the system in the state ϕ. This function is defined by

$$F_\phi(E) = \sum_{E<E_i} |a_i|^2 \quad . \tag{2}$$

In terms of $F_\phi(E)$ the moments are

$$H_n = \int E^n d F_\phi(E) \quad .$$

The function $F_\phi(E)$ has three important properties. $F_\phi(E)$ is a nondecreasing function of its argument E; it is a function of bounded variation, i.e., $F_\phi(+\infty) - F_\phi(-\infty) < \infty$; and $F_\phi(E)$ is zero for all values of E less then a certain minimum value E_{min}. The first two properties characterize $F_\phi(E)$ as a probability-distribution function and are a consequence of the previously defined relationship (2) between the function $F_\phi(E)$ and the operator H and the state vector ϕ. The monotonic property follows, since $F_\phi(E)$ changes only at the points E_i, and there by the amounts $|a_i|^2$, which are positive numbers. Since ϕ was assumed to be normalized, $F_\phi(E)$ is of bounded variation for

$$F_\phi(+\infty) - F_\phi(-\infty) = \Sigma |a_i|^2 = (\phi | \phi).$$

The third property, finally, is of purely physical origin and is not shared by arbitrary Hermitian operators. The eigenvalues of H are the allowable energy levels of a physical system and they must have a lower limit E_{min}.

The enclosure of the system in a box serves to insure the second property rather than to produce a discontinuous function $F_\phi(E)$. All the results of this paper hold if the operator H has a continuous spectrum, provided the vectors ϕ that are chosen are normalizable to unity. If the vector chosen has a delta-function normalization, then this infinity must be suitably treated.

If ϕ had been an eigenfunction of H, $F_\phi(E)$ would have had a single point of increase at the eigenvalue to which ϕ belonged. The aim of any approximation technique is to produce an energy-distribution function that approximates as closely as possible a single step. A suitable measure of the degree of approximation is the standard deviation $\sigma(\phi)$, where $\sigma(\phi)$ is the positive square root of $\sigma^2(\phi)$, where

$$\sigma^2(\phi) = \frac{H_2}{H_0} - \left(\frac{H_1}{H_0}\right)^2 .$$

Since $\sigma^2(\phi)$ can be written as the norm of the vector

$$\left[H - \frac{(\phi|H|\phi)}{(\phi|\phi)}\right]\phi ,$$

it is a nonnegative number. It is zero only for an eigenfunction. In any state ϕ, the mean value of the energy distribution in that state, $\overline{E(\phi)}$, will be used as an estimate of an eigenvalue. The expression for $\overline{E(\phi)}$ is

$$\overline{E(\phi)} = \frac{(\phi|H|\phi)}{(\phi|\phi)} = \frac{H_1}{H_0} .$$

The amount to which eigenfunctions remote in energy from $E(\phi)$ enter into the distribution can be estimated from the Tchebycheff-Bienaymé inequality,[1]

$$\sum_{|\overline{E}-E_i|\geq k\sigma} |a_i|^2 = \int_{|\overline{E}-E|\geq k\sigma} dF_\phi(E) \leq \frac{1}{k^2} .$$

Similar inequalities can be worked out for the higher even moments. For example, defining $\rho(\phi)$ by

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[1] Harald Cramér, Mathematical Methods of Statistics (Princeton University Press, 1946) p. 182.

$$\rho^4(\phi) = \int (E - E(\phi))^4 \, dF_\phi(E) ,$$

we find that the corresponding inequality is

$$\sum_{|E(\phi)-E_i| \geq k\rho} |a_i|^2 = \int_{|E(\phi)-E_i| \geq k\rho} dF_\phi(E) \leq \frac{1}{k^4} .$$

TIME-INDEPENDENT METHODS

The foregoing remarks suggest that the determination of $F_\phi(E)$ would be desirable. Actually this amounts to an almost complete solution of the problem of finding the eigenvalues of H. $F_\phi(E)$ has the eigenvalues of H as discontinuities, and hence they could be read off if $F_\phi(E)$ were known. However, there are two serious drawbacks to this approach. First, an approximation technique yields a sequence of approximating functions $F^{(n)}_\phi(E)$, and even provided these converge to $F_\phi(E)$ it may be very difficult to determine from the approximating sequence the points of discontinuity of $F_\phi(E)$. Secondly, if the only data available are the moments of the operator H in the state ϕ then it is possible that there may exist several distinct distribution functions with the same moment sequence.[2] In this event it is impossible for an approximating sequence of functions based only on the moments to converge to all the possible different distribution functions that could have given rise to the moments. Methods for constructing an approximating sequence of functions from the moments have been given by Tchebycheff, Markov, and Stieltjes.[3] The decision whether a moment sequence uniquely determines a distribution function or not is quite technical and is not given here, but is related to the rate of increase of the moments. For the reasons outlined above, the function $F_\phi(E)$ is utilized only to assist in the discussion rather than as a point of departure for practical methods.

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[2] For an example of this see D. V. Widder, The Laplace Transform (Princeton University Press, 1946) p. 142.

[3] References to these earlier works will be found in the bibliography of Reference 5.

A more modest goal is this: given a state ϕ with distribution function $F_\phi(E)$, to manipulate ϕ in such a fashion that the modified distribution function that is generated resembles the distribution of an eigenfunction more closely than did the original $F_\phi(E)$. Two methods in this category are developed. The chief difficulty underlying both of them is the possibility that the distribution is not determined by its moments. The choice of initial state is crucial in all these considerations, and given a state such that its moments determine the distribution, both methods are feasible. It is possible that even if the distribution is not uniquely determined by the moments these methods may produce a state whose standard deviation is small compared with any of the characteristic energies in the problem, and that this state is then a satisfactory approximation to an eigenfunction.

The problem of determining $F_\phi(E)$ and the related problem of convergence will be ignored for the present. With these reservations methods will be described that will alter any vector and produce one with a smaller standard deviation. Only a single-state vector ϕ is assumed given, and the only way to modify it is to operate on it with the Hamiltonian or the Hamiltonian plus a constant. Thus one is led to consider the new state vector $\phi' = (H - c)\phi$ and to inquire under what circumstances its standard deviation is smaller than that of ϕ. The expansion of ϕ in terms of the eigenstates of H was

$$\phi = \Sigma\, a_i\, \psi(E_i)$$

and

$$F_\phi(E) = \sum_{E_i < E} \left| a_i \right|^2 \quad . \tag{3}$$

The effect of operating on ϕ with $(H - c)$ may be calculated:

$$\phi' = (H - c)\phi = \Sigma\, a_i (E_i - c)\, \psi(E_i) = \Sigma\, a_i'\, \psi(E_i),$$

where we have

$$a_i' = (E_i - c)\, a_i \quad .$$

By use of Eq. (3) with a_i replaced by a_i' one obtains the expression for $F_{\phi'}(E)$

$$F_{\phi'}(E) = \sum_{E_i < E} \left| a_i' \right|^2 = \sum_{E_i < E} (E_i - c)^2 \left| a_i \right|^2 .$$

Thus the vector ϕ' has in its expansion the same component eigenfunctions $\psi(E_i)$ as the vector ϕ but they occur with different weights unless c equals one of the E_i, in which case this component is completely removed.

The standard deviation of this new vector ϕ' can be computed, and when expressed in terms of the moments H_n of the original vector ϕ it becomes

$$\left[\sigma'(c)\right]^2 = \frac{H_4 - 2H_3c + H_2c^2}{H_2 - 2H_1c + H_0c^2} - \left(\frac{H_3 - 2H_2c + H_1c^2}{H_2 - 2H_1c + H_0c^2}\right)^2 .$$

As $\left| c \right|$ approaches infinity σ'^2 approaches

$$\frac{H_2}{H_0} - \left(\frac{H_1}{H_0}\right)^2$$

or just σ^2. If $\left| c \right|$ is very large all the components of ϕ are influenced equally.

The derivative of $\left[\sigma'(c)\right]^2$ with respect to c may be computed and is

$$\frac{d(\sigma')^2}{dc} = \frac{2}{(H_2 - 2H_1c + H_0c^2)^3} \Big\{ \left[H_0^2H_3 + 2H_1^3 - 3H_0H_1H_2\right] c^4$$

$$+ \left[5H_0H_2^2 - 4H_2H_1^2 - H_0^2H_4\right] c^3 + \left[3H_0H_1H_4 + 3H_1H_2^2 - 6H_0H_2H_3\right] c^2$$

$$+ \left[4H_1H_2H_3 + 2H_0H_3^2 - H_0H_2H_4 - 2H_1^2H_4 - 3H_2^3\right] c$$

$$+ \left[H_1H_2H_4 + H_2^2H_3 - 2H_1H_3^2\right] \Big\} .$$

The quantity $(H_2 - 2H_1c + H_0c^2)$ is always positive and its minimum value, which occurs at $c = H_1/H_0$, is equal to $\sigma^2 H_0$. If it were zero there would be no problem, ϕ would have been an eigenfunction of H. Thus the sign of $d(\sigma'^2)/dc$ is determined by the term inside the braces. Since the leading term is an even power of c, the derivative has the same sign at both plus and minus infinity. Since $\sigma'(\pm\infty) = \sigma$, the derivative cannot always have the same sign. As it has the same sign at plus and minus infinity it must have the opposite sign for some finite values of c. Thus there are at least two real roots to the equation

$$\frac{d(\sigma')^2}{dc} = 0 \quad .$$

One of them is the abscissa of a maximum and the other is the abscissa of a minimum.

If $d(\sigma'^2)/dc$ is positive at infinity, then $\sigma'(c)$ monotonically increases from $\sigma'(-\infty) = \sigma$ to the relative maximum, and from the minimum it increases monotonically to $\sigma'(+\infty) = \sigma$. If the derivative is negative at infinity then the reverse situation holds. In either event the minimum value of σ' is smaller than σ, and choosing c to be this optimum value produces a better vector ϕ'. If the equation has four real roots the situation is unchanged.

The procedure can now be repeated. Starting with ϕ', a c' can be found such that $(H - c')\phi'$ has a smaller standard deviation than ϕ'. The procedure can thus be iterated and vectors of the type

$$\phi_n = (H - c_n)(H - c_{n-1}) \ldots (H - c_0)\,\phi \qquad (4)$$

are to have their standard deviations minimized with respect to $c_1, c_2, \ldots, c_n$. There are a variety of ways in which the sequence of constants $c_1, c_2, \ldots, c_n$ can be chosen. The process outlined above essentially consists of choosing them one at a time on the basis of the previous choices. A more efficient way of choosing them consists in finding σ_n as a function of the c's and then choosing all the c's simultaneously. This leads to considerably more complicated equations for the c's, but reduces the standard deviation more rapidly.

Since all the factors in Eq. (4) commute it is clear that σ_n is also a function of the elementary symmetric functions in the c's, and in fact ϕ_n can be written in terms of the n symmetric functions

$$\phi_n = (S_0H^n - S_1H^{n-1} + S_2H^{n-1} + \ldots + (-1)^n S_n H^0)\,\phi,$$

where the S's are the elementary symmetric functions,

$$S_0 = 1$$

$$S_1 = c_0 + c_1 + c_2 + \ldots + c_n,$$

$$\ldots\ldots\ldots\ldots\ldots$$

$$S_n = c_0 c_1 c_2 \ldots c_n.$$

The c's are then the roots of the equation $\Sigma\,(-1)^{n-t} S_t c^t = 0$, and using the S's rather than the c's avoids solving this equation.

The derivatives of $\sigma_2^{\,2}$ with respect to the symmetric functions S_1 and S_2 are

$$\frac{d(\sigma_2^{\,2})}{dS_1} = \frac{2}{(H_4 - 2S_1H_3 + (S_1^{\,2} + 2S_2)H_2 - 2S_1S_2H_1 + S_2^{\,2}H_0)^3}$$

$$\Big\{\Big[3H_0H_1H_2 - 2H_1^{\,3} - H_0^{\,2}H_3\Big]S_2^{\,5} + \Big[4H_1^{\,2}H_2 + H_0^{\,2}H_4 - 5H_0H_2^{\,2}\Big]S_2^{\,4}S_1$$

$$+ \Big[6H_1H_2^{\,2} + 4H_0H_1H_4 + H_0H_2H_3 - 10H_1^{\,2}H_3 - H_0^{\,2}H_5\Big]S_2^{\,4}$$

$$+ \Big[6H_0H_2H_3 - 3H_0H_1H_4 - 3H_1H_2^{\,2}\Big]S_2^{\,3}S_1^{\,2}$$

$$+ \Big[16H_1H_2H_3 + 2H_0H_1H_5 - 10H_2^{\,3} - 4H_1^{\,2}H_4 - 2H_0H_2H_4 - H_0H_3^{\,2}\Big]S_2^{\,3}S_1$$

$$+ \Big[11H_1H_2H_4 + 6H_2^{\,2}H_3 + 4H_0H_3H_4 + H_0H_1H_6 - 16H_1H_3^{\,2} - 4H_1^{\,2}H_5$$

$$- 2H_0H_2H_5\Big] S_2^{\,3} + \Big[3H_2^{\,3} + 2H_1^{\,2}H_4 + H_0H_2H_4 - 4H_1H_2H_3 - 2H_0H_3^{\,2}\Big] S_2^{\,2}S_1^{\,3}$$

$$+ \Big[3H_0H_3H_4 + 3H_2^{\,2}H_3 - 6H_1H_2H_4\Big] S_2^{\,2}S_1^{\,2} + \Big[12H_1H_2H_5 + 10H_2H_3^{\,2}$$

$$+ 4H_1H_3H_4 - 21H_2^{\,2}H_4 - 2H_0H_4^{\,2} - 2H_1^{\,2}H_6 - H_0H_2H_6\Big] S_2^{\,2}S_1$$

$$+ \Big[13H_2H_3H_4 + 4H_1H_4^{\,2} + 2H_1H_2H_6 + H_0H_3H_6 - 12H_1H_3H_5 - 8H_3^{\,3}\Big] S_2^{\,2}$$

$$+ \Big[2H_1H_3^{\,2} - H_2^{\,2}H_3 - H_1H_2H_4\Big] S_2S_1^{\,4} + \Big[8H_2^{\,2}H_4 - 6H_2H_3^{\,2} - 2H_1H_2H_5\Big] S_2S_1^{\,3}$$

$$+ \Big[7H_2H_3H_4 + 3H_1H_2H_6 - 7H_2^{\,2}H_5 - 3H_1H_4^{\,2}\Big] S_2S_1^{\,2} + \Big[12H_2H_3H_5$$

$$+ 6H_1H_4H_5 + 2H_3^{\,2}H_4 - 14H_2^{\,2}H_4 - 4H_1H_3H_6 - 2H_2^{\,2}H_6\Big] S_2S_1$$

$$+ \Big[5H_3H_4^{\,2} + 2H_2H_4H_5 + 2H_2H_3H_6 + H_1H_4H_6 - 8H_3^{\,2}H_5 - 2H_1H_5^{\,2}\Big] S_2$$

$$+ \Big[2H_3^{\,3} + H_2^{\,2}H_5 - 3H_2H_3H_4\Big] S_1^{\,4} + \Big[5H_4^{\,2}H_2 - 4H_4H_3^{\,2} - H_2^{\,2}H_6\Big] S_1^{\,3}$$

$$+ \Big[3H_3^{\,2}H_4 + 3H_2H_3H_6 - 6H_2H_5H_6\Big] S_1^{\,2} + \Big[4H_3H_4H_5 + 2H_2H_5^{\,2} - 3H_4^{\,3}$$

$$- 2H_3^{\,2}H_6 - H_2H_4H_6\Big] S_1 + \Big[H_3H_4H_6 + H_4^{\,2}H_5 - 2H_5^{\,2}H_3\Big]\Big\}.$$

$$\frac{d(\sigma_2^{\,2})}{dS_2} = \frac{2}{(H_4 - 2S_1H_3 + (S_1^{\,2} + 2S_2)H_2 - 2S_1S_2H_1 + S_2^{\,2}H_0)^3}$$

$$\Big\{\Big[2H_1^{\,3} + H_0^{\,2}H_3 - 3H_0H_1H_2\Big] S_2^{\,4}S_1 + \Big[2H_0H_1H_3 + H_0H_2^{\,2} - 2H_1^{\,2}H_2$$

$$- H_0^2H_4\Big] S_2^4 + \Big[5H_0H_2^2 - 4H_1^2H_2 - H_0^2H_4\Big] S_2^3S_1^2$$

$$+ \Big[8H_1^2H_3 + 2H_0^2H_5 - 8H_0H_2H_3 - 2H_0H_1H_4\Big] S_2^3S_1$$

$$+ \Big[4H_0H_3^2 + 2H_0H_1H_5 + 2H_2^3 - 4H_1H_2H_3 - 2H_1^2H_4 - H_0^2H_6 - H_0H_2H_4\Big]S_2^3$$

$$+ \Big[3H_1H_2^2 + 3H_0H_1H_4 - 6H_0H_1H_6\Big] S_2^2S_1^3$$

$$+ \Big[9H_0H_2H_4 + 6H_0H_3^2 + 3H_2^2 - 12H_1H_2H_3 - 6H_0H_1H_5\Big] S_2^2S_1^2$$

$$+ \Big[8H_1H_3^2 + 5H_1H_2H_4 + 3H_0H_1H_6 + 2H_1^2H_5 - 12H_0H_3H_4 - 6H_2^2H_3\Big] S_2^2S_1$$

$$+ \Big[6H_0H_3H_5 + 3H_2^2H_4 - 6H_1H_3H_4 - 3H_0H_2H_6\Big] S_2^2$$

$$+ \Big[4H_1H_2H_3 + 2H_0H_3^2 - 3H_2^3 - 2H_1^2H_4 - H_0H_2H_4\Big] S_2S_1^4$$

$$+ \Big[4H_1^2H_5 + 6H_2^2H_3 + 2H_0H_2H_5 - 2H_1H_2H_4 - 6H_0H_3H_4 - 4H_1H_3^2\Big]S_2S_1^3$$

$$+ \Big[4H_1H_3H_4 + 6H_2^2H_4 + 7H_0^2H_4 - 8H_2H_3^2 - 6H_1H_2H_5 - 2H_1^2H_6$$

$$- H_0H_2H_6\Big] S_2S_1^2 + \Big[4H_1H_2H_6 + 4H_1H_4^2 + 8H_3^3 + 2H_0H_3H_6 - 6H_0H_4H_5$$

$$- 10H_2H_3H_4 - 2H_1H_4^2\Big] S_2S_1 + \Big[4H_2H_3H_5 + 2H_0H_5^2 + 3H_2H_4^2 - 4H_3^2H_4$$

$$- 2H_1H_4H_5 - 2H_2^2H_0 - H_0H_4H_5\Big] S_2 + \Big[H_2^2H_3 + H_1H_2H_4 - 2H_1H_3^2\Big] S_1^5$$

$$\Big[6H_1H_3H_4 - 4H_2^2H_4 - 2H_1H_2H_5\Big] S_1^4$$

$$+ \left[4H_2^{\,2}H_5 + 2H_2H_3H_4 + H_1H_2H_6 - 7H_1H_4^{\,2}\right] S_1^{\,3} + \left[5H_2H_4^{\,2} + 4H_2^{\,2}H_5\right.$$

$$\left. + 2H_1H_4H_5 - 6H_2H_3H_5 - 2H_3^{\,2}H_4 - 2H_1H_3H_5 - H_2^{\,2}H_6\right] S_1^{\,2}$$

$$+ \left[4H_3^{\,2}H_5 + 2H_2H_3H_6 + H_1H_4H_6 - 4H_2H_4H_5 - 2H_1H_5^{\,2} - H_3H_4^{\,2}\right] S_1$$

$$\left. + \left[2H_2H_5^{\,2} + H_4^{\,3} - 2H_3H_4H_5 - H_2H_4H_6\right] \right\} .$$

Since the algebra is quite complicated, as evidenced by the preceding two formulas, it is desirable to find an alternative mode of approach. The opportunity is provided by the third condition imposed on $F_\phi(E)$, namely that it be constant for $E < E_{min}$, and the utility is indicated by the observation that in most physical problems it is the low-lying eigenstates that are of greatest interest. This can be taken advantage of by constructing from ϕ states with minimum energy rather than minimum standard deviation. This process can lead to more than one state, since a minimum-energy state exists for each combination of the auxiliary variables.

The estimate of the energy E in the state is just the mean value of the distribution $F_\phi(E)$,

$$\overline{E}(\phi) = \frac{\int E dF_\phi(E)}{\int dF_\phi(E)} = \frac{H_1}{H_0} .$$

The first improvement on this is found by considering the function $\phi' = (H - c)\phi$. This function has energy $\overline{E'(c)}$, which may be expressed in terms of the moments of ϕ:

$$\overline{E'}(c) = \frac{H_3 - 2cH_2 + c^2H_1}{H_2 - 2cH_1 + c^2H_0} .$$

Again this expression may be differentiated to determine the minimum value.

The derivative is

$$\frac{d\overline{E'}(c)}{dc} = \frac{2(H_2H_0 - H_1^2)c^2 + 2(H_2H_1 - H_3H_0)c + 2(H_3H_1 - H_2^2)}{(H_2 - 2cH_1 + H_0c^2)^2}. \quad (5)$$

The same arguments used in discussing the standard deviation apply again. That is, $\overline{E'}(\pm\infty) = \overline{E}$ and $\frac{d\overline{E'}(c)}{dc}(\pm\infty) > 0$. Hence the derivative must be negative for some finite values of c, and there are two real roots corresponding to a maximum and a minimum of the expression for $\overline{E'}(c)$. The only difference is that the coefficient of c^2 in the derivative, $(H_2H_0 - H_1^2)$, is positive, so that the $\overline{E'}(c)$ is increasing at both $\pm\infty$ and the minimum is given by the larger root. Again the conclusion is that there exists a c that reduces the energy.

The formulas for the iterated results can be developed, and are somewhat less complicated than those for the standard deviation. There is, however, an easier way to get at the results. If an estimate is going to be made using n c's then the moments $H_0, H_1, \ldots H_{2n+1}$ will have to be used. It is possible to find a unique distribution function $F_\phi^n(E)$ having n + 1 points of increase, which will have the same first (2n + 2) moments as $F_\phi(E)$. Then as long as no more than the (2n + 2) moments $H_0, \ldots H_{2n+1}$ are under consideration, $F_\phi^{(n)}(E)$ and $F_\phi(E)$ are indistinguishable. Since there are n constants c available it is clear that the way to minimize the final energy is to choose the constants c at the n largest points of increase of f(E). Then the modification of $F_\phi^{(n)}(E)$ has a single point of increase, and this smallest point of increase is an estimate of the eigenvalue, and the corresponding approximate eigenfunction can be found.

It can be shown[4] that the n + 1 points of increase of f(E) are the n + 1 solutions, E of the equation

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[4] The proofs of this and the following statements are essentially contained in J. V. Uspensky, Introduction to Mathematical Probability, First Edition (McGraw-Hill, New York, 1937) Appendix II. He treats the case in which the highest moment is even, i.e., H_{2n}. The odd case is slightly simpler and almost identical proofs apply.

$$\begin{vmatrix} 1 & E & E^2 & \cdots & E^{n+1} \\ H_0 & H_1 & H_2 & \cdots & H_{n+1} \\ H_1 & H_2 & H_3 & \cdots & H_{n+2} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ H_n & H_{n+1} & H_{n+2} & \cdots & H_{2n+1} \end{vmatrix} = 0 .$$

This equation has $(n+1)$ real distinct roots and they lie between the smallest and largest eigenvalues represented in the distribution function $F_\phi(E)$. The appropriate c's are the n largest roots of this equation, and the estimate of the energy is the smallest solution. In this aspect the formula constitutes a generalization of the Rayleigh-Ritz principle, which states that the solution E of the linear equation

$$\begin{vmatrix} 1 & E \\ H_0 & H_1 \end{vmatrix} = 0$$

lies between the least and greatest eigenvalues,

$$E_{min} \leqslant E = \frac{H_1}{H_0} \leqslant E_{max} .$$

A simple interpretation of this statement is that the mean value of a distribution is in its interior.

The discussion of convergence is most advantageously carried on from the point of view of orthogonal polynomials. Given the distribution $F_\phi(E)$ with moments H_n, then the polynomials

$$P_n(E) = \begin{vmatrix} 1 & E & E^2 & \cdots & E^n \\ H_0 & H_1 & H^2 & \cdots & H_n \\ H_1 & H_2 & H_3 & \cdots & H_{n+1} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ H_{n-1} & \cdots & \cdots & \cdots & H_{2n-1} \end{vmatrix}$$

are known to be the orthogonal polynomials associated with the distribution $F_\phi(E)$.[5] That is, they satisfy the relation

$$\int_{-\infty}^{\infty} P_n(E)\, P_{n'}(E)\, d\, F_\phi(E) = C_{nn'}\, \delta_{nn'} \ ,$$

where $\delta_{nn'}$ is the Kronecker delta, and $C_{nn'}$ is a normalization constant. The determinental form is essentially the result of the Schmidt orthogonalization procedure applied to the functions $1, E, E^2, \ldots$ with the weight function $d\, F_\phi(E)$.

The problem of convergence can now be stated as a problem on the roots of the orthogonal polynomials $P_n(E)$ associated with the distribution function $F_\phi(E)$. The polynomial $P_n(E)$ has n real distinct roots, $E_{n1}, E_{n2}, \ldots, E_{nn}$. The sequence of smallest roots is known to be a decreasing sequence, that is,

$$E_{11} > E_{21} > E_{31} > \ldots > E_{n1} \ .$$

Since this sequence is bounded from below by the smallest eigenvalues it is convergent. It can either converge to the smallest eigenvalue or to some other value larger than the smallest eigenvalue. For orthogonal polynomials in a finite interval it is known that the sequence of smallest roots converges to the smallest point of increase of the function $F_\phi(E)$, i.e., to the smallest eigenvalue.[6] In the infinite interval the result is that if the sequence of largest roots E_{nn} has the property

$$\lim_{n \to \infty} \frac{E_{nn}}{n^2} \to 0$$

then the smallest roots approach the smallest eigenvalue.[7] This is of

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[5] G. Szegö, Orthogonal Polynomials, Am. Math. Soc. Colloquium Publications 23, 26 (1939).

[6] G. Szegö, Ibid, p. 107.

[7] Ibid p. 108. See footnote 29.

little practical value for solving the physical problem. It does indicate that the difficulties may arise because the distribution function $F_\phi(E)$ does not become constant at infinity with sufficient rapidity.

Another more intuitive way to get at the same idea is to notice that the effect of operating on ϕ with $(H - c_1)(H - c_2) \ldots (H - c_n)$ is to multiply $F_\phi(E)$ by $(E - c_1)^2 (E - c_2)^2 \ldots (E - c_n)^2$. Any point of F near a c is deemphasized, those remote from all c's are emphasized. The intent of the process is to increase the magnitude of $F_\phi(E)$ for very small values of E. The c's are chosen in the intermediate range of values; this emphasizes the very small and the very large values in $F_\phi(E)$. If $F_\phi(E)$ is sufficiently constant for large values of E this accentuation of the high-E portions is unimportant. On the other hand, if $F_\phi(E)$ varies too rapidly for large E, then it will be necessary for the c's to be a more quickly increasing sequence in order that the high E values of $F_\phi(E)$ are not too greatly emphasized. However, as c becomes infinite the change in the energy becomes smaller, as pointed out earlier. This is because all points close to the origin are treated equivalently. The result is that the minimum energy estimate has a lower bound greater than the actual energy minimum. Thus not only must all the moments be finite, but they must not be too rapidly increasing for the method to be successful.

There probably is a minimum rate at which $F_\phi(E)$ must approach $F_\phi(\infty)$ as E approaches infinity and this in turn causes a maximum rate of increase of the moments. Either of these conditions is probably sufficient to cause the moment sequence and distribution to be in a unique relationship.

SOME APPLICATIONS OF THE METHOD OF MOMENTS

In this section three problems are treated by the method of moments. The first two are not particularly interesting, but they do have the virtue of being soluble. The third problem is difficult and has not yet been solved by any technique.

The first example is the case in which the initial state ϕ is a linear combination of two eigenfunctions of the Hamiltonian

$$\phi = \alpha\psi(E_1) + \beta\psi(E_2) \quad .$$

So far as ϕ is concerned H is the two-by-two matrix,

$$H = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix} .$$

The function $F_\phi(E)$ has steps of magnitude $|\alpha|^2$ at E_1 and $|\beta|^2$ at E_2. The moments are given by

$$H_n = |\alpha|^2 E_1{}^n + |\beta|^2 E_2{}^n \quad .$$

The lowest-order approximation (Rayleigh - Ritz) would estimate an eigenvalue by the solution of the linear equation

$$\begin{vmatrix} 1 & E \\ |\alpha|^2 + |\beta|^2 & |\alpha|^2 E_1 + |\beta|^2 E_2 \end{vmatrix} = 0 \quad .$$

The root is

$$E = \frac{|\alpha|^2 E_1 + |\beta|^2 E_2}{|\alpha|^2 + |\beta|^2} \quad .$$

The second-order approximation requires a solution of the equation

$$\begin{vmatrix} 1 & E & E^2 \\ |\alpha|^2 + |\beta|^2 & |\alpha|^2 E_1 + |\beta|^2 E_2 & |\alpha|^2 E_1{}^2 + |\beta|^2 E_2{}^2 \\ |\alpha|^2 E_1 + |\beta|^2 E_2 & |\alpha|^2 E_1{}^2 + |\beta|^2 E_2{}^2 & |\alpha|^2 E_1{}^3 + |\beta|^2 E_2{}^3 \end{vmatrix} = 0.$$

This reduces to

$$|\alpha|^2 |\beta|^2 (E_1 - E_2)^2 E^2 - |\alpha|^2 |\beta|^2 (E_1 - E_2)^2 (E_1 + E_2) E + |\alpha|^2 |\beta|^2 (E_1 - E_2) E_1 E_2 = 0.$$

This is the characteristic equation of the two-by-two matrix provided $\alpha, \beta \neq 0$, and $E_1 \neq E_2$. If either of these two conditions had been violated then ϕ itself would have been an eigenfunction, and this in turn would have been indicated by the identical vanishing of the above determinant. The roots of the equation are E_1 and E_2. Thus the first modification of ϕ is $\phi' = (H - E_2)\phi$,

$$\phi' = \begin{bmatrix} E_1 - E_2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} (E_1 - E_2)\alpha \\ 0 \end{bmatrix}.$$

As expected, ϕ' is an eigenfunction and the problem is solved.

As a second example consider the one-dimensional wave packet

$$\phi(x) = \sqrt{2 m a^2} \int_0^\infty dk \; e^{-ikx\sqrt{k/m}} \; e^{-(ak)^2}.$$

The Hamiltonian of the system will be taken to be just the kinetic energy $p^2/2m$. The moments of the Hamiltonian in this state are easily written

$$H_n = (\phi | H^n | \phi)$$

$$= \sqrt{2m}\ a^2 \int_{-\infty}^{\infty} dx \int_0^{\infty} dk\ e^{ikx\sqrt{k/m}}\ e^{-(ak)^2} \int_0^{\infty} dk' \left(\frac{k'^2}{2m}\right)^n e^{-ik'x\sqrt{k'/m}}\ e^{-(ak')^2}$$

$$= 2a^2 \int_0^{\infty} dk\ e^{-2(ak)^2}\ k \left(\frac{k^2}{2m}\right)^n .$$

The integral is now simplified by the substitution $E = \frac{k^2}{2m}$. With this change it becomes

$$H_n = 2ma^2 \int_0^{\infty} dE\ E^n\ e^{-2ma^2 E} .$$

This can easily be converted into an integral with respect to a distribution,

$$H_n = \int E^n\ d\left\{1 - e^{-2ma^2 E}\right\} .$$

With the moments in this form $F_\phi(E)$ is obviously given by

$$F_\phi(E) = \begin{cases} 0 & E < 0 \\ 1 - e^{-2ma^2 E} & 0 \leqslant E \end{cases}$$

This is a continuous distribution but, as has been indicated previously, the method of moments as developed is applicable since H_0 is finite. Since every nonnegative value of E is a point of increase of $F_\phi(E)$, the Hamiltonian $\frac{p^2}{2m}$ has all the numbers from 0 to ∞ as eigenvalues.

The calculation can also be carried out in the more routine fashion. The integral above can be done giving the moments

$$H_n = \left(\frac{1}{2ma^2}\right)^{n+1} n!$$

It should be noted at this point that the moment sequence above and the sequence n! are equivalent. In general, a constant or a constant to the nth power times the nth moment makes no difference in the orthogonal polynomials calculated from the moments. The independence of the method from factors of this form is the justification for the statement that the method of moments is independent of the size of coupling constants.

In the above problem it is sufficient to take the moments as n! . To borrow from prior knowledge, the orthogonal polynomials associated with the distribution function $dF_\phi(E) = e^{-2m\alpha^2 E}dE$ are the Laguerre polynomials. Since the smallest root of the nth Laguerre polynomial is of the order of $1/n$ and the lowest energy level is 0, the method is convergent. The first several Laguerre polynomials, with their zeros, are

$L_0(E)$	$= 1$	
$L_1(E)$	$= 1 - E$	1
$L_2(E)$	$= 2 - 4E + E^2$	0.58578643, 3.41421356
$L_3(E)$	$= 24 - 60E + 24E^2 - 2E^3$	0.41577455, 2.29428036, 6.28994508

These have been computed directly from the determinental form and are not normalized. The largest roots are used as the c's and this leads to the modified distribution functions. The first two modified distributions based on L_2 and L_3 are

$$dF_{\phi'}(E) = (1.7071 - E + .1464\,E^2)\,e^{-E}dE,$$

$$\phi' = (H - 3.4142)\,\phi\ ,$$

$$dF_{\phi''}(E) = (2.6501 - 3.1527E + 1.3049E^2 - .2185E^3 + .01273E^4)\,e^{-E}dE,$$

$$\phi'' = (H - 6.2899)(H - 2.2943)\,\phi\ .$$

These functions have been normalized. To indicate the rapidity of convergence, Table I lists the smallest roots of the fourth through fifteenth Laguerre polynomials.

Table I

Smallest roots of Laguerre polynomials	
n	Smallest root
4	0.32254769
5	0.26356032
6	0.22284660
7	0.19304368
8	0.17027963
9	0.15232222
10	0.13779347
11	0.12579644
12	0.11572212
13	0.10714239
14	0.09974750
15	0.09330781

The third example is an application of the method of moments to the phonon-polaron problem. The motion of slow electrons in polar crystals has been described by the motion of a polaron, a bare electron surrounded by polarization waves (phonons).[8] The Hamiltonian for this system may be reduced to[9]

$$H = \frac{p^2}{2m} + \omega \sum_{|\vec{k}|<K} a_{\vec{k}}^{\dagger} a_{\vec{k}}$$

$$+ \sum_{|\vec{k}|<K} \left(a_{\vec{k}}^{\dagger} V_{|\vec{k}|}^{*} e^{-i\vec{k}\vec{r}} + a_{\vec{k}} V_{|\vec{k}|} e^{i\vec{k}\vec{r}}\right)$$

[8] H. Frohlich, Advances in Physics 3, 325, (1954).

[9] Lee, Low, and Pines, Phys. Rev. 90, 297 (1953).

and

$$V_{|\vec{k}|} = -i\sqrt{\frac{\omega^2}{2m\omega}}\left(\frac{4\pi a}{V}\right)^{1/2}\frac{1}{|\vec{k}|} .$$

The usual commutation rules $\left[a_{\vec{k}}, a^{\dagger}_{\vec{k}'}\right] = \delta_{\vec{k},\vec{k}'}$ apply, and p^2 is the operator $-\nabla^2$. The first two terms describe the noninteracting systems, free electrons, and polarization waves. The second part describes the ability of the electron to absorb or emit phonons accompanied by recoil. The problem is to find the minimum energy of the system.

The state ϕ treated consists of one electron with momentum p' and no phonons; $a_{\vec{k}}\,\phi = 0, \quad \frac{p^2}{2m}\,\phi = \frac{p'^2}{2m}\,\phi = E_0\,\phi$.

The first four moments of the Hamiltonian H in this state are

$$H_0 = 1,$$

$$H_1 = E_0,$$

$$H_2 = E_0^{\,2} + \frac{\omega^2}{\sqrt{2m\omega}}\,\frac{2a}{\pi}\,K,$$

$$H_3 = E_0^{\,3} + \frac{\omega^2}{\sqrt{2m\omega}}\,\frac{2a}{\pi}\,K\,(2\,E_0 + E_0 + \omega + 1/3\,\frac{K^2}{2m}) .$$

Equation (5) is employed to find the value of c. After some simplification it becomes

$$c^2 - (2E_0 + \omega + 1/3\,\frac{K^2}{2m})\,c + E_0\,(E_0 + \omega + \frac{1/3\,K^2}{2m}) - \frac{\omega^2}{2m\omega}\,\frac{2a}{\pi}K = 0.$$

The solutions of this equation are

$$c = E_0 + 1/2(\omega + \frac{1}{3}\,\frac{K^2}{2m}) \pm 1/2\sqrt{(\omega + \frac{1}{3}\,\frac{K^2}{2m})^2 + \frac{4\omega^2}{\sqrt{2m\omega}}\,\frac{2a}{\pi}\,K} .$$

The larger root is the c to be used in computing ϕ', and the smaller the estimate of the energy. For small a the estimate of the energy is

$$E = E_0 - a\omega \left(\frac{2}{\pi} \frac{\frac{K}{\sqrt{2m\omega}}}{1 + \frac{K^2}{6m\omega}} \right) .$$

For large a the estimate becomes

$$E = E_0 - \frac{1}{\sqrt{\frac{\omega^2}{\sqrt{2m\omega}} \frac{2a}{\pi} K}}$$

$$\left[\frac{\omega^2}{\sqrt{2m\omega}} \frac{2a}{\pi} K - 1/2 \sqrt{\frac{\omega^2}{\sqrt{2m\omega}} \frac{2a}{\pi} K} \left(\omega + \frac{1}{3}\frac{K^2}{2m}\right) + \left(\omega + \frac{1}{3}\frac{k^2}{2m}\right)^2 \right] .$$

These results should be compared with several earlier calculations. The perturbation theory treatment[8] gives

$$E = E_0 - a\omega$$

for small a. This is very similar to the result attained above for small a. There are two differences, the constant multiplying a is 1 in perturbation theory compared with a number less than 1 from the moment technique, and secondly the perturbation result is valid only when a is small, while the moment-technique answer is valid for all values of a. Intermediate coupling theory[9] has also been applied to this problem and yields the same answer as perturbation theory. However, the range of validity is extended up to $a = 6$ or 7. The same comparisons apply to intermediate coupling as to perturbation theory. The amount of work involved in the perturbation-theory treatment is about equal to the moment technique, while the intermediate-coupling-theory method is an order of magnitude more difficult. The strongest results so far achieved have been obtained by considering path integrals.[10] In this method terms have been produced proportional to the higher powers of a. The first two terms above are reproduced. The only drawback of this method is its apparent inability to construct the state vectors corresponding to the energy estimate. The effort involved is again quite moderate in the path-integral method.

[10] R. P. Feynman, Phys. Rev. 97, 660 (1955).

In higher orders of the moment method based on the initial state considered above, neither the linear dependence on α for small α nor the one-half-power dependence on α for large α is changed. This is easily seen because each successive even moment is one power of α higher than the preceding even one, whereas each of the odd moments is of the same order in α as the preceding even moment. By entering in the determinant either the highest or lowest power of α occurring in the moment the dependence of the successive orthogonal polynomials on α for large and small α can be determined. As stronger results are available, it would appear that the state chosen is not an appropriate one.

TIME-DEPENDENT METHODS

There is a series solution for the time-dependent Schrödinger Equation which is related to the preceding discussion of time-independent methods in that the approximation to the actual temporal development is the temporal development of a finite operator having its first n moments equal to the Hamiltonian in question. A state vector $\phi(t_0)$ is specified at an initial time t_0, and it is desired to know ϕ at a later time t; the vector ϕ develops according to the time-dependent Schrödinger equation,

$$i \frac{\partial \phi}{\partial t} = H\phi \quad . \tag{6}$$

In accordance with previous work, $H\phi(t)$ is written as $c\,\phi(t) + \phi'(t)$. The equation can then be solved for $\phi(t)$ in terms of $\phi'(t)$, an unknown state. It turns out that $\phi'(t)$ again satisfies a Schrödinger equation and therefore the process may be iterated.

It is convenient to add certain factors to the notation suggested above. Thus $\phi_n(t)$ will be defined

$$\phi_n(t) = \frac{H - c_{n-1}}{c_n - c_{n-1}} \phi_{n-1}(t) e^{i(c_{n-1} - c_{n-2})t} \tag{7}$$

and $\phi_0(t) = \phi(t)$. With these definitions each ϕ satisfies the time-dependent Schrödinger equation

$$i \frac{\partial \phi_n(t)}{\partial t} = (H - c_{n-1})\phi_n(t) . \qquad (c_{-1} \equiv 0) \quad (8)$$

This may be proved by an induction on n. For $n = 0$, since $c_{-1} \equiv 0$, this is the Schrödinger Eq. (6), which was assumed. Assume the result is true for n-1:

$$i \frac{\partial \phi_{n-1}(t)}{\partial t} = (H - c_{n-2})\phi_{n-1}(t) .$$

The unknown vector $\phi_n(t)$ is now introduced on the right-hand side:

$$i \frac{\partial \phi_{n-1}(t)}{\partial t} = (H - c_{n-1} + c_{n-1} - c_{n-2})\phi_{n-1}(t) ,$$

$$= (c_{n-1} - c_{n-2})\phi_{n-1}(t) + (c_n - c_{n-1})\phi_n(t) e^{-i(c_{n-1} - c_{n-2})t} ,$$

where use has been made of Eq. (7). This equation may now be integrated $\phi_{n-1}(t)$

$$= e^{-i(c_{n-1} - c_{n-2})(t - t_0)} - i(c_n - c_{n-1}) e^{-i(c_{n-1} - c_{n-2})} \int_{t_0}^{t} \phi_n(t_n)\, dt_n . \quad (9)$$

If $\frac{H - c_{n-1}}{c_n - c_{n-1}}$ is now applied to both sides this reduces to Eq. (8), and the induction is proved.

Equation (9) may be used as the basis for a series expansion of $\phi_0(t)$. Repeated application yields

$$\phi(t) = \sum_{n=0}^{n=N} (-i)^n \prod_{j=1}^{n} (c_j - c_{j-1}) e^{-i\left[c_0 t - (c_n - c_{n-1})t_0\right]} \phi_n(t_0) \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots$$

$$\int_{t_0}^{t_{n-1}} dt_n \exp\left\{-i\sum_{j=1}^{n}(c_j-c_{j-1})t_j\right\} + (-i)^{N+1}\prod_{j=1}^{N+1}(c_j-c_{j-1})e^{-ic_0t}\int_{t_0}^{t} dt_1$$

$$\int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_N} dt_{N+1} \exp\left\{-i\sum_{j=1}^{n}(c_j-c_{j-1})t_j\,\phi_{N+1}(t_{N+1})\right\} .$$

Again the proof follows easily by induction.

The integration over time can be carried out except for the unknown function $\psi_{N+1}(t_{N+1})$. The resulting series is

$$\phi(t) = \sum_{n=0}^{N}(-i)^n\prod_{j=1}^{n}(c_j-c_{j-1})e^{-i\left[c_0t-(c_n-c_{n-1})t_0\right]}\phi_n(t_0)$$

$$\times \sum_{k=0}^{n}\frac{e^{-i\left[(c_{n-k}-c_0)t+(c_n-c_{n-k+1})t_0\right]}}{\prod_{i\neq n-k}(c_{n-k}-c_i)} + (-i)^{N+1}\sum_{j=1}^{N+1}(c_j-c_{j-1})e^{-ic_0t}$$

$$\int_{t_0}^{t}\sum_{k=0}^{N}\frac{e^{-i\left[(c_{N-k}-c_0)t+(c_N-c_{N-k+1})t_{N+1}\right]}}{\prod_{N-k\neq i}(c_{N-k}-c_i)}\phi(t_{N+1})\,dt_{N+1} \quad . \quad (10)$$

The magnitude of the term $\prod_{j=1}^{n}(c_j-c_{j-1})\phi_n(t_0)$ can be found readily in terms of the moments. The magnitude of $\phi_n(t_0)$ is

$$\left|\phi_n(t_0)\right| = \sqrt{(\phi_n(t_0)\,|\,\phi_n(t_0))} \quad .$$

This may be expanded by use of the recursion relation for the ϕ's,

$$(\phi_n(t_0)\,|\,\phi_n(t_0)) = (\phi_{n-1}(t_0)\left|\frac{(H-c_{n-1})^2}{(c_n-c_{n-1})^2}\right|\phi_{n-1}(t_0))$$

$$= \frac{(\phi_0(t_0)\left|(H-c_{n-1})^2(H-c_{n-2})^2\ldots(H-c_0)^2\right|\phi_0(t_0))}{(c_n-c_{n-1})^2(c_{n-1}-c_{n-2})^2\ldots(c_1-c_0)^2},$$

so that the magnitude of $\prod_{j=1}^{n}(c_j-c_{j-1})\phi_n(t_0)$ becomes

$$\left|\prod_{j=1}^{n}(c_j-c_{j-1})\phi_n(t_0)\right| = \sqrt{(\phi_0\left|(H-c_0)^2(H-c_1)^2\ldots(H-c_{n-1})^2\right|\phi_0)},$$

which is a polynomial in the moments. Since all the ϕ's satisfy the Schrödinger equation, their magnitudes are time-independent. On the basis of these results the magnitude of the remainder R_N after N terms is

$$R_N = \sqrt{(\phi_0\left|(H-c_{n-1})^2(H-c_{n-2})^2\ldots(H-c_0)^2\right|\phi_0)}\,(t-t_0)\sum_{k=0}^{N}\frac{1}{\prod_{n-k=i}\left|c_{N-k}-c_i\right|}.$$

It is possible to minimize the entire expression involving c's, but to do so again leads to complicated expressions. Minimizing just the magnitude of $(\phi_0\left|(H-c_0)^2\ (H-c_n)^2\right|\phi_0)$ is probably almost as good, and the problem can then be solved explicitly. Again it is easier to deal with the symmetric functions in the c's rather than with the c's themselves.

To minimize the magnitude of ϕ_n, the symmetric functions in the c's are chosen to satisfy the following linear equations:

$$\sum_{r=0}^{n-1}(-1)^{r+s}H_{2n-1-r-s}S_{r+1} = (-1)^{s+1}H_{2n-s}\quad(s=1,2,\ldots n).$$

This system always has a nonvanishing determinant.[11] Again an approximation is made to the actual Hamiltonian by the finite matrix having the identical first 2n moments, and all the comments of the preceding sections apply. Again the c's have to be the zeros of the asso-

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[11] Widder, loc. cit. p. 136. The same determinant, modified by the transformation E goes to -E so that all the odd moments change sign, is shown to be positive.

ciated orthogonal polynomials. Canceling the n points of increase of the function $F_{\phi}^{(n)}(E)$ associated with the finite matrix having the same first 2n moments as H makes $F_{\phi}^{(n)}(E)$ identically 0. The equation for the c's in terms of the S's

$$S_0 c^n - S_1 c^{n-1} + \ldots\ldots + (-1)^n S_n c^0 = 0 ,$$

must be the characteristic equation of the finite matrix having the same first 2n moments, since the eigenvalues of this matrix are the points of increase of $F_{\phi}^{(n)}(E)$. Thus the time-dependent theory has led to the same equations as the time-independent one. It should be noted that the highest moment that appears in the magnitude of ϕ_n, H_{2n} disappears in the minimization criteria, emphasizing the analogy with energy minimization.

If the other terms are considered in the minimization then more complicated equations are obtained, resembling the standard deviation equation. They are slightly stronger results; there is no reason to believe this method will converge if the simpler methods fail. This follows since convergence is intimately associated with whether or not the distribution with a finite number of points of increase will approach the one representing the physical problem.

The transition from time-dependent back to time-independent formalism can be made by observing that a solution $\phi(t)$ of the time-dependent equation may be expanded in a series of eigenfunctions,

$$= \Sigma (\psi(E_i) \,|\, \phi)\, \psi(E_i)\, e^{-iE_i t} \quad .$$

This is an expansion in almost periodic functions, and if it is multiplied by e^{iEt} and averaged over time, a nonzero result occurs only if E is an eigenvalue and the result extracted is just the eigenfunction. For example:

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \phi(t) e^{iEt}\, dt = \lim_{T\to\infty} \Sigma\, (\psi(E_i) \,|\, \phi)\psi(E_i \frac{1}{T}\int_0^T e^{i(E-E_i)t}\, dt$$

$$= \Sigma\, (\psi(E_i)\,|\,\phi)\,\psi(E_i)\,\delta_{EE_i}$$

$$= \begin{cases} 0 & E \neq E_i \\ (\psi(E_i)\,|\,\phi)\;\psi(E_i) & E = E_i \end{cases} .$$

A more conventional averaging is

$$\lim_{\epsilon \to 0} \int_0^\infty e^{iEt} e^{-\epsilon t}\; \phi(t)dt \quad ;$$

the result is the same. Formally applying an averaging process to the series Eq. (10) for $\phi(t)$ yields the result

$$\lim_{T\to\infty} \frac{1}{T}\int \phi(t)e^{iEt}dt = \begin{cases} 0 & E \neq c_i \\ \sum\limits_{n=i}^{\infty} \prod\limits_{j=1}^{n} (c_j - c_{j-1}) \dfrac{1}{\prod\limits_{i\neq j} (c_i - c_j)} \phi_n(0) & E = c_i \end{cases} .$$

The series on the right is formally an eigenfunction. The series converges moderately well, but after it has been operated on with H it seems to always diverge and hence is of no value unless it can be explicitly summed.

II. THE π-MESIC DISINTEGRATION OF THE DEUTERON

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ABSTRACT

An investigation of the higher-order corrections to the mesic disintegration of deuterons is considered. It is found that the corrections are small, quite independently of the description employed.

II. THE π-MESIC DISINTEGRATION OF THE DEUTERON

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INTRODUCTION

Among the earliest experiments carried out with π mesons were the slowing down and absorption of negative π mesons in hydrogen and deuterium.[1] These experiments had originally been suggested as a means of determining the spin and parity of the meson and the nature of its nuclear interaction.[2] Calculations had been carried out which indicated that the moderation time for negative π mesons was small compared with the π-μ decay time, thus permitting an appreciable fraction of the mesons to reach the inner atomic orbits.[3] Many survey calculations of a semi-empirical nature were carried out to determine the spin and parity of the meson[4] from the experimental results. These

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[1] Panofsky, Aamodt, and York, Phys. Rev. 78, 825 (1950); Panofsky, Aamodt, Hadley, and Phillips, Phys. Rev. 80, 94 (1950); Aamodt, Hadley, and Panofsky, Phys. Rev. 80, 282 (1950), Panofsky, Aamodt, and Hadley, Phys. Rev. 81, 565 (1951).

[2] B. Ferretti, Report of a Conference on Fundamental Particles and Low Temperatures, p. 75 The Physical Soc., London (1947).

[3] A. Wightman, Phys. Rev. 77, 521 (1950).

[4] R. Marshak and A. Wightman, Phys. Rev. 76, 114 (1949); C. Marty and J. Prentki, J.phys. et radium X 156 (1949); R. Marshak and A. Wightman, Phys. Rev. 79, 220 (1950); S. Tamor, Phys. Rev. 79, 221 (1950); S. Tamor and R. Marshak, Phys. Rev. 80, 766 (1950); Marshak, Tamor and Wightman, Phys. Rev. 80, 765 (1950); Brueckner, Serber and Watson, Phys. Rev. 81, 575 (1951); S. Tamor, Phys. Rev. 82, 38 (1951); R. Marshak, Revs. Modern Phys. 23, 137 (1951).

experiments and calculations all tended to indicate that the meson is captured from the K shell, and that the π meson is a pseudoscalar with either pseudoscalar or pseudovector coupling to the nucleon. Later experiments were conducted on the absorption of low-energy positive mesons by deuterium.[5] By use of detailed balancing arguments and the cross sections for the inverse processes, the spin of the π^+ meson was found to be zero.

The experimental work over the ensuing years tended to indicate that the dominant interaction of the moderate-energy π meson with nucleons was in the p state.[6] Since, to the lowest order in the coupling constant, the nonrelativistic limits of both pseudoscalar and pseudovector coupling are identical and describe p-wave mesons,[7] this common limit was extensively investigated and has been found to give reasonable agreement with the scattering,[8] photoproduction[9], and other simple properties[10] of the meson-nucleon system up to several hundred Mev.

On the other hand there exist S-wave effects that are not negligible.[11] As the relativistic meson-nucleon theory has never been satisfactorily treated, and as S-wave effects are absent from the nonrelativistic limits, the significance of the S-wave interaction has remained obscure. Several attempts have been made to remedy this defect. In the conventional reduction of the relativistic theory the nucleon-recoil terms are usually dropped. The inclusion of these terms is necessary to make the interaction a Galilean invariant, and does contribute S-wave effects. For scattering, these effects tend to make the agreement be-

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[5] Durbin, Loar, and Steinberger, Phys. Rev. 83, 646 (1951); Clark, Roberts, and Wilson, Phys. Rev. 83, 649 (1951); Durbin, Loar, and Steinberger, Phys. Rev. 84, 581 (1951).

[6] Anderson, Fermi, Martin, and Nagle, Phys. Rev. 91, 167 (1953).

[7] F. J. Dyson, Phys. Rev. 73, 929 (1948).

[8] G. Chew and F. Low, Phys. Rev. 101, 1570 (1956); G. Chew, Phys. Rev. 95, 1669 (1954).

[9] G. Chew and F. Low, Phys. Rev. 101, 1579 (1956).

[10] H. Miyazawa, Phys. Rev. 101, 1564 (1956).

[11] H. Bethe and F. DeHoffman, Mesons and Fields, Vol. II Mesons (Row Peterson, Evanston 1956).

tween theory and experiment worse.[12] These terms were also used in some of the earlier phenomenological calculations of the π^+-deuteron interaction,[13, 14] and were found to be dominant for very low meson energies.[14]

Another aspect of the meson-nucleon absorption interaction was the early recognition that some of the mesic interactions could give information about nuclear structure. Thus the gamma rays emitted in the reaction $\pi^- + d \rightarrow n + n + \gamma$ give information on the existence of a dineutron.[15]

More recently π-mesic atoms have been made and their X-ray spectra have been measured. The nonelectromagnetic corrections to the 1 S level have been determined.[16] These offer additional information on the S-wave interaction of the meson-nucleon system. The first interpretation of the nonelectromagnetic level shift related these to virtual scattering of the meson and thus to the S-wave meson-nucleon scattering lengths.[17] This interpretation has been criticized because it takes into account only elastic processes, whereas virtual inelastic processes are also possible.[18] That this must be so is evident from the fact that real absorption takes place; the spectral lines have a finite width and the atoms a finite lifetime. The contribution of the inelastic events to the level shift has been calculated in a phenomenological way,[18] and does, according to this calculation, make a substantial contribution to the level shift.

The basic inelastic process is the absorption of a negative meson by a nucleon pair, and thus it appears valuable to investigate this event more carefully. However, as in the earlier investigation of the deuteron,[15] the situation seems to have turned about. As will be shown, the significant parameter in the ability of a nucleon pair to absorb a

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[12] E. Henley and M. Ruderman, Phys. Rev. 90, 719 (1953).

[13] W. B. Cheston, Phys. Rev. 83, 1118 (1951).

[14] Chew, Steinberger, Goldberger, and Yang, Phys. Rev. 84, 581 (1951).

[15] K. Watson and R. Stuart, Phys. Rev. 82, 738 (1951); Aamodt, Hadley, and Panofsky, Phys. Rev. 83, 1057 (1951).

[16] Stearns, De Benedetti, and Leipuner, Phys. Rev. 96, 804 (1954).

[17] Deser, Goldberger, Baumann, and Thiring, Phys. Rev. 96, 774 (1954).

[18] K. Brueckner, Phys. Rev. 98, 769 (1955).

meson is the magnitude of the momentum component in its wave function corresponding to the rest mass of the meson. As this number is poorly known for complex nuclei and the deuteron, the experiment may be used as a momentum spectrometer within the limits of validity of the impulse approximation.

In the lowest order of perturbation theory the relative momentum component corresponding to the meson rest mass is the only feature of the nuclei which enters into the calculation. The purpose of this investigation is to see to what extent this dependence is modified in higher-order processes.

The mesic disintegration of deuterium is quite closely related to the photodisintegration of deuterium which has been more extensively investigated.[19, 20] In a recent calculation the corrections introduced by virtual meson processes to the deuteron photodisintegration have been calculated[20] by use of symmetric pseudoscalar meson theory with cutoff pseudovector interactions. The calculation in this paper is, to a large extent, patterned after the former in its treatment of the intermediate states. As indicated earlier,[8, 9, 10] the pseudovector form of meson theory appears to explain moderately accurately the low-energy meson-nucleon effects. The use of an S-wave coupling to accomplish the absorption and then the neglect of virtual S-wave mesons in the intermediate state is rather artificial. It may be partly justified by the conventional observation that the p-wave effects are larger.

The principal conclusion of the calculation is that the absorption of the meson at rest is quite insensitive to the effects of virtual mesons in the intermediate states. This is to be expected because the large p-wave effects generally occur at energies that are about a meson mass above threshold.

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[19] J. Marshall and E. Guth, Phys. Rev. 78, 738 (1950); L. Schiff, Phys. Rev. 78, 733 (1950).

[20] F. Zachariasen, Phys. Rev. 101, 371 (1956).

THE ABSORPTION MATRIX ELEMENT

The existence in the nonrelativistic limit of a meson-nucleon coupling involving the nucleon velocity was noted in early work.[13, 14] It was also pointed out that the strength of this term relative to the p-wave term is determined by the requirement that the interaction be a Galilean invariant.[12] Thus the form of the interaction is

$$(4\pi)^{1/2} \frac{f}{\mu} \tau_i \quad \vec{\sigma} \cdot (\vec{\nabla}_{meson} - \frac{\mu}{m} \vec{\nabla}_{nucleon}) \phi_i \quad .$$

The difference in the gradients is the meson-nucleon relative velocity and thus a Galilean invariant. The coupling constant is taken as $f^2 = 0.08$, where μ is the meson mass and m the nucleon mass. For processes involving virtual mesons, the meson field is expanded in plane waves, while for the absorption the meson field is expanded in hydrogenic wave functions divided by $\sqrt{2\mu}$. The meson field is then given by its value at the origin. This is

$$\phi(0) = \left(\frac{\mu^3 \tilde{\alpha}^3}{\pi}\right)^{1/2}$$

for the 1s orbit from which the meson is absorbed. The symbol $\tilde{\alpha}$ is used for the fine-structure constant to avoid confusion with the parameter α of the Hulthén wave function. The first portion of the interaction is the p-wave interaction that will be used to describe all virtual mesons. The second portion is an S-wave coupling and will be used to describe only the absorption of the external meson. The justification for this is the observed predominance of p-wave phenomena at low energy.

Since the theory is divergent a cutoff will be used where necessary. The value chosen is the nucleon mass, since this value is about that indicated by scattering theory. The result is quite insensitive to cutoff, because the first two orders of perturbation theory are independent of the cutoff.

Now that the form of the interaction to be used has been chosen, it is necessary to decide which terms in the perturbation expansion are to be included. There are three considerations that govern this

choice. First, in the spirit of the impulse approximation, the number of virtual mesons exchanged between the nucleons is held to the minimum necessary to achieve any process. That is, each process is considered only with the least possible number of exchanged mesons. Secondly, from prior experience with low-energy meson theory, only the angular momentum 3/2 isotopic spin 3/2 state is considered in higher-order processes. Finally, in any possible sequence of processes, the external vertex is always chosen as near the start of the process as possible, since this produces as many vanishing energy denominators as possible. This means that absorption is always the second process.

The exact expression for the transition operator desired can now be reduced by formal arguments similar to those given for the photodisintegration.[20] The result is that all possible meson exchanges between two nucleons, such that there is always at least one meson in the field, should be considered. The external vertex should be joined to these diagrams in all possible ways, and the matrix element taken between an initial deuteron state and a final scattering state. Figure 1 lists that subset of these diagrams selected according to the three rules stated above which are to be calculated. The heavy dot on the nucleon line indicates a virtual (3/2, 3/2) scattering of the meson. These diagrams will initially be calculated between plane-wave nucleon states and then averaged over the deuteron and scattering states. The deuteron will be represented by a Hulthén wave function,

$$\psi_D = \left(\frac{2\alpha\beta(\alpha+\beta)}{\alpha^2+\beta^2}\right)^{1/2} (e^{-\alpha r} - e^{-\beta r}) ,$$

where the constants α and β have the values[21]

$$\alpha = 0.32738,$$
$$\beta = 1.91844,$$

in units of the reciprocal meson Compton wavelength. The final state is taken as an undistorted expanding spherical wave.

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[21] Maso Sugawara, Handbuch der Physik 39 (to be published).

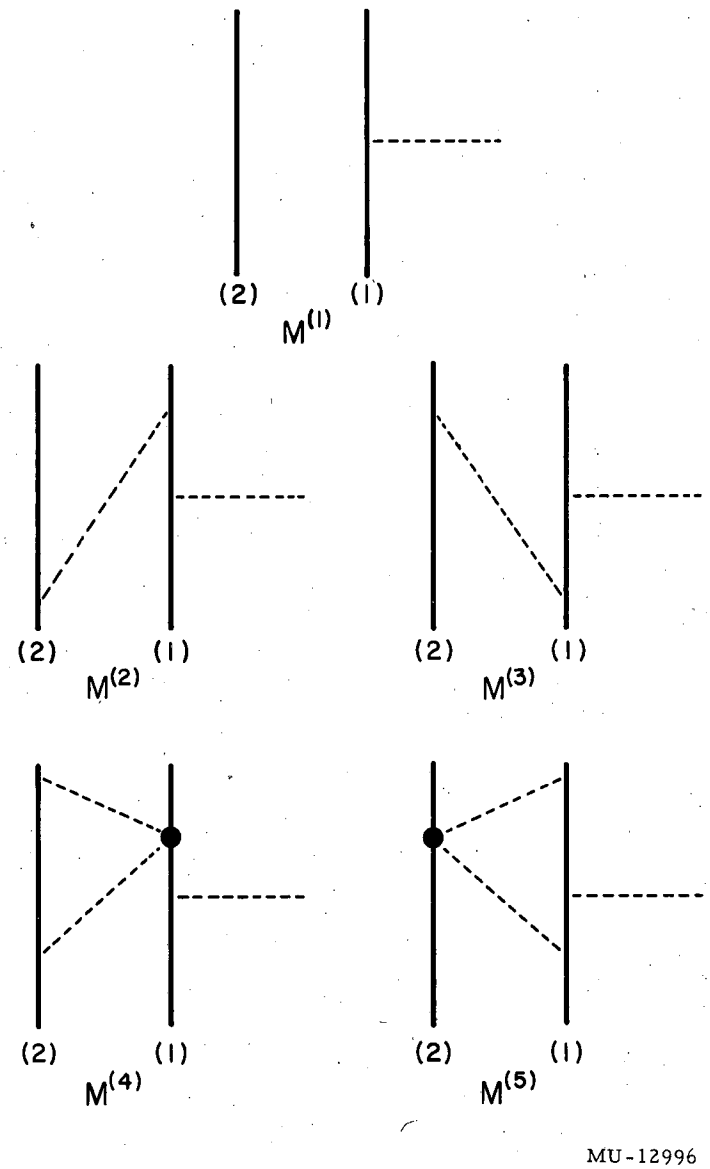

Fig. 1. Interaction diagrams representing the nuclear absorption of the negative π meson.

The general form of the interaction Hamiltonian has already been given. The expansion of the usual pseudovector portion in plane waves is

$$H_I = H_1 + H_2,$$

$$H_1 = (4\pi)^{1/2} \frac{f}{\mu} \sum_{k,i} \tau_i^{(1)} a_{\vec{k}\,i} \; \vec{\sigma}(1) \cdot i\vec{k} e^{ikr^{(1)}} \frac{1}{\sqrt{2\omega_k}} + \text{complex conjugate.}$$

The indices (1) refer to the coordinates or operators of nucleon (1). H_2 is identical except for the replacement of the (1)'s by (2)'s. The $a_{\vec{k},\,i}$ ($a_{\vec{k},\,i}^{*}$) are the absorption (emission) operators for mesons of momentum $\vec{k}$ and isotopic spin i. This portion of the Hamiltonian is used to describe the virtual mesons. The absorption of the real 1S meson is described by the single term in the expansion of H_I into hydrogenic wave functions,

$$H_{abs} = \frac{\sqrt{2}\,\phi(0)}{\sqrt{2\mu}} (4\pi)^{1/2} \frac{f}{m} \sigma^{(1)} \cdot (\nabla^{(1)} - i\frac{P}{2}) .$$

The isotopic spin operator has been replaced by the $\sqrt{2}$, since only negative mesons are absorbed. Nucleon (1) will always be taken as the nucleon that absorbs the meson, and consequently H_{abs} has no (2) portion. The only momentum that the 1s meson can have is the translational momentum of the center of gravity of the deuteron $\vec{P}/2$ that has been subtracted from the gradient of the nucleon wave function to maintain the Galilean invariance of the interaction.

The lowest-order contribution to the absorption is the matrix element of H_{abs} between the initial and final states. Because of the simplicity of the operator the matrix element could be directly evaluated between the exact nucleon states, but to be consistent with the treatment of the higher-order processes, it will first be evaluated between the plane-wave nucleon states,

$$\phi_i = \frac{1}{(2\pi)^3} e^{i(p_1 r_1 + p_2 r_2)} \chi_{1/2}^{n}(2) \, \chi_{1/2}^{m}(1) ,$$

$$\phi_f = \frac{1}{(2\pi)^3} e^{i(p_1'r_1 + p_2'r_2)} \chi^{n'}_{1/2}(2)\, \chi^{m'}_{1/2}(1) \ .$$

The $\chi^m_{1/2}(1)$ and $\chi^n_{1/2}(2)$ are two component spinors for nucleons (1) and (2) respectively.

The matrix element between the plane-wave states is

$$M_{if}^{(1)} = \int d^3r_1 d^3r_2 \ \frac{1}{(2\pi)^3} e^{-i(\vec{p}_1'\vec{r}_1 + \vec{p}_2'\vec{r}_2)}$$

$$\times (\chi^{n'}_{1/2}(2)\, \chi^{m'}_{1/2}(1) \left| \vec{\sigma}_1 \cdot i(\vec{p}_1 - \frac{\vec{P}}{2}) \right| \chi^n_{1/2}(2)\, \chi^m_{1/2}(1))$$

$$\times \ (\sqrt{4\pi})^{1/2} \frac{f}{m} \frac{\sqrt{2}\,\phi(0)}{\sqrt{2\mu}} \frac{1}{(2\pi)^3} \ e^{i(\vec{p}_1\vec{r}_1 + \vec{p}_2\vec{r}_2)}$$

$$= \delta(\vec{p}_1 - \vec{p}_1')\, \delta(\vec{p}_2 - \vec{p}_2')\, (4\pi)^{1/2} \frac{f}{m} \frac{\sqrt{2}\,\phi(0)}{\sqrt{2\mu}} (\chi^{n'}_{1/2}(2)\, \chi^{m'}_{1/2}(1) \left| \vec{\sigma}_1 \cdot i(\vec{p}_1 - \frac{\vec{P}}{2}) \right| \chi^n_{1/2}(2)\, \chi^m_{1/2}(1)).$$

The transformations to the center-of-mass coordinates of the two nucleons is convenient, and are contained in the formulas

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \ , \qquad \vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2} \ ,$$

$$\vec{p} = 1/2\,(\vec{p}_1 - \vec{p}_2) \ , \qquad \vec{P} = \vec{p}_1 + \vec{p}_2 \ ,$$

$$\vec{p}' = 1/2\,(\vec{p}_1' - \vec{p}_2') \ , \qquad \vec{P}' = \vec{p}_1' + \vec{p}_2' \ .$$

With these substitutions the matrix element becomes

$$M_{if}^{(1)} = \delta(\vec{p} + \frac{\vec{P}}{2} - \vec{p}' - \frac{\vec{p}'}{2})\, \delta(\frac{\vec{P}}{2} - \vec{p} - \frac{\vec{p}'}{2} + \vec{p}')\, (4\pi)^{1/2} \frac{f}{m} \frac{\sqrt{2}\phi(0)}{m\sqrt{2\mu}}$$

$$i(\chi^{n'}_{1/2}(2)\, \chi^{m'}_{1/2}(1) \left| \vec{\sigma}_1 \cdot \vec{p} \right| \chi^n_{1/2}(2)\, \chi^m_{1/2}(1)) \ .$$

The exact initial and final states are

$$\psi_I = \frac{1}{(2\pi)^{3/2}} e^{i\vec{K}\vec{R}} \Phi_I(r) \chi_1^m 1/\sqrt{4\pi} ,$$

$$\psi_F = \frac{1}{(2\pi)^{3/2}} e^{i\vec{K}'\vec{R}} \Phi_F(r) \sqrt{\frac{3}{8\pi}} \left(\frac{\vec{S}\cdot\vec{r}}{r}\right) \chi_1^{m'} .$$

The vectors $\vec{K}$ and $\vec{K}'$ are the initial and final momenta of the center of mass of the system. The matrix $\vec{S} = 1/2(\vec{\sigma}_1 + \vec{\sigma}_2)$. The expression $\sqrt{\frac{3}{8\pi}} \frac{\vec{S}\cdot\vec{r}}{r} \chi^{m_1}$ represents a normalized $^3P_1$ state.[22] The deuteron is taken as a $^3S_1$ state. The D-state admixture is neglected. Since it absorbs a pseudoscalar particle having zero orbital angular momentum its final state must be $^3P_1$. The choice of constants requires both radial functions to be normalized to one,

$$\int_0^\infty r^2 \left| \phi_I(r) \right|^2 dr = \int_0^\infty r^2 \left| \phi_F(r) \right|^2 dr = 1.$$

The matrix element $M_{IF}^{(1)}$ between the deuteron and scattering states can be expressed as

$$M_{FI}^{(1)} = \sum_{spin} \int (\psi_F \left| \phi_f \right) M_{fi}' (\phi_i \left| \psi_I \right) d^3P\, d^3p\, d^3P'\, d^3p' .$$

A similar equation holds, of course, for any of the other matrix elements. The transformation functions $(\psi_F \left| \phi_f \right)$ and $(\phi_i \left| \psi_I \right)$ can be calculated, and are

$$(\phi_i \left| \psi_I \right) = \delta(\vec{K}-\vec{P}) \frac{1}{\sqrt{4\pi}} (\chi_{1/2}^n(2)\, \chi_{1/2}^m(1) \left| \chi_1^m \right) \sqrt{\frac{2}{\pi}} \int dr\, r^2\, j_0(pr) \Phi_I(r) ,$$

$$(\psi_F \left| \phi_f \right) = -\delta(\vec{K}'-\vec{P}') \sqrt{\frac{3}{8\pi}} (\chi_1^{m'} \left| \frac{\vec{S}\cdot\vec{p}'}{i\, p'} \right| \chi_{1/2}^{n'}(2)\, \chi_{1/2}^{m'}(1)) \int dr' r'^2 \Phi_F^*(r') j_1(p'r'). \tag{1}$$

[22] W. Rarita and J. Schwinger, Phys. Rev. 59, 556 (1941).

With the help of these, $M_{FI}^{(1)}$ becomes

$$M_{FI}^{(1)} = -(4\pi)^{1/2}\frac{f}{m}\frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}}\int d^3p\,d^3p'\,d^3P\,d^3P'\;\delta\left[\vec{p}-\vec{p}' + 1/2\,(\vec{P}-\vec{P}')\right]$$

$$\delta\left[1/2(\vec{P}-\vec{P}') + (\vec{p}'-\vec{p})\right]\sum_{\text{spin}}\left(\chi_1^{m'}\left|\frac{\vec{S}\cdot\vec{p}'}{i\;p'}\right|\chi_{1/2}^{n'}(2)\,\chi_{1/2}^{m'}(1)\right)\left(\chi_{1/2}^{n'}(2)\,\chi_{1/2}^{m'}(1)\right|i\vec{\sigma}_1$$

$$\cdot\,\vec{p}\left|\chi_{1/2}^{n}(2)\,\chi_{1/2}^{m}(1)\right)\left(\chi_{1/2}^{n}(2)\,\chi_{1/2}^{m}(1)\right|\chi_1^{m}\Big)\frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{8\pi}}\,\delta(\vec{K}-\vec{P})\,\delta(\vec{K}'-\vec{P}')$$

$$\sqrt{\frac{2}{\pi}}\int r^2 dr\, j_0(pr)\,\Phi_I(r)\sqrt{\frac{2}{\pi}}\int r'^2 dr'\;\Phi_F^*(r')\,j_1(p'r')\,.$$

The integrals over the delta functions and the sum over the spins can be easily carried out. After these operations have been performed, the matrix element becomes

$$M_{FI}^{(1)} = -(4\pi)^{1/2}\frac{f}{m}\frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}}\frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{8\pi}}\,\delta(\vec{K}-\vec{K}')$$

$$\cdot\,\frac{2}{\pi}\int d^3\vec{p}\,dr\,dr'\;\left(\chi_1^{m'}\left|\left(\frac{\vec{S}\cdot\vec{P}}{p}\right)(\vec{\sigma}_1\cdot\vec{p})\right|\chi_1^{m}\right)r^2 j_0(pr)$$

$$\times\qquad \Phi_I(r)\,r'^2\,\Phi_F^*(r')\,j_1(p\,r')\,.$$

The integrals over the angles of $\vec{p}$ can also be carried out without specifying the radial functions ϕ_I and ϕ_F. This gives for the matrix element

$$M_{FI} = -(4\pi)^{1/2}\frac{f}{m}\frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}}\frac{1}{\sqrt{4\pi}}\sqrt{\frac{3}{8\pi}}\,\delta(\vec{K}-\vec{K}')$$

$$\frac{4\pi}{2}\left(\chi_1^{m'}\left|\left[1 + 1/3\,(\vec{\sigma}_1\cdot\vec{\sigma}_2)\right]\right|\chi_1^{m}\right)$$

$$\frac{2}{\pi}\int dp\,dr\,dr'\;p^3 r^2 r'^2\,j_0(pr)\,\Phi_I(r)\,\Phi_F^*(r')\,j_1(pr')\,.$$

This can be simplified further, since $(\chi_i^{m'} | (\vec{\sigma}_1 \cdot \vec{\sigma}_2) | \chi_i^m) = \delta_{mm'}$. The final form for M_{FI} before specifying the radial functions is

$$M_{FI} = -(4\pi)^{1/2} \frac{f}{m} \frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}} \frac{1}{\sqrt{4\pi}} \sqrt{\frac{3}{8\pi}} \frac{8\pi}{3} \delta(\vec{K}-\vec{K}')$$

$$\delta_{mm'} \frac{2}{\pi} \int dp\,dr\,dr'\, p^3 r^2 r'^2 j_0(pr) \Phi_I(pr) \Phi_F^*(r') j_1(pr)$$

$$= M \frac{2}{\pi} \int dp\,dr\,dr'\, p^3 r^2 r'^2 j_0(pr) \Phi_I(r') \Phi_F^*(r') j_1(pr) .$$

The constant M is used for

$$M = -(4\pi)^{1/2} \frac{f}{m} \frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}} \sqrt{\frac{3}{8\pi}} \frac{1}{\sqrt{4\pi}} \frac{8\pi}{3} \sqrt{\frac{2}{\pi}} \delta(\vec{K}-\vec{K}') \delta_{mm'} , \quad (2)$$

which is also common to all the higher-order matrix elements.

It is now necessary to make a choice of the functions Φ_I and Φ_F. If Φ_F is chosen to be an expanding spherical wave

$$\Phi_F = \sqrt{\frac{2}{\pi}}\, j_1(\bar{p} r') ,$$

then it is not necessary to determine Φ_I, but only the Fourier transform for one value of the momentum. With the above choice of Φ_F the r' integral becomes

$$\sqrt{\frac{2}{\pi}} \int dr'\, r'^2 \phi_F(r) j_1(pr) = \frac{2}{\pi} \int dr'\, r'^2 j_1(\bar{p}r') j_1(pr') = \frac{\delta(p-\vec{p})}{p^2},$$

and with the aid of the delta function all but one of the remaining integrals can be done:

$$M_{FI} = M \int dp\,dr\, r^2 p^3 \frac{\delta(p-\bar{p})}{p^2} j_0(pr) \Phi_I(r) = M \bar{p} \int dr\, r^2 j_0(\bar{p}r) \Phi_I(r).$$

The remaining integral is just the expression for the momentum component of the deuteron at the momentum $\overline{p}$. The value of $\overline{p}$ is, of course, determined by the energy-conservation condition

$$\overline{p}^2 = m\mu \ .$$

The absorption rate to first order, R_1, is given by the usual formula,

$$R_1 = 2\pi \left| M_{FI}^{(1)} \right|^2 \rho\,(E) \ .$$

Two factors of $\delta(K-K')$ occur in the square of the matrix element. The first of these gives unity when an integral is taken over an interval of final states. The other factor $\delta(K-K')$ is to be interpreted as the volume of the region in which the reaction occurs. The quantity computed without this factor of the volume is the transition rate per unit volume. Since the wave function for the center of mass of the deuteron has been normalized to one deuteron per unit volume, this transition rate is actually the desired transition rate per deuteron. The density of states is

$$\rho\,(E) = \sum_{l,m} \int p^2\, dp\, \delta\,(E-\mu) = \int p^2\, dp\ \delta\,(\frac{p^2}{m} - \mu) = 1/2\sqrt{m\mu}\ m \ ;$$

the transition rate becomes

$$R_1 = 2\pi\ 4\pi\left(\frac{f}{m}\right)^2 \frac{\left|\phi(0)\right|^2}{\mu}\ \frac{2}{3}\,\frac{2}{\pi}\left|\int dr\, r^2\, j_0\,(\overline{p}r)\,\overline{\Phi}_I\,(r)\right|^2 (m\mu)^{3/2}\, m\,\frac{1}{2} \ .$$

After $\frac{\mu^3\tilde{\alpha}^3}{\pi}$ is substituted for $\left|\phi(0)\right|^2$, this becomes

$$R_1 = \frac{8\pi}{3} f^2 \sqrt{m\mu}\ \mu^3\tilde{\alpha}^3\,\frac{2}{\pi}\left|\int dr\, r^2\, j_0\,(\overline{p}r)\,\overline{\Phi}_I\,(r)\right|^2 \ .$$

For the Hulthén wave function the integral is easily done, and gives

$$\int dr\, r^2\, j_0\,(\overline{p}r)\,\overline{\Phi}_I\,(r) = \left\{\frac{1}{\alpha^2+\overline{p}^2} - \frac{1}{\beta^2+\overline{p}^2}\right\}\sqrt{\frac{2\alpha\beta\,(\alpha+\beta)}{(\beta-\alpha)}} \ .$$

After the numerical values for the various constants are substituted, R_1 becomes, in units in which the meson mass is unity,

$$R_1 = 0.098 \times 10^{-8} ,$$

or in conventional units

$$R_1 = 2.1 \times 10^{14}/\text{sec.}$$

The higher-order corrections can easily be included in the transition rate by multiplying R_1 by the square of the ratio of the R matrix to the already computed matrix element of the interaction. The factors M and the normalization constant for the Hulthén wave function are common to both and are dropped. If these factors are neglected the matrix element of the interaction is

$$M_{FI}^{(1)} \sim \frac{\overline{p}}{\alpha^2 + \overline{p}^2} - \frac{\overline{p}}{\beta^2 + \overline{p}^2} .$$

This factor has the value $1.3049 \times 10^{-1}/\mu$.

RADIATIVE CORRECTIONS

The second-order processes are those for which there is one meson exchanged between the nucleons while the absorption takes place. For $M_{fi}^{(2)}$ the exchanged meson must clearly be a neutral one. After the absorption of the external negative meson, the absorbing nucleon is a neutron, and must undergo an even number of changes of charge to remain a neutron at the end of the process. It is clear that the nucleon that did not directly enter the absorption process must have been a neutron. Thus the exchanged neutral meson is both emitted and absorbed by neutrons. The isotopic spin contribution to the matrix element is therefore one. Between the plane-wave states the matrix element $M_{fi}^{(2)}$ is

$$M_{fi}^{(2)} = \int \frac{d^3k}{(2\pi)^3} d^3r_1 d^3r_2 \left\{ \frac{1}{(2\pi)^3} e^{-i(\vec{p}_1'\vec{r}_1+\vec{p}_2'\vec{r}_2)} \chi_{1/2}^{n'}(2)\, \chi_{1/2}^{m'}(1) \right.$$

$$(4\pi)^{1/2}\frac{f}{\mu}\frac{\vec{\sigma}_1\cdot\vec{k}}{\sqrt{2\omega_k}} e^{i\vec{k}\vec{r}_1} \frac{1}{\mu-\omega_k-E_k} (4\pi)^{1/2}\frac{f}{m}\frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}}\vec{\sigma}_1\cdot\left(\vec{\nabla}_1-i\frac{\vec{p}}{2}\right)\frac{1}{-\omega_k-E_k}$$

$$\left. \frac{\vec{\sigma}_2\cdot\vec{k}}{\sqrt{2\omega_k}} e^{-i\vec{k}\vec{r}_2} \frac{1}{(2\pi)^3} e^{i(\vec{p}_1\vec{r}_1+\vec{p}_2\vec{r}_2)} \chi_{1/2}^{n}(2)\, \chi_{1/2}^{m}(1) \right\} ;$$

here E_k is the nucleon recoil energy and is equal to $\mu/2$. The integrals over r_1 and r_2 are easily carried out and give

$$M_{fi}^{(2)} = (4\pi)^{1/2}\frac{f}{m}\frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}}\left[(4\pi)^{1/2}\frac{f}{\mu}\right]^2 \int \frac{d^3k}{(2\pi)^3}\, \delta(\vec{p}_1+\vec{k}-\vec{p}_1')\,\delta(\vec{p}_2-\vec{k}-\vec{p}_2')$$

$$\frac{1}{2\omega_k}\frac{1}{\omega_k+E_k}\frac{1}{\omega_k+E_k-\mu}\left(\chi_{1/2}^{n'}(2)\,\chi_{1/2}^{m'}(1)\right|\left.(\vec{\sigma}_1\cdot\vec{k})\, i(\vec{\sigma}_1\cdot\vec{p}_1-\frac{\vec{p}}{2})(\vec{\sigma}_2\cdot\vec{k})\right|\chi_{1/2}^{n}(2)\chi_{1/2}^{m}(1)\Big).$$

With the help of the δ functions the final integral is performed and, after the transformation to center-of-mass coordinates is made, $M_{fi}^{(2)}$ becomes

$$M_{fi}^{(2)} = (4\pi)^{1/2} \frac{f}{m} \frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}} \left[(4\pi)^{1/2} \frac{f}{\mu}\right]^2 \frac{1}{(2\pi)^3} \delta(\vec{P}-\vec{P}') \frac{1}{2\omega_{\vec{p}-\vec{p}'}} \frac{1}{\omega_{\vec{p}-\vec{p}'}+\frac{\mu}{2}}$$

$$\frac{1}{(\omega_{\vec{p}-\vec{p}'}-\frac{\mu}{2})} (\chi^{n'}_{1/2}(2)\, \chi^{m'}_{1/2}(1) \left| (\vec{\sigma}_1 \cdot \vec{p}'-\vec{p})(i\vec{\sigma}_1 \cdot \vec{p})(\sigma_2 \cdot \vec{p}'-\vec{p}) \right| \chi^{n}_{1/2}(2)\, \chi^{m}_{1/2}(1)).$$

As for the first-order contribution, this plane-wave matrix element must now be averaged over the actual initial and final states. The transformation functions are the same as used before Eq. (1).

After the δ-function integrals have been performed the matrix element is

$$M_{FI}^{(2)} = -(4\pi)^{1/2} \frac{f}{m} \frac{\sqrt{2}\phi(0)}{\sqrt{2\mu}} \left[(4\pi)^{1/2} \frac{f}{\mu}\right]^2 \frac{1}{(2\pi)^3} \delta(K-K') \int d^3p\, d^3p' \frac{1}{2\omega_{\vec{p}-\vec{p}'}}$$

$$\frac{1}{\omega_{\vec{p}-\vec{p}'}+\frac{\mu}{2}} \frac{1}{\omega_{\vec{p}-\vec{p}}-\frac{\mu}{2}} \sqrt{\frac{3}{8\pi}} \sqrt{\frac{1}{4\pi}} (\chi^{m'}_1 \left| \frac{\vec{S}\cdot\vec{p}'}{p'} (\vec{\sigma}_1 \cdot \vec{p}'-\vec{p})(\vec{\sigma}_1 \cdot \vec{p})(\vec{\sigma}_2 \cdot \vec{p}'-\vec{p}) \right| \chi^{m}_1)$$

$$\frac{2}{\pi} \int dr' r'^2 \Phi_F^*(r') j_1(p'r') \int dr\, r^2 j_0(pr) \Phi_I(r) . \qquad (3)$$

The substitution $\vec{p}-\vec{p}'=\vec{l}$ is now introduced and the variables $\vec{l}$ and $\vec{p}'$ retained. The Jacobian of the transformation is $+1$. The angular portion of the matrix element in the new coordinate system is now extracted. It is

$$\int d\Omega_l\, d\Omega_{p'}\, (\chi^{m'}_1 \left| (\vec{S}\cdot\vec{p}')(\vec{\sigma}_1 \cdot \vec{l})(\vec{\sigma}_1 \cdot \vec{p}'+\vec{l})(\vec{\sigma}_2 \cdot \vec{l}) \right| \chi^{m}_1)\, j_0(\left|\vec{p}'+\vec{l}\right| r) .$$

The direction of $\vec{l}$ is chosen as the polar axis in $\vec{p}'$ space. The azimuthal integral can be done, and gives

$$\int d\Omega_l \left\{ \int_0^\pi \sin\theta_{p'}\, d\theta_{p'}\, (\chi^{m'}_1 \left| 2\pi \frac{(\vec{S}\cdot\vec{l})(\vec{l}\cdot\vec{p}')}{l^2} (\vec{\sigma}_1 \cdot \vec{l})(\vec{\sigma}_1 \cdot \vec{l})(\vec{\sigma}_2 \cdot \vec{l}) \right.\right.$$

$$+ \; 2\pi \frac{(\vec{S}\cdot\vec{l})(\vec{l}\cdot\vec{p}')}{l^2} (\vec{\sigma}_1\cdot\vec{l}) \frac{(\vec{\sigma}_1\cdot\vec{l})(\vec{l}\cdot\vec{p}')}{l^2} (\vec{\sigma}_2\cdot\vec{l}) + \pi p^2 \left[1 - \frac{(\vec{l}\cdot\vec{p}')^2}{(lp')^2}\right]$$

$$\left[S_i (\vec{\sigma}_1\cdot\vec{l})\sigma_{1i} (\vec{\sigma}_2\cdot\vec{l}) - \left(\frac{\vec{S}\cdot\vec{l}}{l}\right) (\vec{\sigma}_1\cdot\vec{l}) \left(\frac{\vec{\sigma}_1\cdot\vec{l}}{l}\right)(\vec{\sigma}_2\cdot\vec{l})\right] \Big| \chi_1^m) \; j_0 (\left|\vec{p}' + \vec{l}\right| r) \; .$$

The summation convention is implied where repeated indices occur. After some simplification and inversion of the order of integration, this becomes

$$(\chi_1^{m'} \Big| \pi \int_0^{\pi} \sin\theta_{p'} d\theta_{p'} \int d\Omega_l \left\{ 2(\vec{S}\cdot\vec{l})(\sigma_2\cdot l) l p' \left[1 + \frac{\vec{l}\cdot\vec{p}'}{l^2}\right] + p'^2 \left[1 - \left(\frac{\vec{l}\cdot\vec{p}'}{lp}\right)^2\right]\right.$$

$$\left. \left[S_i (\vec{\sigma}_1\cdot\vec{l})\sigma_{1i} (\vec{\sigma}_2\cdot\vec{l}) - (\vec{S}\cdot\vec{l})(\vec{\sigma}_2\cdot\vec{l})\right]\right\} j_0 (\left|\vec{p}' + \vec{l}\right| r) \Big| \chi_1^m) \; .$$

The integration over the angles of $\vec{l}$ can now be carried out, and yields

$$\frac{4\pi^2}{3} \int_{-1}^{1} dx \, (\chi_1^{m'} \Big| 2(\vec{S}\cdot\vec{\sigma}_2) l^3 p' \left[x + \frac{p'}{l} x^2\right]$$

$$+ p'^2 l^2 \left[1 - x^2\right] \left[S_i (\sigma_1\cdot\sigma_2)\sigma_{1i} - (S\cdot\sigma_2)\right] \Big| \chi_1^m) \; j_0 (\sqrt{p'^2 + 2p'lx + l^2} r)$$

after the substitution $\cos\theta = x$.

The commutation rules for the σ's can be employed to simplify the term multiplied by $1-x^2$, and it becomes

$$(\vec{S}\cdot\vec{\sigma}_2) - (\vec{S}\cdot\vec{\sigma}_1) \; .$$

It is clear from symmetry considerations that this vanishes. The expression thus reduces to

$$l^2 p' \frac{8\pi^2}{3} \int_{-1}^{1} dx \, (lx + p' x^2) \, j_0 (\sqrt{p'^2 + 2p'lx + l^2} r) \, (\chi_1^{m'} \Big| \vec{S}\cdot\vec{\sigma}_2 \Big| \chi_1^m).$$

Finally

$$(\chi_1^{m'} \Big| \vec{S}\cdot\vec{\sigma}_2 \Big| \chi_1^m) = 1/2 \, (3+1) \, \delta_{mm'} \; .$$

The results are substituted into the earlier Eq. (3), and it becomes

$$M_{FI}^{(2)} = M\left[(4\pi)^{1/2}\frac{f}{\mu}\right]^2 \frac{2\pi}{(2\pi)^3}\sqrt{\frac{2}{\pi}}\int l^4 dl\, p'^2 dp' \int_{-1}^{1} dx(lx+p'x^2)\frac{1}{2\omega_l}\frac{1}{\omega_l^2-\frac{\mu^2}{4}}$$

$$\int dr\, r^2 j_0\left(\sqrt{p'^2+2p'lx+l^2}\right)\Phi_I(r)\int dr'\, r'^2\, \phi_F^*(r')\, j_1(p'r) \quad .$$

It is now necessary to substitute in the initial and final radial-wave functions. With these substitutions, and if we make use of the δ function resulting from the r' integral, the matrix element becomes

$$M_{FI}^{(2)} = M\left[(4\pi)^{1/2}\frac{f}{\mu}\right]^2 \frac{1}{(2\pi)^2}\int l^4 dl\, \frac{1}{2\omega_l}\frac{1}{\omega_l^2-\frac{\mu^2}{4}}\int_{-1}^{1} dx(lx+p'x^2)$$

$$\left\{\frac{1}{\alpha^2+p'^2+2p'lx+l^2} - \frac{1}{\beta^2+p'^2+2p'lx+l^2}\right\} \quad .$$

The normalization constant has been dropped in accordance with previous comments. The x integration can be easily performed, and yields

$$M_{FI}^{(2)} = \frac{M}{p}\left[(4\pi)^{1/2}\frac{f}{\mu}\right]^2 \frac{1}{(2\pi)^2}\,\frac{1}{4}\int \frac{l^2 dl}{\omega_l(\omega_l^2-\frac{\mu}{4})}\left\{(\alpha^2+\bar{p}^2-l^2)\left[\frac{\alpha^2+\bar{p}^2-l^2}{4l\bar{p}}\right.\right.$$

$$\left.\left.\times\log\frac{\alpha^2+(l+\bar{p})^2}{\alpha^2+(l-\bar{p})^2} - 1\right] - (\beta^2+\bar{p}^2+l^2)\left[\frac{\beta^2+\bar{p}^2+l^2}{4l\bar{p}}\log\frac{\beta^2+(l+\bar{p})^2}{\beta^2+(l-\bar{p})^2} - 1\right]\right\} . \quad (4)$$

This is as far as it is possible to go analytically. The remaining integral has been carried out numerically.

Identical methods suffice for the reduction of $M_{FI}^{(3)}$ to the form

$$M_{FI}^{(3)} = \left(\frac{M}{\bar{p}}\right)\left[(4\pi)^{1/2}\frac{f}{\mu}\right]^2 \frac{1}{(2\pi)^2}\frac{1}{4}\int \frac{l^2 dl}{\omega_l(\omega_l^2 - \frac{\mu^2}{4})}\left\{(a^2+p^2+l^2)\left[\frac{a^2+\bar{p}^2+l^2}{4l\bar{p}}\right.\right.$$

$$\left.\left.\log\frac{a^2+(l+\bar{p})^2}{a^2+(l-\bar{p})^2} - 1\right] - (\beta^2+\bar{p}^2+l^2)\left[\frac{\beta^2+\bar{p}^2+l^2}{4l\bar{p}}\log\frac{\beta^2+(l+\bar{p})^2}{\beta^2+(l-\bar{p})^2} - 1\right]\right\}. \quad (5)$$

The final result for the one meson in the field contribution is the sum of Eqs. (4) and (5), and is

$$M_{FI}^{(2)} + M_{FI}^{(3)} = \left(\frac{M}{\bar{p}}\right)\left[(4\pi)^{1/2}\frac{f}{\mu}\right]^2 \frac{2}{(4\pi)^2}$$

$$\int_0^\infty \frac{l^2 dl}{\omega_l(\omega_l^2 - \frac{\mu^2}{4})}\left\{(a^2+p^2)\left[\frac{a^2+\bar{p}^2+l^2}{4l\bar{p}}\log\frac{a^2+(l+\bar{p})^2}{a^2+(l-\bar{p})^2}\right]\right.$$

$$\left. - (\beta^2+p^2)\left[\frac{\beta^2+\bar{p}^2+l^2}{4l\bar{p}}\log\frac{a^2+(l+\bar{p})^2}{a^2+(l-\bar{p})^2}\right]\right\},$$

or

$$M_{FI}^{(2)} + M_{FI}^{(3)} = \frac{M}{\bar{p}}\frac{f^2}{2\pi} I_0 .$$

The integral I_0 is dimensionless and has been evaluated numerically (using Simpson's rule) with an asymptotic estimate of the remainder for $l > 100\mu$. In terms of the matrix element,

$$M_{IF}^{(1)}; \quad M_{IF}^{(2)}, \text{ and } M_{IF}^{(3)} \text{ are}$$

$$M_{IF}^{(2)} + M_{IF}^{(3)} = 0.134 \; M_{IF}^{(1)} .$$

The transition rate R to the same order is then

$$R = 1.286 \; R_0 = 2.67 \times 10^{14}/\text{sec.}$$

The higher-order processes involve the virtual scattering of mesons. As has been pointed out earlier, experience indicates that the state in which both the angular momentum and the isotopic spin are equal to 3/2 is the dominant state for low-energy scattering. This then is the only state considered in the scattering processes. If a meson is created on a nucleon it will be necessary for it to scatter off the other nucleon in order to scatter in the resonant state. If a nucleon emits a meson, the nucleon-meson pair must be in a (1/2, 1/2) state, because the initial nucleon was. The absorption of the external pion can not change this to (3/2, 3/2), since the external meson has zero angular momentum. Similarly if a meson is scattered in a (3/2, 3/2) state by a nucleon it must be absorbed by the nucleon by which it was originally created. Thus only those scattering diagrams enter in which the meson crosses twice between the nucleons. Of these only the two illustrated in Fig. 1 are compatible with the last of the conditions, that is, that the absorption is the second process in the sequence.

To treat the scattering as realistically as possible, it is necessary to use the transition operator rather than the Born approximation for the scatterings. Since these scatterings are off the energy shell, there is no direct way to compare them with experiment. However, a simple integral has been suggested that agrees well with the scattering on the energy shell.[23] This form for the virtual scattering has also been used with good results in the study of deuteron photodisintegration.[20] The suggested form is

$$R_{3/2\ 3/2}(\vec{k},\vec{k}') = P_{II'}\left[3\vec{k}\cdot\vec{k}' - (\sigma\cdot k')(\sigma\cdot k)\right]\frac{8\pi f^2}{3\mu^2}\ \frac{1}{\sqrt{\omega\omega'}\,(\mu-\omega-\omega')}$$

$$\times\ 1 + \left\{\frac{\dfrac{4f^2}{3\pi\mu}\ (\mu-\omega-\omega')\displaystyle\int \frac{L^4\,dL}{\omega_L(\mu-\omega_L)(\mu-\omega-\omega_L)(\mu-\omega'-\omega_L)}}{1 - \displaystyle\int_0^m \frac{L^4\,dL}{(2\pi)^3}\ \frac{32\pi^2 f^2}{3\mu^2}\ \frac{1}{\omega_L(\mu-\omega_L)(\mu-2\omega_L)}}\right\}, \qquad (6)$$

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[23] J. L. Gammel, Phys. Rev. 95, 209 (1954).

where $P_{II'}$ is the projection operator for the isotopic spin (3/2) state.

The recoil energy of the nucleons has been neglected in this expression since no very reasonable method of including it is available. The effect of including any nucleon recoil energy would be to decrease the results. The present results are an upper limit for the matrix element. That the nucleon recoil effects are small has been verified by computing the second-order processes with and without recoil included in the energy denominators.

The expression (6) for the transition operator can be considerably simplified. First, the denominator of the term in brackets is independent of the k's and can be calculated numerically. Its value is $1 - 0.692 = 0.371$. The numerator is a function of the variables ω and ω'. By changing the variable of integration to $\omega_L = \sqrt{\mu^2 + L^2}$ and separating the denominator into partial fractions one can bring it into the form

$$4\pi \frac{8\pi f^2}{3\mu^2} \frac{1}{(2\pi)^3} \frac{\omega + \omega' - \mu}{\omega - \omega'} \left\{ \int \frac{d\omega_L \sqrt{\omega_L^2 - \mu^2}(\omega_L + \mu)}{(\omega_L + \omega' - \mu)} - \int \frac{d\omega_L \sqrt{\omega_L^2 - \mu^2}(\omega_L + \mu)}{\omega_L + \omega - \mu} \right\}.$$

The dependence on the variables ω and ω' inside the integral has been separated. The function of a single variable

$$f(\omega) = \int \frac{d\omega_L \sqrt{\omega_L^2 - \mu^2}(\omega_L + \mu)}{\omega_L + \omega - \mu}$$

is easily evaluated as a function of ω by numerical integration in the range of interest $\mu < \omega < m$. It is graphed in Fig. 2. This curve can be fitted exceedingly well by the parabola,

$$0.311\ \omega^2 - 4.70\ \omega + 28.99\ ,$$

which is also graphed in Fig. 2. The parabola is then used for $f(\omega)$ and Eq. (6) reduces to

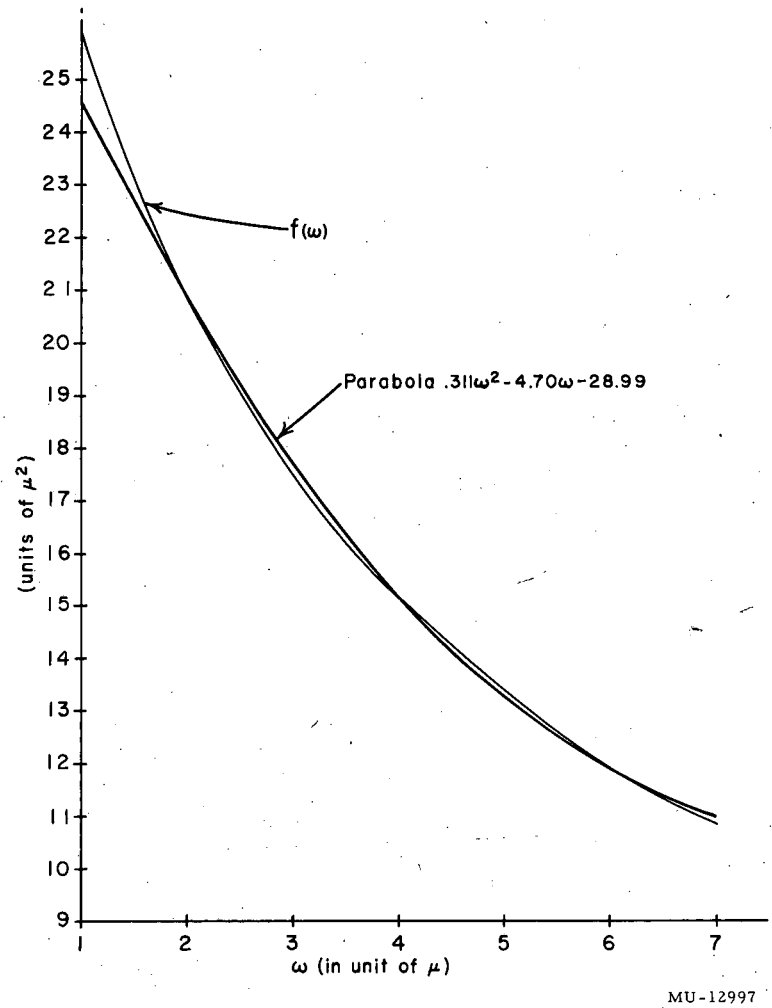

Fig. 2. A comparison of the function $f(\omega)$ and the approximating parabola.

$$R_{3/2\ 3/2}(k',k) = P_{II'} \frac{8\pi f^2}{3\mu^2} \sqrt{\frac{1}{\omega\omega'(\mu-\omega-\omega')}}$$

$$\left[3k'\cdot k - (\sigma\cdot k')(\sigma\cdot k)\right] \left\{ I + \frac{\omega+\omega'-\mu}{\mu} \left(.430 - .0285 \frac{\omega+\omega'}{\mu} \right) \right\} . \quad (7)$$

This is the form finally taken for the off-the-energy-shell-scattering amplitude.

With this form for the scattering amplitude, techniques similar to those employed in the previous computation reduce the matrix elements to double integrals. The chief difference is that, as might be expected with gradient coupling, the integrals are divergent. A cutoff of the virtual pion momenta at the nucleon mass is introduced. The final results are

$$M_{IF}^{(4)} + M_{IF}^{(5)} = .053\ M \ .$$

The transition R is then

$$R = 1.408\ R_0 = 2.9 \times 10^{14}/\text{sec.}$$

CONCLUSIONS

The order-of-magnitude agreement between the calculated value R_{calc} 2.9×10^{14} and the measured value R_{exp} 7.0×10^{14}/sec appear to be due not so much to the model as to the circumstances that largely divorce the numerical results from the underlying model. The failure to get closer agreement is undoubtedly due to the failure of the Hulthén wave function to describe the high-momentum components of the deuteron. The details of the model might be expected to be most strongly exhibited in the higher-order processes, but to the accuracy available in both the theory and the experiment these make negligible contributions. Since the cutoff is used only in the highest-order term, the calculation is largely independent of the cutoff. Again, because the scattering of the virtual meson is remote from the scattering resonance, the contributions from this source are small. This would be true whether the present form of the scattering operator or some other one were used. The deuteron wave function appears principally through one number, the value of its momentum component at the rest mass of the meson.

The calculation becomes in effect a test of only two numbers, the coupling constant and the indicated deuteron-momentum component. As the coupling constant is rather well-determined from scattering experiments, the results should be interpreted as a failure of the Hulthén function to describe the high-momentum spectra of the deuteron. The absorption of mesons by larger nuclei probably is accomplished by high-energy pairs, and it seems reasonable that this calculation may be extended, and the absorption rate of mesons by a nucleus taken as a measure of its high-momentum components.

Because the result is so independent of the details it is also reasonably free of the errors inherent in the approximations used. For example, there might be serious doubts on the validity of using an impulse-approximation treatment, but in view of the small size of the contributions of the higher-order processes the use of this approximation would appear justified. The same remark applies to the form of the scattering operator employed for the virtual mesons.

The lowest-order calculation has also been carried out for a

variety of other momentum distributions. In all these distributions it is of course necessary to specify a parameter, the mean momentum. For equivalent choices of this parameter the lowest-order contribution to the matrix element is not particularly altered. As has been indicated earlier, the absorption process may be a step in a higher-order calculation leading to a level shift in a mesic atom. The level shift does distinguish more adequately between the various wave functions, as the entire function rather than just a single Fourier component enters. Since it is not clear experimentally what portion of the level shifts in mesic atoms is to be attributed to virtual absorptions no definite choice of wave function can be made.

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