The Interaction of Nuclear Electric Quadrupole Moments with Molecular Rotation in Asymmetric-Top Molecules. I*

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The theory of the interaction of nuclear electric quadrupole moments with molecular rotation is extended to asymmetric-top molecules containing one or two quadrupolar nuclei. The first-order theory is developed in detail, and in a form which makes use of published numerical tables of line strengths of asymmetric-top pure rotation transitions, and involves the second derivatives of the electrostatic potential V taken along the three principal axes of inertia. Only two of these are independent, and $(\partial^2V/\partial z'^2)$ and $(\partial^2V/\partial x'^2)-(\partial^2V/\partial y'^2)$ are a convenient choice of the parameters of the problem. A general formulation of the theory, which includes higher order effects, is given. In case a molecule contains only one quadrupolar nucleus, the structure of the quadrupole multiplets should be sufficient to identify pure rotation transitions.

1. INTRODUCTION

THE theory of the electric quadrupole interaction of nuclei and molecular rotation has been developed for linear and for symmetric top molecules containing one or two quadrupolar nuclei.[1–4] This paper extends the theory to asymmetric-rotor molecules containing one or two such nuclei, in a form which makes use, for first-order work, of previously published numerical tables of line strengths of asymmetric rotors.[5] These tables extend to rotational levels involving $J=12$; a second paper will be concerned with developing convenient asymptotic expressions to be used for rotational levels for which $J>12$. The effects of accidental near degeneracy and the small splitting of the higher levels for a given J are considered.

2. THE FIRST-ORDER HAMILTONIAN

The first-order interaction of nuclear electric quadrupole moments with the electric field of an atom or a molecule is described by the Hamiltonian[1, 6]

$$\sum_i[(eQ_i\langle(\partial^2V/\partial z^2)_i\rangle_{Av})/2J(2J-1)I_i(2I_i-1)]\times[3(\mathbf{I}_i\cdot\mathbf{J})^2+\tfrac{3}{2}(\mathbf{I}_i\cdot\mathbf{J})-\mathbf{I}_i^2\mathbf{J}^2] \quad (1)$$

where the $\mathbf{I}_i$ are the nuclear spin angular momentum operators and $\mathbf{J}$ the molecular angular momentum operator. The summation extends over all quadrupolar nuclei present. Q_i, the quadrupole moment of the nucleus, is defined by[1]

$$eQ_i=e\langle 3z_i^2-r_i^2\rangle_{Av}$$

where $\mathbf{r}_i$ is referred to the center of the ith nucleus as origin. The average is taken over the nuclear state $M_I=I$. Also we have[7]

$$\langle\partial^2V/\partial z^2\rangle_{Av}=\langle\textstyle\sum_j e_j(3\cos^2\theta_j-1)/r_j^3\rangle_{Av}.$$

The average is taken over the state $M_J=J$. Here $\mathbf{r}_j$ is the vector from the center of the ith nucleus as origin to the molecular charge e_j; θ_j is the angle between $\mathbf{r}_j$ and the space-fixed z axis.

The first-order problem consists of two parts, (i) the evaluation of the dependence of the $\langle(\partial^2V/\partial z^2)_i\rangle$ on the rotational state, and (ii) the approximate or exact solution of the secular equation obtained from Eq. (1), which involves obtaining the matrices of the operators in square brackets.

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[4] J. Bardeen and C. H. Townes, Phys. Rev. **73**, 97 (1948).

[5] P. C. Cross, R. M. Hainer, and G. W. King, J. Chem. Phys. **12**, 219 (1944): hereafter called CHK.

[6] H. B. G. Casimir, *On the Interaction between Atomic Nuclei and Electrons*, (E. F. Bohn, Haarlem, 1936).

[7] The components of the dyadic ∇E have everywhere been written in explicitly. For a linear molecule or symmetric top $(\partial^2V/\partial z'^2)$, where z' is a molecule-fixed axis, becomes the q of Bardeen and Townes (see reference 4). In the present problem z' will not in general coincide with an internuclear bond.

The result of the second part is obtained by the same methods used for simpler molecules. This rests on the independence of the operators in square brackets of the symmetric-rotor quantum number K, and hence also of the asymmetric rotor pseudo-quantum number τ. The special dependence of $\langle\partial^2V/\partial z^2\rangle_{Av}$ for the various molecular types introduces only a scale factor into the expressions for the splitting of an energy level.

For molecules containing one quadrupolar nucleus the characteristic value[6] of the operator in square brackets in Eq. (1) is

$$\tfrac{3}{4}C(C+1)-I(I+1)J(J+1), \qquad (2)$$

where $C=F(F+1)-I(I+1)-J(J+1)$ and F takes the values $J+I, J+I-1, \cdots |J-I|$. If two quadrupolar nuclei are present, explicit expressions can be written only in some special cases.[8] In general one may set up the secular equation by the method of Bardeen and Townes.[4] It is also possible to write the secular equation in either of the two vector coupling representations $\mathbf{I}_1+\mathbf{I}_2=\mathbf{I}$, $\mathbf{J}+\mathbf{I}=\mathbf{F}$ or $\mathbf{I}_1+\mathbf{J}=\mathbf{F}_1$, $\mathbf{F}_1+\mathbf{I}_2=\mathbf{F}$. The former scheme is convenient for identical nuclei.[9] The matrices of $\mathbf{I}_1\cdot\mathbf{J}$ and $\mathbf{I}_2\cdot\mathbf{J}$ in these schemes can be obtained from previous work on atomic spectra.[10,11]

The energies for molecules containing three quadrupolar nuclei may also be obtained by using the four-vector scheme of reference (10), but the resulting expressions will be complicated, and their application in analysis of spectra very laborious.

3. ROTATIONAL DEPENDENCE OF $\langle\partial^2V/\partial z^2\rangle_{Av}$

A principal task of this paper is the evaluation of the average value of $(\partial^2V/\partial z^2)$ in terms of rotational quantum numbers and quantities which are constants for a given vibrational and electronic state. In work with asymmetric tops, the expression obtained involves a transformation which depends on the asymmetry of the molecule and the J-value in question. Therefore an equation is derived which involves only quantities which have been tabulated for $J<12$ in CHK in connection with other work on asymmetric tops.

$(\partial^2V/\partial z^2)$ is the zz-component of the dyadic $\nabla\mathbf{E}$ (z here is a space-fixed axis). We may obtain it in terms of the components along molecule-fixed axes $x'y'z'$ (which will be chosen as the principal axes of inertia) by a transformation involving the direction cosines between z and $x'y'z'$. The result is

$$\begin{aligned}\partial^2V/\partial z^2=&\alpha_{zx'}{}^2(\partial^2V/\partial x'^2)+\alpha_{zy'}{}^2(\partial^2V/\partial y'^2)\\&+\alpha_{zz'}{}^2(\partial^2V/\partial z'^2)\\&+2\alpha_{zx'}\alpha_{zy'}(\partial^2V/\partial x'\partial y')\\&+2\alpha_{zx'}\alpha_{zz'}(\partial^2V/\partial x'\partial z')\\&+2\alpha_{zy'}\alpha_{zz'}(\partial^2V/\partial y'\partial z') \qquad (3)\end{aligned}$$

where the α's are direction cosines. According to the definition of $\langle\partial^2V/\partial z^2\rangle_{Av}$, the right side is to be averaged over the state J, τ for which $M_J=J$, and also over the vibrational and electronic state. (This latter averaging is only implicit in our work).

In averaging the right side of Eq. (3), considerable simplification occurs. The matrix elements of $\alpha_{zx'}$ and $\alpha_{zy'}$ in a symmetric rotor representation vanish except for $K'=K\pm1$, and those of $\alpha_{zz'}$ except for $K'=K$.[12] Thus the matrices $\alpha_{zx'}\alpha_{zz'}$ and $\alpha_{zy'}\alpha_{zz'}$ in this representation have non-vanishing elements only for $K'=K\pm1$. They have therefore no diagonal elements in an asymmetric rotor representation, since the transformation to this representation involves either only odd or only even K. The average value of $\alpha_{zx'}\alpha_{zy'}$ is zero in either representation since it is a purely imaginary Hermitian matrix.

Equation (3) thus reduces on averaging to

$$\begin{aligned}\langle\partial^2V/\partial z^2\rangle_{Av}=&\langle\alpha_{zx'}{}^2\rangle_{Av}(\partial^2V/\partial x'^2)\\&+\langle\alpha_{zy'}{}^2\rangle_{Av}(\partial^2V/\partial y'^2)+\langle\alpha_{zz'}{}^2\rangle_{Av}(\partial^2V/\partial z'^2). \qquad (4)\end{aligned}$$

The average is over the state J, τ with $M_J=J$. The fact that the components of $\nabla\mathbf{E}$ are averages over vibrational and electronic states is not

[8] If two identical nuclei of spin 1 or $\frac{3}{2}$ are present in a molecule with C_2 axis, the secular equation factors sufficiently to give explicit expressions for the energies.

[9] H. M. Foley, Phys. Rev. **71**, 751 (1947).

[10] M. H. Johnson, Jr., Phys. Rev. **38**, 1635 (1931).

[11] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Teddington, England, 1935) Chapter III.

[12] The properties of these matrices are given, for instance, in CHK, in addition to a table of the elements in a symmetric rotor representation. All the properties of asymmetric rotors used here are expressed in the formulation of CHK; the notation as regards direction cosines and axes is different, however.

explicitly indicated. Approximate numerical computation of $\langle \partial^2 V/\partial z^2 \rangle_{Av}$ will be described first, since the discussion will indicate in which cases more detailed expressions may be required.

The average of a squared direction cosine appearing in Eq. (4) may be written

$$\langle \alpha^2 \rangle_{Av} = \sum_{J'\tau'} |\alpha_{J\tau J;J'\tau' J}|^2. \quad (5)$$

The direction cosine elements in general exist for $J'=J$ or $J\pm 1$. The restriction that $M_J=J$, however, eliminates the elements $\alpha_{J;J-1}$ and gives

$$\langle \alpha^2 \rangle_{Av} = \sum_{\tau'} \{ |\alpha_{J\tau J;J+1\tau' J}|^2 + |\alpha_{J\tau J;J\tau' J}|^2 \}. \quad (6)$$

However, the line strength of an asymmetric rotor transition $J\tau \rightarrow J'\tau'$ is, in a rigid rotor approximation, proportional to the quantity

$$\lambda_{J\tau;J'\tau'} = 3 \sum_{MM'} |\alpha_{J\tau M;J'\tau' M'}|^2 \quad (7)$$

where α is the direction cosine between z and whichever of x', y', or z' coincides with the dipole moment. The quantities (7) are tabulated numerically in CHK for $J \leq 12$ and for asymmetries $\kappa = -1.0$, -0.5, 0, 0.5, and 1.0, where κ is Ray's asymmetry parameter, defined for instance in CHK.

In order to obtain the average value of a squared direction cosine in terms of these tabulated quantities,[13] we must undo the summation over the Zeeman components in Eq. (7). This can be done explicitly since the M-dependence of the matrix elements of the direction cosines of the asymmetric rotor may be written down in terms of the factors in Table I of CHK. In addition we can make use of a sum rule (Eq. (21), CHK) to eliminate the $J; J+1$ matrix elements in Eq. (6).

The result of all this is

$$\left\langle \frac{\partial^2 V}{\partial z^2} \right\rangle_{Av} = \frac{2J}{(2J+1)(2J+3)} \times \sum_{\tau'} [(\partial^2 V/\partial x'^2)\lambda^{x'}_{J\tau;J\tau'} + (\partial^2 V/\partial y'^2)\lambda^{y'}_{J\tau;J\tau'} + (\partial^2 V/\partial z'^2)\lambda^{z'}_{J\tau;J\tau'}], \quad (8)$$

where the $\lambda^i_{J\tau;J\tau'}$ are Q-branch entries in the table of CHK. These entries are subdivided into a, b, and c sub-branches, where a, b, and c are the principal axes of inertia. The moments of inertia about these axes satisfy $I_a < I_b < I_c$. The $x'y'z'$ axes are to be identified with a, b, and c according to this restriction. In using the tables one must remember, in order to get all the $\lambda^i_{J\tau;J\tau'}$, that $\lambda^i_{J\tau;J\tau'} = \lambda^i_{J\tau';J\tau}$. In practice, the summations seldom include more than two important terms.

The accuracy of any result obtained in this manner depends upon the accuracy with which interpolation may be made in the table. Because of the coarseness of the tabulation this may in many cases not be sufficient, and an expression is desirable which involves explicitly the transformation from a symmetric rotor representation to the representation which diagonalizes the energy of the asymmetric top in question, since the coefficients of this transformation depend upon the particular value of the asymmetry parameter κ.

One may derive such an expression by writing down the complete matrices of the squared direction cosines of Eq. (4) in a symmetric rotor representation, for instance by matrix multiplication of the direction cosine matrices given in Table I of CHK; then using the transformation mentioned above. Using the relation[14]

$$\partial^2 V/\partial x'^2 + \partial^2 V/\partial y'^2 + \partial^2 V/\partial z'^2 = 0 \quad (9)$$

one obtains by this procedure

$$\left\langle \frac{\partial^2 V}{\partial z^2} \right\rangle_{Av} = \frac{1}{(J+1)(2J+3)} \times \sum_K [S_{K\tau}{}^2 (3K^2 - J(J+1))(\partial^2 V/\partial z'^2) - 2 S_{K\tau} S_{K+2\tau} f^{\frac{1}{2}}(J, K+1) \times ((\partial^2 V/\partial x'^2) - (\partial^2 V/\partial y'^2))], \quad (10)$$

where

$$f(J, n) = \tfrac{1}{4}[(J+n)(J+n+1)(J-n)(J-n+1)].$$

[13] The procedure for obtaining squares of individual direction cosine matrix elements from the CHK tables is given by S. Golden and E. Bright Wilson, Jr. in "The Stark Effect for a Rigid Asymmetric Rotor," Appendix C (to be published).

[14] This relation holds because of the way in which the average over the electronic state is carried out. A small sphere surrounding the nucleus is excluded from the integration. The electron distribution within the sphere has spherical symmetry, and its interaction with the nucleus does not affect the fine structure formulas, nor the values of the constants obtained from the measurements of the fine structure.

Here the $S_{K\tau}$ must be evaluated for the asymmetry and the J in question. Such an expression will probably only be useful when, for a low J, a higher degree of precision is required than is available from the CHK table for the particular asymmetry involved. It is completely unsuited for use in analysis of rotational spectra. It furnishes, however, a starting point for development of asymptotic approximations which will be given in the second paper. It should be observed that, for a symmetric rotor, Eq. (10) reduces to the relation

$$\left\langle \frac{\partial^2 V}{\partial z^2} \right\rangle_{Av} = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} \frac{\partial^2 V}{\partial z'^2}$$

and this could have been obtained from Eq. (4) by writing in the diagonal elements of the α^2 in a symmetric rotor representation. (There are, however, easier methods of obtaining this expression). It further reduces to

$$\left\langle \frac{\partial^2 V}{\partial z^2} \right\rangle_{Av} = -\frac{J}{2J+3} \frac{\partial^2 V}{\partial z'^2}$$

for linear molecules.

Since the CHK tables extend only to $J=12$, and Eq. (10) should be especially tedious to apply for $J>12$, it has seemed advisable to develop asymptotic approximations to $\langle \partial^2 V/\partial z^2 \rangle_{Av}$ for these higher levels. It has so far been possible to obtain such approximation for slight asymmetry and for these levels which are highest or lowest for a given J. These approximations will be published in a later paper.

4. IDENTIFICATION OF ASYMMETRIC ROTOR SPECTRA

One of the uses to which this theory may be put is that of identification and analysis of pure rotation spectra of asymmetric tops containing one quadrupolar nucleus. The structure of a quadrupole multiplet arising from a given transition depends on the scale factors $eQ\langle \partial^2 V/\partial z^2 \rangle_{Av}$ of the initial and final states and on the characteristic value of the operator in square brackets of Eq. (1), given in Eq. (2). This characteristic value depends on I and J, but I is assumed known. The structure thus depends on three unknowns, J and the quadrupole coupling parameters $eQ\langle \partial^2 V/\partial z^2 \rangle_{Av}$. Since for $I=1$ the multiplet will consist of five ($\Delta J=\pm 1$) or six ($\Delta J=0$) components, for $I=\frac{3}{2}$ either nine ($\Delta J=\pm 1$) or ten ($\Delta J=0$) components, and so on, one should in principle have a highly overdetermined set of equations giving the separations of components in terms of the three unknowns.

If the J-values of the transition can be determined in this way, one should also be able to get τ and τ' by a process of elimination in which approximate expected frequencies and selection rules are used, or by comparison of observed values of $eQ\langle \partial^2 V/\partial z^2 \rangle_{Av}$ for initial and final states with those predicted from Eq. (8). In order to make such predictions, there must be available estimates of the second derivatives of the potential along the principal axes.

Dr. C. H. Townes has suggested a way in which to make such guesses. We assume that the component of $\nabla\mathbf{E}$ along the bond from the nucleus in question is the same as that observed experimentally in a linear molecule in which the same nucleus appears, similarly bonded. If we in addition make the approximate assumption that the charge distribution in the vicinity of the nucleus is symmetrical about the bond and use the relation $\nabla^2 V=0$, we can obtain the components of $\nabla\mathbf{E}$ along the principal axes in terms of the components along the bond and the direction cosines between the bond and the principal axes. Then, approximately,

$$\frac{\partial^2 V}{\partial x_i'^2} = -\frac{1}{2} \frac{\partial^2 V}{\partial \zeta^2} [3\alpha_{i\zeta}^2 - 1], \quad i=1, 2, 3 \qquad (11)$$

where ζ is an axis along the bond and x_1', x_2', x_3' are the principal axes of inertia.

5. HIGHER-ORDER TERMS IN QUADRUPOLE COUPLING

The preceding sections have been concerned with developing in detail formulas for the first-order quadrupole contributions to the energy. The problem of calculating higher order contributions will be outlined here. Only the one-nucleus case will be discussed; the extension to

molecules containing two quadrupolar nuclei is immediate.

Bardeen and Townes have developed formulas for the elements of the symmetric rotor quadrupole Hamiltonian which are off-diagonal in J.[15] Their formulas apply when the nucleus in question is on the symmetry axis, so that

$$\partial^2 V/\partial x'^2 = \partial^2 V/\partial y'^2,$$
$$\partial^2 V/\partial x'\partial y' = \partial^2 V/\partial x'\partial z' = \partial^2 V/\partial y'\partial z' = 0. \quad (12)$$

The matrix then turns out to be diagonal in K.

In the present problem these simplifications are absent. In general the quadrupole Hamiltonian will have non-vanishing elements connecting different values of J and τ. While for most nuclei in linear and symmetric tops the second-order effects are small, in asymmetric tops there exists the possibility of near accidental degeneracies, $E_{J\tau} \cong E_{J'\tau'}$, which will make the second-order corrections important. Furthermore, for a given J the highest levels are essentially degenerate in pairs (small K-type doubling) so that for these levels elements off-diagonal in τ must always be taken into account.

The complete quadrupole Hamiltonian may be written

$$\mathbf{H} = \tfrac{1}{6}\mathbf{Q}:\nabla\mathbf{E} \quad (13)$$

where

$$Q_{\mu\nu} = \int \rho(3x_\mu x_\nu - \delta_{\mu\nu} r^2) d\tau,$$

$$(\nabla E)_{\mu\nu} = \textstyle\sum_j (e_j/r_j^3)(3x_{j\mu}x_{j\nu} - \delta_{\mu\nu} r_j^2), \quad \mu, \nu = 1, 2, 3$$

and the symbol : indicates the inner product of the two dyadics. The matrices of the "scalar product" of two tensors in the $FIJM_F$ scheme have been developed by Racah[16] and his formulas may be used here. The Hamiltonian has the following non-vanishing matrix elements.

TABLE I.

		E	$C_{z'}$	$C_{y'}$	$C_{z'}$
$\alpha_{zz'}^2\alpha_{zy'}^2\alpha_{zz'}^2$	A	1	1	1	1
$\alpha_{zz'}\alpha_{zy'}\ \alpha_{zz'}$	$B_{x'}$	1	1	−1	−1
$\alpha_{zz'}\alpha_{zz'}\ \alpha_{zy'}$	$B_{y'}$	1	−1	1	−1
$\alpha_{zy'}\alpha_{zz'}\ \alpha_{zz'}$	$B_{x'}$	1	−1	−1	1

[15] J. Bardeen and C. H. Townes, Phys. Rev. **73**, 627 (1948), as corrected in an erratum, p. 1204.

[16] G. Racah, Phys. Rev. **52**, 438 (1942). Racah's formulas were first applied to the quadrupole problem by Bardeen and Townes, reference 5.

$$\begin{aligned}
&(J\tau F|H|J+2\tau' F) \\
&= \frac{eQ(J_\tau J|\nabla E_{zz}|J+2\tau' J)}{16I(2I-1)[(2J+1)(J+1)]^{\frac{1}{2}}} \\
&\quad\times[(I+J+F+2)(I+J+F+3) \\
&\quad\times(I-J+F-1)(I-J+F) \\
&\quad\times(J-I+F+1)(J-I+F+2) \\
&\qquad\times(I+J-F+1)(I+J-F+2)]^{\frac{1}{2}}, \\
&(J\tau F|H|J+1\tau' F) \\
&= \frac{eQ(J\tau J|\nabla E_{zz}|J+1\tau' J)}{8I(2I-1)J(2J+1)^{\frac{1}{2}}} \\
&\quad\times[F(F+1)-I(I+1)-J(J+2)] \\
&\quad\times[(I+J+F+2)(I-J+F) \\
&\qquad\times(J-I+F+1)(J+I-F+1)]^{\frac{1}{2}}, \\
&(J\tau F|H|J\tau' F) = \frac{eQ(J\tau J|\nabla E_{zz}|J\tau' J)}{8I(2I-1)J(2J-1)} \\
&\qquad\times[3C(C+1)-4I(I+1)J(J+1)],
\end{aligned} \quad (14)$$

where Q is defined in Eq. (1). The matrix is diagonal in F and M_F. The $J;J-1$ and $J;J-2$ elements may be determined from Eq. (14) by the Hermitian property of $\mathbf{H}$. The evaluation of the matrix elements of $\nabla E_{zz} = (\partial^2 V/\partial z^2)$ is the difficult problem here, as before. For symmetric tops, using the substitution of Eq. (3), one finds

$$(JKJ|\nabla E_{zz}|J+1KJ) = \frac{3K[(J+1)^2-K^2]^{\frac{1}{2}}}{(J+1)(J+2)[2J+3]^{\frac{1}{2}}} \frac{\partial^2 V}{\partial z'^2},$$

$$(JKJ|\nabla E_{zz}|J+2KJ) = \frac{3[\{(J+1)^2-K^2\}\{(J+2)^2-K^2\}]^{\frac{1}{2}}}{(J+2)(2J+3)[(J+1)(2J+5)]^{\frac{1}{2}}} \frac{\partial^2 V}{\partial z'^2}.$$

Substitution of these into Eqs. (14) leads to the expressions of Bardeen and Townes.

For asymmetric tops the evaluation of $(J\tau J|\nabla E_{zz}|J'\tau' J)$ may be simplified by the use of group theory. The asymmetric top wave functions belong to representations of the four-group D_2; so also do the direction cosines α appearing in Eq. (3). Table I gives the symmetries of the direction cosines and their

products. Thus if the two states have the same symmetry, only those combinations of direction cosines belonging to representation A give non-vanishing elements. If the two states have different symmetries, one of the combinations $\alpha_{zz'}\alpha_{zy'}$, $\alpha_{zx'}\alpha_{zz'}$, $\alpha_{zy'}\alpha_{zz'}$ will give non-vanishing elements.

It is this latter case which is involved in the near degeneracies due to slight K-doubling. This should make possible the individual determination of $(\partial^2 V/\partial x'\partial y')$, etc. It seems reasonable that these "cross-derivates" should be small, but by how much they deviate from the 0 value in symmetric rotors must be found from experiment. Equation (14) shows that in this case the multiplet will have the appearance of a "first-order" quadrupole multiplet, only the scale factor differing. Accidental degeneracy arising from levels involving different J may, however, occur between levels of arbitrary relative symmetries.

The matrices Eq. (14) may be used in the above cases, either to evaluate the second-order energy corrections, or to make possible the treatment of near-degenerate levels by degenerate perturbation theory.

The evaluation of the various matrix elements of the combinations of direction cosines which may occur will not be discussed in detail. Unforunately, it seems that the line-strength tables can no longer be used. Expressions analogous to Eq. (10) may be derived involving explicitly the transformation from symmetric to asymmetric rotor basis. Finally, approximation procedures such as will be the subject of the second paper should be applicable.

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The Meson Field and Equations of Motion of Point Particles

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The equation of motion of a point particle possessing a charge and interacting with a meson field (both vector and scalar) is derived from a generalization of the scheme of Infeld and Wallace for determining the equation of a point electron in an electromagnetic field. The retarded and advanced meson fields of the point particle and the nature of the simultaneous expressions for the symmetric, $\frac{1}{2}$(ret+adv), and radiation, $\frac{1}{2}$(ret−adv), potentials and field intensities are investigated. The simultaneous radiation field is found to be always finite for $r\rightarrow 0$, whereas the corresponding symmetric field allows expansion in powers of r with -2 as the lowest, r being the radius of the 3-dimensional sphere surrounding the singularity which represents the point particle. It is shown that the removal of the singularities from the symmetric field leads to the equation of motion given by Bhabha for the vector meson field in the case of the retarded field; the symmetric field, on the other hand, leads to the equation of motion in which the radiation damping is absent. The corresponding equation of motion of a point particle in a scalar meson field is also given.

I. INTRODUCTION

INVESTIGATIONS of the meson field and its scattering by nuclear particles in recent years have led to important developments in the theory of fundamental particles. The highly divergent nature of scattering cross sections for large energies of the meson wave was a puzzle for a long time and was considered to set a limit to the validity of quantum mechanics. It was first realized by Heisenberg[1] and Bhabha[2]

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