

absorption and the measurements of energy distribution were taken each on a different surface in a different tube. Further, there is good evidence that the parameters, particularly  $h$ , vary with the preparation of the surface.<sup>8</sup> One does not seem to be justified, therefore, in attempting a more accurate determination of the constants.

The principal feature of the experimental curve, namely, the steep rise at low energies, is well represented by the theoretical curve. It is not at all surprising that in other respects there are some differences between them. It should be remarked that the comparison of the energy distributions is a more severe test of the theory than comparison of yields, since the latter is a comparison of the integral of the former. Further, to determine the energy distribution, it is necessary to assume an explicit form for the connection between age and energy which is not required for the yield.

The differences between the curves of Fig. 2 can be explained in a reasonable way in terms of the model which we have used. There are two considerations that have been left out of account that will raise the calculated distribution at the high end where it is too low. First, one should expect a gradual transition from the surface dead layer to the active material in the crystal. Thus, some electrons will be able to originate at depths less than  $h$ , and these will lose less energy in reaching the surface. Second, one can expect the electrons to be produced with an initial spread in energy of several

tenths of a volt.<sup>6</sup> Those that are abnormally energetic at birth will be likely to reach the surface with an excess of energy. Neither of these effects can make any noticeable change in the course of the yield.

At  $E=0$  the theoretical curve drops discontinuously to zero. This is to be attributed to our assumption that an electron reaching the surface with  $\epsilon > A$  will surely surmount the surface barrier and escape. Actually, when  $\epsilon - A$  is small, the chance of escape in a single encounter  $(\epsilon - A)/\epsilon$  becomes so small that a large fraction of electrons will lose their extra energy without getting over the barrier. The resulting distribution would decrease continuously to zero in better agreement with observation.

The distribution to be expected when there is no dead layer but destruction of excitons at the surface (mechanism A) has also been calculated. In this case, diffusion of the excitons is taken into account. It turns out then that the distribution in age decreases with increasing age. With the linear connection (9) between age and energy, this means that the energy distribution rises with energy in violent contradiction with experiment. We conclude that a dead layer is essential to the explanation of both the energy distribution and the yield.

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## Consequences of Gauge Invariance for Radiative Transitions\*

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Consideration is given to any system of particles whose behavior under the influence of an external electromagnetic field can be described by a gauge invariant Schroedinger equation. Detailed restrictions on the form of the hamiltonian which are imposed by the condition of gauge invariance are derived. These provide a simple means to the solution of many problems of the interaction of a system with the electromagnetic field. In particular the following consequences are established: (1) In multipole expansions for single photon processes the electric multipole operators have the usual form but the form of the magnetic multipole operators may depend in a detailed way on the interactions between particles and electromagnetic field. (2) The  $f$ -sum rule can be expressed in closed form in terms of the interactions. (3) A generalization of the  $f$ -sum rule to all electric multipole orders is given. (4) The cross section for scattering of a low energy photon can be expressed in terms of the electrostatic polarizability quite independently of the interactions. Applications of these methods to problems in nuclear physics are given in an accompanying paper.

### I. INTRODUCTION

IT is generally assumed for any molecular, atomic, or nuclear system that, to the approximation in which it can be described by a Schroedinger equation, the electromagnetic interactions of the system must

appear in such a way as to leave the equations of motion gauge invariant. The purpose of this note is to show that this assumption has many general consequences for radiative transitions. For example, the well known  $f$ -sum rule for the oscillator strengths can be obtained directly from the gauge property as can similar sum rules for the other electric multipole orders.

Since nuclear processes involve charge-bearing quanta

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(mesons) in a manner which has not yet been adequately described, little is known about the electromagnetic interactions of nuclei. To the extent that these properties can be incorporated into a Schroedinger equation (phenomenological theory) tentative theoretical discussions<sup>1,2</sup> usually assume that the system must be gauge invariant. The radiative properties of nuclei are thereby affected in a manner which can be discovered by application of the general results given here. That application is made in the following paper.

For molecular and atomic systems, the electromagnetic interactions are well known so that no information of a fundamental nature can be expected to ensue from this study. However a somewhat deeper understanding of well-known relationships is provided. Furthermore, for the treatment of certain molecular problems it is convenient to replace the interactions by approximate interactions which involve exchange or velocity dependence.<sup>3</sup> To this approximation, results obtained here serve as a convenient device for the study of electromagnetic properties.<sup>4</sup>

## II. GENERAL PROPERTIES OF THE HAMILTONIAN

It will be found convenient to make an explicit separation of the center of mass variables and the relative coordinates. The coordinate and momentum of the center of mass are denoted by  $\mathbf{R}$  and  $\mathbf{P}$  respectively. The internal variables will be denoted symbolically by a set of operators  $\varphi_\lambda$  which, for different values of  $\lambda$ , may include relative coordinates, relative momenta, spin variables, exchange operators, and so on. The essential property of  $\varphi_\lambda$  is that it commutes with  $\mathbf{R}$  and  $\mathbf{P}$ .

In the absence of an electromagnetic field the hamiltonian of the system is

$$T_0(\mathbf{P}) + H_0(\varphi_\lambda).$$

We now assume that in the presence of an external electromagnetic field described by a vector potential  $\mathbf{A}(\mathbf{r})$ , the Hamiltonian is written as<sup>5</sup>

$$T\{\mathbf{P}, \mathbf{A}(\mathbf{r})\} + H\{\varphi_\lambda, \mathbf{A}(\mathbf{r})\},$$

with

$$T\{\mathbf{P}, \mathbf{A}(\mathbf{r})\} = T_0(\mathbf{P} - \sum_\alpha (e_\alpha/c)\mathbf{A}_\alpha), \quad (1)$$

where  $e_\alpha$  is the charge on the  $\alpha$ th particle, and  $\mathbf{A}_\alpha = \mathbf{A}(\mathbf{r}_\alpha)$ ,  $\mathbf{r}_\alpha$  being the position of that particle. The operator  $H$  includes the internal kinetic energy and terms involving the interactions between the particles. However, the latter terms need not be obtainable by a simple prescription from the field free interactions in  $H_0$ .

<sup>1</sup> R. G. Sachs, Phys. Rev. **74**, 433 (1948).

<sup>2</sup> R. K. Osborne and L. L. Foldy, Phys. Rev. **79**, 795 (1950).

<sup>3</sup> The introduction of a velocity dependent interaction to facilitate the treatment of electrons in a periodic lattice serves as an example. See J. C. Slater, Phys. Rev. **76**, 1592 (1949).

<sup>4</sup> In this connection see the discussion of the modification of sum rules in atomic systems given by V. Fock, Z. Physik **89**, 744 (1934).

<sup>5</sup> The braces are used to indicate that  $H$  and  $T$  are functionals of the vector field  $\mathbf{A}(\mathbf{r})$ .

In most problems concerning the interaction of the field with atomic systems, the field is weakly coupled to the system and  $H\{\varphi_\lambda, \mathbf{A}\}$  can be expanded in powers of the coupling coefficient. This expansion into terms of successively higher order is then taken to be

$$H\{\varphi_\lambda, \mathbf{A}\} = H_0(\varphi_\lambda) + H_1\{\varphi_\lambda, \mathbf{A}(\mathbf{r})\} + (1/2!)H_2\{\varphi_\lambda, \mathbf{A}(\mathbf{r})\} + \cdots, \quad (2)$$

where the  $H_n$  are hermitian operators.

Particular properties of the operator  $H_1$  are of interest since this term represents the interaction responsible for emission or absorption of a single photon. It can be seen easily that  $H_1$  is linearly dependent on  $\mathbf{A}(\mathbf{r})$ :

$$H_1\{\varphi_\lambda, \epsilon\mathbf{A} + \epsilon'\mathbf{A}'\} = \epsilon H_1\{\varphi_\lambda, \mathbf{A}\} + \epsilon' H_1\{\varphi_\lambda, \mathbf{A}'\}. \quad (3)$$

Furthermore, the magnetic moment of the system about its center of mass may be defined in terms of  $H_1$ . For a weak uniform magnetic field  $\mathbf{H}$ , we set

$$\mathbf{A} = -\frac{1}{2}[(\mathbf{r} - \mathbf{R}) \times \mathbf{H}]$$

and the first-order interaction energy is

$$-(\mathbf{M} \cdot \mathbf{H}) = -\frac{1}{2}H_1\{\varphi_\lambda, (\mathbf{r} - \mathbf{R}) \times \mathbf{H}\}, \quad (4)$$

where  $\mathbf{M}$  is the magnetic moment operator. Note that the introduction of  $\mathbf{R}$  in this way is possible because  $\mathbf{R}$  can be treated as a number in  $H_1$  by virtue of its commutation with all the  $\varphi_\lambda$ . Since  $H_1$  is linear, we can divide by the magnitude of the magnetic field and obtain

$$(\mathbf{M} \cdot \mathbf{n}) = \frac{1}{2}H_1\{\varphi_\lambda, \varrho \times \mathbf{n}\} \quad (5)$$

for the definition of an arbitrary component of the magnetic moment in terms of the unit vector  $\mathbf{n}$ . The definition of  $\varrho$  is

$$\varrho = \mathbf{r} - \mathbf{R}, \quad (6)$$

the coordinate relative to the center of mass.

## III. GENERAL CONSEQUENCES OF GAUGE INVARIANCE

The requirement of gauge invariance can be presented in terms of an arbitrary gauge function  $G(\mathbf{r})$  and the associated expression

$$g = (i/\hbar c) \sum_\alpha e_\alpha G(\mathbf{r}_\alpha). \quad (7)$$

The hamiltonian is gauge invariant if<sup>6</sup>

$$T\{\mathbf{P}, \mathbf{A} + \text{grad}G\} + H\{\varphi_\lambda, \mathbf{A} + \text{grad}G\} = e^\sigma [T\{\mathbf{P}, \mathbf{A}\} + H\{\varphi_\lambda, \mathbf{A}\}]e^{-\sigma}. \quad (8)$$

By the definition, Eq. (1), the operator  $T$  is independently gauge invariant so the terms in  $T$  may be dropped from Eq. (8) to give

$$H\{\varphi_\lambda, \mathbf{A} + \text{grad}G\} = e^\sigma H\{\varphi_\lambda, \mathbf{A}\}e^{-\sigma}. \quad (9)$$

With  $\mathbf{A} = 0$  the left side of Eq. (9) can be expanded in

<sup>6</sup> H. Weyl, *Theory of Groups and Quantum Mechanics* (Dover Publications Inc., New York), p. 100.

accordance with Eq. (2) while the right side can be expanded in terms of commutators of  $g$  with  $H_0$ :

$$H_0(\varphi_\lambda) + H_1\{\varphi_\lambda, \text{grad}G\} + (1/2!)H_2\{\varphi_\lambda, \text{grad}G\} + \dots \\ = H_0(\varphi_\lambda) + [g, H_0] + (1/2!)[g, [g, H_0]] + \dots \quad (10)$$

By equating terms of equal order from Eq. (10) gauge invariance is seen to imply the conditions

$$H_1\{\varphi_\lambda, \text{grad}G\} = [g, H_0], \quad (11)$$

$$H_2\{\varphi_\lambda, \text{grad}G\} = [g, [g, H_0]], \quad (12)$$

and, in general,

$$H_n\{\varphi_\lambda, \text{grad}G\} = c^n H_0 / c g^n, \quad (13)$$

where the expression on the right denotes the commutator of  $H_0$  taken  $n$  times with respect to  $g$ .

All of the consequences of gauge invariance relevant to problems discussed here are expressed by Eqs. (13). These equations are conditions on the form of the hamiltonian and can henceforth be used freely without regarding  $G$  as a gauge function.

Note that, subsequent to writing down a hamiltonian of a given form, the electromagnetic field can be quantized without modification of the equations. This is correct if the hamiltonian involves only variables that commute with  $\mathbf{A}$ .

#### IV. SINGLE PHOTON PROCESSES

For the sake of definiteness we consider the emission of a single photon. The vector potential for the radiation field is taken to be

$$\mathbf{A} = c(2\pi\hbar/V)^{\frac{1}{2}} \sum_{\mathbf{k}, \mathbf{u}} q_{\mathbf{k}, \mathbf{u}} \omega^{-\frac{1}{2}} \mathbf{u} \exp(i\mathbf{k} \cdot \mathbf{r}), \quad (14)$$

with  $q_{\mathbf{k}, \mathbf{u}} = a_{\mathbf{k}, \mathbf{u}} + a_{-\mathbf{k}, \mathbf{u}}^*$  where  $a_{-\mathbf{k}, \mathbf{u}}^*$ ,  $a_{\mathbf{k}, \mathbf{u}}$  are the creation and annihilation operators for a photon of propagation vector  $\mathbf{k}$  and polarization  $\mathbf{u}$  with  $(\mathbf{u} \cdot \mathbf{k}) = 0$ ;  $\omega = ck$  is the angular frequency of the photon, and  $V$  is the volume of the enclosure introduced for purposes of normalization. For single photon processes,  $\mathbf{A}$  is to be treated only in first order. Then, by Eq. (2), the interaction of the radiation field with the internal motion of the system is

$$I = \sum_{\mathbf{k}, \mathbf{u}} c(2\pi\hbar/V\omega)^{\frac{1}{2}} q_{\mathbf{k}, \mathbf{u}} H_1\{\varphi_\lambda, \mathbf{u} \exp(i\mathbf{k} \cdot \mathbf{r})\}. \quad (15)$$

Denoting by  $I'$ , the matrix element of  $I$  with respect to the radiation field for emission of the photon  $(\mathbf{k}, \mathbf{u})$ ,

$$I' = c(2\pi\hbar/V\omega)^{\frac{1}{2}} H_1\{\varphi_\lambda, \mathbf{u} \exp(-i\mathbf{k} \cdot \mathbf{r})\}. \quad (16)$$

The radiative transition probabilities may then be obtained in terms of the matrix element of  $I'$  with respect to wave functions of the system of particles. Since  $\mathbf{R}$  commutes with the  $\varphi_\lambda$ , it may be treated as a constant with the result

$$I' = c(2\pi\hbar/V\omega)^{\frac{1}{2}} \\ \times \exp(-i\mathbf{k} \cdot \mathbf{R}) H_1\{\varphi_\lambda, \mathbf{u} \exp(-i\mathbf{k} \cdot \boldsymbol{\rho})\}, \quad (17)$$

where  $\boldsymbol{\rho} = \mathbf{r} - \mathbf{R}$ . This form is convenient since the external factor merely establishes the conservation of total momentum while the argument appearing in  $H_1$  depends only on the internal variables of the system.

The wave functions of the system can be written as the product of  $\exp(i\mathbf{K} \cdot \mathbf{R})$  with a function describing the state of the internal motion. The matrix element of  $I'$  will vanish unless  $\mathbf{K}$  decreases by the amount  $\mathbf{k}$  in the emission process. Taking this change of momentum into account, the transition probability is determined by the matrix element of

$$I'' = c(2\pi\hbar/V\omega)^{\frac{1}{2}} H_1\{\varphi_\lambda, \mathbf{u} \exp(-i\mathbf{k} \cdot \boldsymbol{\rho})\} \quad (18)$$

with respect to the internal wave functions only. The operator  $I''$  will be called the *effective* interaction.

A multipole expansion of the effective interaction about the center of mass can now be made. Introducing the definitions

$$G_l(\mathbf{r}) = (\mathbf{u} \cdot \boldsymbol{\rho})(\mathbf{k} \cdot \boldsymbol{\rho})^{l-1} / l! k^{l-1}, \quad (19)$$

and

$$\mathbf{W}_l(\mathbf{r}) = l \boldsymbol{\rho} (\mathbf{k} \cdot \boldsymbol{\rho})^{l-1} / (l+1)! k^{l-1}, \quad (20)$$

then

$$\mathbf{u} \exp(-i\mathbf{k} \cdot \boldsymbol{\rho}) \\ = \sum_{l=1}^{\infty} (-ik)^{l-1} \{ \text{grad}G_l + i[\mathbf{u} \times \mathbf{k}] \times \mathbf{W}_l \}. \quad (21)$$

The gradient is taken with respect to  $\mathbf{r}$ . Substitution into Eq. (18) and use of the linear property of  $H_1$ , gives the effective interaction as

$$I'' = c(2\pi\hbar/V\omega)^{\frac{1}{2}} \sum_{l=1}^{\infty} (-ik)^{l-1} [H_1\{\varphi_\lambda, \text{grad}G_l\} \\ + iH_1\{\varphi_\lambda, [\mathbf{u} \times \mathbf{k}] \times \mathbf{W}_l\}]. \quad (22)$$

Introducing

$$D_l = \sum_{\alpha} e_{\alpha} G_l(\mathbf{r}_{\alpha}) \quad (23)$$

the gauge condition, Eq. (11), with  $g = (i/\hbar c) \sum_l D_l$ , yields

$$I'' = -(2\pi\hbar/V\omega)^{\frac{1}{2}} \sum_{l=1}^{\infty} (-ik)^{l-1} [(i/k)[H_0, D_l] \\ - icH_1\{\varphi_\lambda, [\mathbf{u} \times \mathbf{k}] \times \mathbf{W}_l\}]. \quad (24)$$

From the definitions Eq. (23) and Eq. (19), we see that

$$D_l = \sum_{\alpha} e_{\alpha} (\mathbf{u} \cdot \boldsymbol{\rho}_{\alpha})(\mathbf{k} \cdot \boldsymbol{\rho}_{\alpha})^{l-1} / l! k^{l-1} \quad (25)$$

is just the electric  $2^l$ -pole moment<sup>7</sup> and the corresponding terms in Eq. (24) are the time derivatives of the electric multipole moments. It is of some conse-

<sup>7</sup> Actually the multipole moments are usually defined in terms of surface harmonics (see Dancoff and Morrison, Phys. Rev. 55, 122 (1939)), which are irreducible representations of the rotation group, rather than these reducible tensors. However, since the multipole expansion is always used in the sense that only the lowest term with nonvanishing matrix element is to be considered, the extra terms which are included here would vanish as a consequence of the selection rules.

quence<sup>8</sup> that the electric multipole terms appear this way whatever the interaction. The other terms, which are magnetic in character, may depend very strongly on the interactions between particles, as shown in the following paper.

Defining a vector  $\mathbf{M}_l$  by

$$(\mathbf{u} \times \mathbf{k} \cdot \mathbf{M}_l) = -H_1 \{ \varphi_\lambda, [\mathbf{u} \times \mathbf{k}] \times \mathbf{W}_l \}, \quad (26)$$

the effective interaction becomes

$$I'' = -(2\pi\hbar/V\omega)^{\frac{1}{2}} \sum_{l=1}^{\infty} (-ik)^{l-1} [\dot{D}_l + ic(\mathbf{u} \times \mathbf{k} \cdot \mathbf{M}_l)]. \quad (27)$$

Equation (20), defining  $\mathbf{W}_l$ , and Eq. (26) show on comparison with Eq. (5) that  $\mathbf{M}_1$  is just the magnetic moment of the system. In general, the  $\mathbf{M}_l$  provide the magnetic multipole moments of order  $2^l$ . To demonstrate this it must be shown that  $\mathbf{M}_l$  transforms under rotation and inversion of the particle variables like a component of a tensor of rank  $l$  with parity  $(-)^{l-1}$ . First consider transformations of *all* vectors, including  $\mathbf{u}$  and  $\mathbf{k}$ . Then

$$(\mathbf{u} \times \mathbf{k} \cdot \mathbf{M}_l) \rightarrow (\mathbf{u} \times \mathbf{k} \cdot \mathbf{M}_l) \quad (28)$$

since  $H_1$  (and each  $H_n$ ) is a scalar operator for transformations of all variables. Now under transformations of  $\mathbf{u}$  and  $\mathbf{k}$  *alone*  $[(\mathbf{u} \times \mathbf{k}) \times \mathbf{W}_l]$  transforms, according to Eq. (20), like a tensor of rank  $l$  with parity  $(-)^{l-1}$ . Since  $H_1$  is linear, the defining Eq. (26) shows that under this transformation  $(\mathbf{u} \times \mathbf{k} \cdot \mathbf{M}_l)$  transforms similarly. If the transformation of  $\mathbf{u}$  and  $\mathbf{k}$  is supplemented by the same transformation of particle variables, Eq. (28) shows that  $(\mathbf{u} \times \mathbf{k} \cdot \mathbf{M}_l)$  must undergo the inverse transformation, which establishes the required property.

The important result is the multipole expansion Eq. (27) of the effective interaction which was obtained only for the internal part,  $H$  of the hamiltonian. It is still to be shown that the interaction terms in  $T\{\mathbf{P}, \mathbf{A}\}$ , given by Eq. (1), have a negligible influence on transitions. Since

$$T_0(\mathbf{P}) = \mathbf{P}^2/2M_0, \quad (29)$$

$M_0$  the total mass of the system, the terms in  $T$  which contribute to single photon processes are

$$T_1 = (-1/M_0)(2\pi\hbar/V\omega)^{\frac{1}{2}} \times \exp(-i\mathbf{k} \cdot \mathbf{R}) \sum_{\alpha} e_{\alpha} \exp(-i\mathbf{k} \cdot \mathbf{q}_{\alpha})(\mathbf{u} \cdot \mathbf{P}). \quad (30)$$

Now the multipole expansion is an expansion of  $\exp(-i\mathbf{k} \cdot \mathbf{q}_{\alpha})$  in powers of  $(\mathbf{k} \cdot \mathbf{q}_{\alpha})$ , and we note that the matrix element of the zero-order term vanishes because the internal wave functions are orthogonal. The first-order term in  $(\mathbf{k} \cdot \mathbf{q}_{\alpha})$  (quadrupole order) makes a contribution only if the dipole selection rules are satisfied; but then there is a contribution of dipole order from  $I''$  so terms of quadrupole order should be neglected. In general we see that  $T_1$  contributes in one

<sup>8</sup> See following paper. Also C. Møller and L. Rosenfeld, *Kgl. Danske Videnskab Selskab Mat.-fys. Medd.* **20**, No. 12 (1943).

higher order than  $I''$  so it may always be neglected for the single photon process.

## V. SUM RULES FOR ELECTRIC MULTIPOLE RADIATION

The transition probability for the emission of electric  $2^l$ -pole radiation in the direction  $d\Omega$  when the system goes from a state  $n$  to a state  $j$  is found by Eq. (27) to be

$$w_{jn}^l = \frac{2\pi}{\hbar} \rho_E |I_{jn}''|^2 = \frac{e^2}{M} \frac{\omega^{2l}}{c^{2l+1}} \left( \frac{\omega_{nj}}{\omega} \right) f_{jn}^l \frac{d\Omega}{4\pi}, \quad (31)$$

where  $M$  is some appropriate particle mass and  $\hbar\omega_{nj}$  is the change in *internal* energy of the system. This energy change differs from  $\hbar\omega$  by the very small recoil energy of the center of mass. The generalized oscillator strength  $f_{jn}^l$  is defined by

$$f_{jn}^l = (2M/\hbar e^2) \omega_{nj} | (D_l)_{jn} |^2, \quad (32)$$

but, for present purposes, it is more conveniently written in the form

$$f_{jn}^l = (-M/\hbar^2 e^2) \{ [H_0, D_l]_{jn} (D_l)_{nj} - (D_l)_{jn} [H_0, D_l]_{nj} \}. \quad (33)$$

Then the sum of the oscillator strength over all initial states  $n$  is

$$\sum_n f_{jn}^l = -(M/\hbar^2 e^2) [[H_0, D_l], D_l]_{jj}, \quad (34)$$

i.e., the expectation value of the double commutator in state  $j$ . However, according to Eq. (12) and the definition, Eq. (23), of  $D_l$ , the double commutator can be expressed directly in terms of  $H_2$ :

$$\sum_n f_{jn}^l = (M c^2 / e^2) \langle H_2 \{ \varphi_\lambda, \text{grad} G_l \} \rangle_{jj} \quad (35)$$

where  $G_l$  is given explicitly in Eq. (19) and the gradient is taken with respect to  $\mathbf{r}$ . Equation (35) is the *generalized  $f$ -sum rule*.

That Eq. (35) leads to the usual  $f$ -sum rule for dipole radiation can easily be established by noting that

$$\text{grad} G_1 = \mathbf{u}. \quad (36)$$

Consider, as a particular example, particles of mass  $m_{\alpha}$  whose mutual interaction can be described by an ordinary potential  $U(\rho_1, \rho_2, \dots)$ .

Then the internal hamiltonian may be written as

$$H\{\varphi_\lambda, \mathbf{A}\} = \frac{1}{4M_0 c^2} \sum_{\alpha, \beta} m_{\alpha} m_{\beta} \left( \frac{c}{m_{\alpha}} \mathbf{p}_{\alpha} - \frac{c}{m_{\beta}} \mathbf{p}_{\beta} - \frac{e_{\alpha}}{m_{\alpha}} \mathbf{A}_{\alpha} + \frac{e_{\beta}}{m_{\beta}} \mathbf{A}_{\beta} \right)^2 + U \quad (37)$$

where  $M_0$  is the total mass of the system. The operator  $H_2$  is

$$H_2\{\varphi_\lambda, \mathbf{A}\} = \frac{1}{2M_0 c^2} \sum_{\alpha, \beta} m_{\alpha} m_{\beta} \left( \frac{e_{\alpha}}{m_{\alpha}} \mathbf{A}_{\alpha} - \frac{e_{\beta}}{m_{\beta}} \mathbf{A}_{\beta} \right)^2. \quad (38)$$

Therefore

$$H_2\{\varphi_\lambda, \mathbf{u}\} = \frac{1}{2M_0c^2} \sum_{\alpha, \beta} m_\alpha m_\beta \left( \frac{e_\alpha}{m_\alpha} - \frac{e_\beta}{m_\beta} \right)^2, \quad (39)$$

and the sum rule for dipole radiation becomes

$$\sum_n f_{jn} = \frac{M}{2M_0e^2} \sum_{\alpha, \beta} m_\alpha m_\beta \left( \frac{e_\alpha}{m_\alpha} - \frac{e_\beta}{m_\beta} \right)^2. \quad (40)$$

For a system of  $Z$  electrons of mass  $m$  in the field of a nucleus of charge  $Ze$ , we choose  $M$  to be  $m/M_0$  times the nuclear mass and find

$$\sum_n f_{jn} = Z \quad (41)$$

in agreement with the usual result. Again note that the mass appearing in the definition of this oscillator strength differs slightly from the electron mass.

## VI. THE SCATTERING OF LIGHT

As a further example of the consequences of gauge invariance, consider the elastic scattering by the system of a photon of propagation vector  $\mathbf{k}$  and polarization vector  $\mathbf{u}$  into the state  $\mathbf{k}'$ ,  $\mathbf{u}'$ . It will be shown that gauge invariance just leads to the cancellation of diamagnetic terms which is required to establish the usual relationship between the static electric polarizability and the cross section for the scattering of a low energy photon.

The second-order terms must be carried for this two-quantum process so the interaction is

$$I = H_1\{\varphi_\lambda, \mathbf{A}\} + \frac{1}{2}H_2\{\varphi_\lambda, \mathbf{A}\} + T\{\mathbf{P}, \mathbf{A}\}. \quad (42)$$

Application of the vector potential, Eq. (14), to the center of mass interaction  $T\{\mathbf{P}, \mathbf{A}\}$  leads directly to the Thomson cross section for the scattering of light by a charged mass point. Consideration is now restricted to the internal part of the hamiltonian. In this case only the terms of electric dipole order are carried in the vector potential, which is then written as

$$\mathbf{A} = c(2\pi\hbar/V)^{\frac{1}{2}} \sum_{\mathbf{k}, \mathbf{u}} \omega^{-\frac{1}{2}} q_{\mathbf{k}, \mathbf{u}} \mathbf{u} \exp(i\mathbf{k} \cdot \mathbf{R}). \quad (43)$$

If a function  $G(\mathbf{r})$  is defined by

$$G = c(2\pi\hbar/V)^{\frac{1}{2}} \sum_{\mathbf{k}, \mathbf{u}} \omega^{-\frac{1}{2}} q_{\mathbf{k}, \mathbf{u}} [\mathbf{u} \cdot (\mathbf{r} - \mathbf{R})] \exp(i\mathbf{k} \cdot \mathbf{R}) \quad (44)$$

then

$$\mathbf{A} = \text{grad}G. \quad (45)$$

The gauge conditions, Eqs. (11) and (12), may therefore be used to transform Eq. (42) to

$$I = (i/\hbar)(2\pi\hbar/V)^{\frac{1}{2}} \sum_{\mathbf{k}, \mathbf{u}} \omega^{-\frac{1}{2}} q_{\mathbf{k}, \mathbf{u}} [D, H_0] \exp(i\mathbf{k} \cdot \mathbf{R}) - (\pi/V\hbar) \sum_{\mathbf{k}, \mathbf{u}} \sum_{\mathbf{k}', \mathbf{u}'} (\omega\omega')^{-\frac{1}{2}} q_{\mathbf{k}, \mathbf{u}} q_{\mathbf{k}', \mathbf{u}'} [D, [D', H_0]] \quad (46)$$

with

$$D = \sum_{\alpha} e_{\alpha}(\mathbf{u} \cdot \boldsymbol{\rho}_{\alpha}), \quad D' = \sum_{\alpha} e_{\alpha}(\mathbf{u}' \cdot \boldsymbol{\rho}_{\alpha}). \quad (47)$$

Now the transition amplitude<sup>9</sup> for the absorption of  $(\mathbf{k}, \mathbf{u})$  and the emission of  $(\mathbf{k}', \mathbf{u}')$  is found from Eq. (46) to be

$$T = -\frac{2\pi}{V\hbar} (\omega\omega')^{-\frac{1}{2}} \left\{ \sum_i \left( \frac{[D, H_0]_{0j} [D', H_0]_{j0}}{\hbar\omega_{0j} + \hbar\omega} + \frac{[D', H_0]_{0j} [D, H_0]_{j0}}{\hbar\omega_{0j} - \hbar\omega'} \right) + \frac{1}{2} [D, [D', H_0]]_{00} + \frac{1}{2} [D', [D, H_0]]_{00} \right\}, \quad (48)$$

if the initial and final internal state of the particle system is denoted by the subscript "0." On using the relationship

$$[D, H_0]_{0j} = -\hbar\omega_{0j} D_{0j}, \quad (49)$$

$T$  becomes

$$T = \frac{\pi}{V\hbar} (\omega\omega')^{-\frac{1}{2}} \left\{ \sum_j \left( \frac{D_{0j} [D', H_0]_{j0} - [D, H_0]_{0j} D_{j0}'}{1 + \omega/\omega_{0j}} + \frac{D_{0j}' [D, H_0]_{j0} - [D', H_0]_{0j} D_{j0}}{1 - \omega'/\omega_{0j}} \right) - [D, [D', H_0]]_{00} - [D', [D, H_0]]_{00} \right\}. \quad (50)$$

Now if an expansion of the energy denominators in powers of  $\omega/\omega_{0j}$  and  $\omega'/\omega_{0j}$  is carried out, the zero-order term in the summation is just cancelled by the diamagnetic terms represented by the double commutators. The first-order term is proportional to the very small difference between  $\omega$  and  $\omega'$  so, neglecting this difference,  $T$  is to second order

$$T = (2\pi/V\hbar) \sum_j (\omega/\omega_{0j}) (D_{0j} D_{j0}' + D_{0j}' D_{j0}). \quad (51)$$

Thus

$$T = -(2\pi/V) \omega \alpha_{\mathbf{u}, \mathbf{u}'}, \quad (52)$$

where  $\alpha_{\mathbf{u}, \mathbf{u}'}$  is the  $(\mathbf{u}, \mathbf{u}')$  component of the electrostatic polarizability tensor. Note that this result is quite independent of the detailed interactions between the particles except through the influence of the interactions on the wave functions which determine the matrix elements.

<sup>9</sup> The term transition amplitude is used here for the quantity  $T$  which appears in the expression for the transition probability,  $w = (2\pi/\hbar) \rho_E |T|^2$ . Sometimes it is referred to as the "matrix element."