

Derivation of Nonrelativistic Hamiltonian for Electrons from Quantum Electrodynamics

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The effective quantum-mechanical Hamiltonian for a system of electrons in static electromagnetic field is derived from quantum electrodynamics for electron velocities small compared with the light velocity. The Hamiltonian obtained is almost identical with the one obtained by Bethe and Salpeter, but there is a small difference, of which an explanation is given.

1. INTRODUCTION

In this paper the effective quantum-mechanical Hamiltonian for a system of electrons in a static electromagnetic field is derived from the quantum electrodynamics for the case in which the velocities of the electrons are sufficiently small compared with the light velocity. It is assumed that the variation of the electromagnetic field through space is moderate in the sense that its Fourier component has an appreciable value only for those wavelengths which are sufficiently larger than the Compton wavelength of the electron.

Different derivations have been given by Bethe and Salpeter¹ and by Slater.² Bethe and Salpeter's derivation of the Hamiltonian is based on Breit's equation, which can be regarded as a generalized Dirac equation. They obtained the Hamiltonian from Breit's equation through a technique which is somewhat similar to the Pauli approximation to the Dirac equation. On the other hand, Slater's derivation is largely based on classical considerations. The result of Bethe and Salpeter and that of Slater are the same. It appears obvious, however, that the derivation from quantum electrodynamics is the most appropriate from the viewpoint of the unified understanding of the basic laws governing nature.

The Hamiltonian obtained here is almost identical with the one obtained by Bethe and Salpeter and by Slater, but there is a small difference, which we discuss later. The Hamiltonian to be derived here is the following:

$$H = \sum_j \frac{1}{2m} \mathbf{p}_j^2 \quad (1a)$$

$$- \sum_j \frac{1}{8m^3 c^2} \mathbf{p}_j^4 \quad (1b)$$

$$+ \sum_j (e/mc) \mathbf{p}_j \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}_j) \quad (1c)$$

$$+ \sum_j (e^2/2mc^2) \mathbf{A}_{\text{ex}}(\mathbf{r}_j)^2 \quad (1d)$$

$$- \sum_j e\phi_{\text{ex}}(\mathbf{r}_j) \quad (1e)$$

$$+ \sum_j (e/mc) \mathbf{s}_j \cdot \mathbf{H}_{\text{ex}}(\mathbf{r}_j) \quad (1f)$$

$$+ \sum_j (e/2m^2 c^2) \mathbf{s}_j \cdot [\mathbf{E}_{\text{ex}}(\mathbf{r}_j) \times \mathbf{p}_j] \quad (1g)$$

$$+ \sum_j (\pi e \hbar^2 / 2m^2 c^2) \rho_{\text{ex}}(\mathbf{r}_j) \quad (1h)$$

$$+ \sum_{j < k} (e^2 / r_{jk}) \quad (2a)$$

$$- \sum_{j < k} \frac{e^2}{2m^2 c^2} \mathbf{p}_j \cdot \left[\frac{(\mathbf{r}_j - \mathbf{r}_k)(\mathbf{r}_j - \mathbf{r}_k)}{r_{jk}^3} + \frac{1}{r_{jk}} \right] \cdot \mathbf{p}_k \quad (2b)$$

$$- \sum_{j \neq k} \frac{e^2}{m^2 c^2} \frac{1}{r_{jk}^3} \mathbf{s}_j \cdot [(\mathbf{r}_k - \mathbf{r}_j) \times \mathbf{p}_k] \quad (2c)$$

$$- \sum_{j \neq k} \frac{e^2}{2m^2 c^2} \frac{1}{r_{jk}^3} \mathbf{s}_j \cdot [(\mathbf{r}_j - \mathbf{r}_k) \times \mathbf{p}_j] \quad (2d)$$

$$- \sum_{j < k} \frac{e^2}{m^2 c^2} \mathbf{s}_j \cdot \left[\frac{3(\mathbf{r}_j - \mathbf{r}_k)(\mathbf{r}_j - \mathbf{r}_k)}{r_{jk}^5} - \frac{1}{r_{jk}^3} \right] \cdot \mathbf{s}_k \quad (2e)$$

$$- \sum_{j < k} (8\pi e^2 / 3m^2 c^2) \delta(\mathbf{r}_j - \mathbf{r}_k) \mathbf{s}_j \cdot \mathbf{s}_k \quad (2f)$$

$$- \sum_{j < k} (\pi e^2 \hbar^2 / m^2 c^2) \delta(\mathbf{r}_j - \mathbf{r}_k). \quad (2g)$$

The notation is as usual: c is the light velocity, $-e$ is the charge of the electron, and m is the mass of the electron. \mathbf{r}_j is the position of the j th electron, \mathbf{p}_j is its momentum, and \mathbf{s}_j its spin. The external electric field $\mathbf{E}_{\text{ex}}(\mathbf{r})$ and the magnetic field $\mathbf{H}_{\text{ex}}(\mathbf{r})$ are in Gaussian units. They are assumed to be independent of time. They are derived from the scalar potential $\phi_{\text{ex}}(\mathbf{r})$ and the vector potential $\mathbf{A}_{\text{ex}}(\mathbf{r})$, respectively, according to

$$\mathbf{E}_{\text{ex}}(\mathbf{r}) = -\nabla\phi_{\text{ex}}(\mathbf{r}), \quad (3a)$$

$$\mathbf{H}_{\text{ex}}(\mathbf{r}) = \nabla \times \mathbf{A}_{\text{ex}}(\mathbf{r}). \quad (3b)$$

$\rho_{\text{ex}}(\mathbf{r})$ is the charge density giving rise to the potential

¹ H. A. Bethe and E. E. Salpeter, *Encyclopedia of Physics*, edited by S. Flügge (Springer-Verlag, Berlin-Göttingen-Heidelberg, 1957), Vol. 35, p. 88.

² J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill Book Company, Inc., New York, 1960), Vol. II.

$\phi_{\text{ex}}(\mathbf{r})$. Thus,

$$\Delta\phi_{\text{ex}}(\mathbf{r}) = -4\pi\rho_{\text{ex}}(\mathbf{r}). \quad (4)$$

The vector potential is so chosen that its divergence is zero:

$$\nabla \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}) = 0. \quad (5)$$

The symbol $\mathbf{1}$ means the unit dyadic, and $\delta(\mathbf{r})$ is the Dirac δ function. \mathbf{p}_j^4 means $(\mathbf{p}_j^2)^2$, and r_{jk} means $|\mathbf{r}_j - \mathbf{r}_k|$.

Each term of the Hamiltonian (1a)–(2g) allows its classical interpretation. The terms (1a), (1c), (1d), and (1e) constitute the well-known Hamiltonian of a system of point particles under the influence of the Lorentz force

$$-e\mathbf{E}_{\text{ex}}(\mathbf{r}_j) - (e/c)[\mathbf{v}_j \times \mathbf{H}_{\text{ex}}(\mathbf{r}_j)], \quad (6)$$

where \mathbf{v}_j is the velocity of the particle j . The term (1b) comes from the variation of mass due to relativity. (2a) is the Coulomb interaction between electrons. (2b) is a term which was derived by Darwin³ using retarded potential, but a simpler explanation is the following. According to the Biot and Savart law, the magnetic field produced by the orbital motion of the electron k is given by

$$\mathbf{H}_k(\mathbf{r}) = (e/c)(\mathbf{r} - \mathbf{r}_k) \times \mathbf{v}_k / |\mathbf{r} - \mathbf{r}_k|^3. \quad (7)$$

This magnetic field is derived from the vector potential

$$\mathbf{A}_k(\mathbf{r}) = -\frac{e}{2c} \left[\frac{(\mathbf{r} - \mathbf{r}_k)(\mathbf{r} - \mathbf{r}_k)}{|\mathbf{r} - \mathbf{r}_k|^3} + \frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}_k|} \right] \cdot \mathbf{v}_k. \quad (8)$$

This $\mathbf{A}_k(\mathbf{r})$ is chosen to be divergence-less. The effect of this field on the motion of the electron j can be taken into account by changing the $\mathbf{A}_{\text{ex}}(\mathbf{r}_j)$ in (1c) and (1d) to $\mathbf{A}_{\text{ex}}(\mathbf{r}_j) + \mathbf{A}_k(\mathbf{r}_j)$. Neglecting the term quadratic in $\mathbf{A}_k(\mathbf{r}_j)$, and the cross term between $\mathbf{A}_{\text{ex}}(\mathbf{r}_j)$ and $\mathbf{A}_k(\mathbf{r}_j)$, the only new term in the Hamiltonian is

$$(e/mc)\mathbf{p}_j \cdot \mathbf{A}_k(\mathbf{r}_j). \quad (9)$$

Putting $\mathbf{v}_k = \mathbf{p}_k/m$ in (8) and using it in (9) and summing it over j and k ($k \neq j$), we obtain twice (2b). This result should be divided by 2, since the sum consists of pairs of identical terms, that is, $\mathbf{p}_j \cdot \mathbf{A}_k(\mathbf{r}_j) = \mathbf{p}_k \cdot \mathbf{A}_j(\mathbf{r}_k)$.

The terms (1h) and (2g) can be interpreted as due to the spread of the charge of the electron, which leads to a modification of the terms (1e) and (2a). In the first approximation, this modification is represented by the addition of (1h) and (2g), respectively, provided that the spread is spherically symmetrical and the mean square radius is $\langle r^2 \rangle_{\text{av}} = \frac{3}{4}(\hbar/mc)^2$.

Now we have finished with those terms that do not contain the spin operators. The remaining terms concern the spin of the electron. The term (1f) is the interaction of the spin magnetic moment of the electron

with the external magnetic field. (1g) is the term that causes the precession of the spin in the external electric field. The explanation of the origin of this term is not simple; readers are referred to the paper by Thomas.⁴ (2c) is the interaction of the spin of the electron with the magnetic field produced by the orbital motion of the other electrons. (2d) is of the same nature as (1g) and expresses the interaction of the spins of electrons with the electric field produced by the other electrons. (2e) is the mutual interaction between spin magnetic moments that are not mutually penetrating, while (2f) takes account of the mutual penetration.

The above Hamiltonian is almost identical with the one derived by Bethe and Salpeter. However, there is a small difference: the terms (1h) and (2g) are absent in the Bethe–Salpeter Hamiltonian, while their Hamiltonian contains

$$\sum_j (ie\hbar/4m^2c^2)\mathbf{p}_j \cdot \mathbf{E}_{\text{ex}}(\mathbf{r}_j) \quad (10a)$$

$$- \sum_{j < k} (ie^2\hbar/4m^2c^2)(\mathbf{p}_j - \mathbf{p}_k) \cdot (\mathbf{r}_{jk}/r_{jk}^3), \quad (10b)$$

which is absent in our Hamiltonian. There is some relation between (1h) and (2g) and (10a) and (10b). Namely, the mean values of (1h) and (2g) for a state represented by a real (not complex) wave function are equal to the mean values of (10a) and (10b) for the same state, respectively. However, the operators (1h) and (2g) themselves are not identical with (10a) and (10b), respectively. That (1h) and (2g) are preferable to (10a) and (10b) is obvious from the fact that (10a) and (10b) are not Hermitian. Thus, (10a) and (10b) do not fit the pattern of quantum mechanics.

The deficiency of (10a) and (10b) comes from the inadequate normalization of the wave functions $\psi_{\pm}(\mathbf{p})$ introduced by Bethe and Salpeter. In their article the $\psi_{\pm}(\mathbf{p})$ are defined from the Fourier component $\psi(\mathbf{p})$ of the Dirac four-component wave function through a transformation which is very similar to the Foldy–Wouthuysen transformation.⁵ Denoting the Foldy–Wouthuysen transformation by e^{iS} , the above transformation is expressed by

$$\begin{pmatrix} \psi_+(\mathbf{p}) \\ \psi_-(\mathbf{p}) \end{pmatrix} = \left(\frac{E_0 + E_p}{2E_p} \right)^{\frac{1}{2}} e^{iS} \psi(\mathbf{p}), \quad (11)$$

where $E_p = c(m^2c^2 + p^2)^{\frac{1}{2}}$ and $E_0 = mc^2$. Since e^{iS} is a unitary transformation, $[(E_0 + E_p)/2E_p]^{\frac{1}{2}} e^{iS}$ is not unitary, so that the Hermitian character of the Hamiltonian is not conserved through this transformation. This is the reason why Bethe and Salpeter obtained the non-Hermitian Hamiltonian. If the transformation e^{iS} itself is used instead of $[(E_0 + E_p)/2E_p]^{\frac{1}{2}} e^{iS}$ to define $\psi_{\pm}(\mathbf{p})$ from $\psi(\mathbf{p})$, the Bethe–Salpeter method would lead to the same result as ours. However, their

³ C. G. Darwin, *Phil. Mag.* **39**, 537 (1920).

⁴ L. H. Thomas, *Nature* **117**, 514 (1926).

⁵ L. L. Foldy and S. A. Wouthuysen, *Phys. Rev.* **78**, 29 (1950).

method of derivation is not identical with ours, and the primary purpose of the present paper is this new derivation.

2. QUANTUM ELECTRODYNAMICS

We start with the quantum electrodynamical Hamiltonian

$$H_{Q.E.} = H_M + H_R + H_C + H_I + H_E, \quad (12)$$

$$H_M = \sum_s \int \hbar c (\kappa^2 + k^2)^{\frac{1}{2}} \times [a^*(\mathbf{k}s)a(\mathbf{k}s) + b^*(\mathbf{k}s)b(\mathbf{k}s)] d^3k, \quad (13a)$$

$$H_R = \sum_\lambda \int \hbar c k c^*(\mathbf{k}\lambda)c(\mathbf{k}\lambda) d^3k, \quad (13b)$$

$$H_C = \frac{1}{2} \int \rho(\mathbf{r})\rho(\mathbf{r}') |\mathbf{r}-\mathbf{r}'|^{-1} d^3r d^3r', \quad (13c)$$

$$H_I = -(1/c) \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d^3r, \quad (13d)$$

$$H_E = \int \rho(\mathbf{r})\phi_{\text{ex}}(\mathbf{r}) d^3r - (1/c) \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}) d^3r, \quad (13e)$$

where H_M is the rest energy plus kinetic energy of electrons and positrons, H_R is the energy of the radiation field, H_C is the mutual interaction of electrons and positrons, H_I is the interaction between the electron-positron current and the radiation field, and H_E is the interaction of electrons and positrons with external field. $a(\mathbf{k}s)$, $b(\mathbf{k}s)$, and $c(\mathbf{k}\lambda)$ are the annihilation operators of an electron, a positron, and a photon, respectively, while $a^*(\mathbf{k}s)$, etc. are the corresponding creation operators. The argument \mathbf{k} of these operators is the momentum of the particle in unit of \hbar . The parameter s designates the spin state of the electron or the positron, $s=1, 2$ corresponding to the values $\pm\frac{1}{2}\hbar$ of the z component of the spin. The parameter $\lambda(=1, 2)$ in $c(\mathbf{k}\lambda)$ and $c^*(\mathbf{k}\lambda)$ designates the polarization of the photon. κ in (13a) is defined by $\kappa=mc/\hbar$.

$\mathbf{A}(\mathbf{r})$ in (13d) is an operator defined by

$$\mathbf{A}(\mathbf{r}) = (2\pi)^{-1} \sum_\lambda \int (\hbar c/k)^{\frac{1}{2}} [c(\mathbf{k}\lambda) + c^*(-\mathbf{k}\lambda)] \cdot \mathbf{e}(\mathbf{k}\lambda) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k, \quad (14)$$

where $\mathbf{e}(\mathbf{k}\lambda)$ is the unit vector in the direction of the polarization. The $\mathbf{e}(\mathbf{k}\lambda)$ are chosen so that $\mathbf{e}(\mathbf{k}\lambda) = \mathbf{e}(-\mathbf{k}\lambda)$. The operators $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ in (13c), (13d), and (13e) are defined by

$$\rho(\mathbf{r}) = -\frac{1}{2}e(1-C)\psi^*(\mathbf{r})\psi(\mathbf{r}), \quad (15)$$

$$\mathbf{j}(\mathbf{r}) = -\frac{1}{2}ec(1-C)\psi^*(\mathbf{r})\boldsymbol{\alpha}\psi(\mathbf{r}), \quad (16)$$

where $\psi(\mathbf{r})$ is a four-component operator

$$\psi(\mathbf{r}) = (2\pi)^{-\frac{3}{2}} \int \left(1 - \frac{\beta\mathbf{k} \cdot \boldsymbol{\alpha}}{\kappa + k_0}\right) \left(\frac{\kappa + k_0}{2k_0}\right)^{\frac{1}{2}} \cdot \begin{pmatrix} a(\mathbf{k}1) \\ a(\mathbf{k}2) \\ b^*(-\mathbf{k}2) \\ -b^*(-\mathbf{k}1) \end{pmatrix} \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k, \quad (17)$$

and C is a symbol which indicates that $a(\mathbf{k}s)$, $a^*(\mathbf{k}s)$, $b(\mathbf{k}s)$, and $b^*(\mathbf{k}s)$ appearing to the right of this symbol should be replaced by $b(\mathbf{k}s)$, $b^*(\mathbf{k}s)$, $a(\mathbf{k}s)$, and $a^*(\mathbf{k}s)$, respectively. In Eq. (17), k_0 means $k_0 = (\kappa^2 + k^2)^{\frac{1}{2}}$. $\boldsymbol{\alpha}$ and β in (16) and (17) are the well-known Dirac matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (18)$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (19)$$

Quantum electrodynamics satisfies the requirement of relativity, though this is not self-evident from the forms of (12)–(13e). The relativistic structure of quantum electrodynamics can be visualized in a formalism which involves the longitudinal and scalar photons, but an appropriate unitary transformation leads to the formalism of (12)–(13e).

Quantum electrodynamics suffers from the well-known divergence difficulties. If the Hamiltonian (12) is to have any mathematical significance, it is necessary to cut the integral (17) at some large value of k . This cutoff destroys the relativistic invariance of the theory, but we adopt this cutoff as an inevitable deviation from relativity.

3. CREATION AND ANNIHILATION OPERATORS AT A POSITION

It is convenient to introduce the operators

$$\phi_a(\mathbf{r}s) = (2\pi)^{-\frac{3}{2}} \int a(\mathbf{k}s) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k, \quad (20a)$$

$$\phi_a^*(\mathbf{r}s) = (2\pi)^{-\frac{3}{2}} \int a^*(\mathbf{k}s) \exp(-i\mathbf{k} \cdot \mathbf{r}) d^3k, \quad (20b)$$

$$\phi_b(\mathbf{r}s) = (2\pi)^{-\frac{3}{2}} \int b(\mathbf{k}s) \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k, \quad (20c)$$

$$\phi_b^*(\mathbf{r}s) = (2\pi)^{-\frac{3}{2}} \int b^*(\mathbf{k}s) \exp(-i\mathbf{k} \cdot \mathbf{r}) d^3k. \quad (20d)$$

These are Fourier transformations of $a(\mathbf{k}s)$, $a^*(\mathbf{k}s)$,

$b(\mathbf{k}s)$, $b^*(\mathbf{k}s)$. Thus, they can be interpreted as the operators which create or annihilate an electron or a positron at a position \mathbf{r} .

We also use the notations

$$\phi_a(\mathbf{r}) = \begin{pmatrix} \phi_a(\mathbf{r}1) \\ \phi_a(\mathbf{r}2) \end{pmatrix}, \quad (21)$$

$$\phi_b(\mathbf{r}) = \begin{pmatrix} \phi_b(\mathbf{r}1) \\ \phi_b(\mathbf{r}2) \end{pmatrix}, \quad (22)$$

$$\phi(\mathbf{r}) = \begin{pmatrix} \phi_a(\mathbf{r}1) \\ \phi_a(\mathbf{r}2) \\ \phi_b^*(\mathbf{r}2) \\ -\phi_b^*(\mathbf{r}1) \end{pmatrix} = \begin{pmatrix} \phi_a(\mathbf{r}) \\ i\sigma_y\phi_b^{*T}(\mathbf{r}) \end{pmatrix}, \quad (23)$$

where T means transposition. From (20a-d) and (23) we have

$$\phi(\mathbf{r}) = (2\pi)^{-3} \int \begin{pmatrix} a(\mathbf{k}1) \\ a(\mathbf{k}2) \\ b^*(-\mathbf{k}2) \\ -b^*(-\mathbf{k}1) \end{pmatrix} \exp(i\mathbf{k}\cdot\mathbf{r}) d^3k. \quad (24)$$

4. NONRELATIVISTIC APPROXIMATION

The integrand of (13a) can be modified to some extent without any influence on the main result to be obtained in this paper. Thus, we can use the approximation

$$H_M = \sum_s \int \hbar c \kappa \left[1 + \frac{1}{2}(k/\kappa)^2 - \frac{1}{8}(k/\kappa)^4 \right] \cdot [a^*(\mathbf{k}s)a(\mathbf{k}s) + b^*(\mathbf{k}s)b(\mathbf{k}s)] d^3k \quad (25)$$

without changing the main result. Similarly, we can put

$$\psi(\mathbf{r}) = (2\pi)^{-3} \int \left[1 - \frac{1}{2}(\beta\mathbf{k}\cdot\boldsymbol{\alpha}/\kappa) - \frac{1}{8}(k/\kappa)^2 \right] \cdot \begin{pmatrix} a(\mathbf{k}1) \\ a(\mathbf{k}2) \\ b^*(-\mathbf{k}2) \\ -b^*(-\mathbf{k}1) \end{pmatrix} \exp(i\mathbf{k}\cdot\mathbf{r}) d^3k. \quad (26)$$

These approximations are called the nonrelativistic approximation in distinction from the nonrelativistic cutoff mentioned at the end of Sec. 2.

From (24) and (26) we have

$$\psi(\mathbf{r}) = [1 + (i/2\kappa)\beta\boldsymbol{\alpha}\cdot\nabla + (1/8\kappa^2)\Delta]\phi(\mathbf{r}). \quad (27)$$

The Hermitian conjugate of (27) is

$$\psi^*(\mathbf{r}) = \phi^*(\mathbf{r}) - (i/2\kappa)\nabla\phi^*(\mathbf{r})\cdot\boldsymbol{\alpha}\beta + (1/8\kappa^2)\Delta\phi^*(\mathbf{r}). \quad (28)$$

Putting (27) and (28) into (15) and neglecting the terms which are proportional to κ^{-3} and κ^{-4} we have

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) + \rho_2(\mathbf{r}), \quad (29)$$

$$\rho_0(\mathbf{r}) = -\frac{1}{2}e(1-C)\phi^*(\mathbf{r})\phi(\mathbf{r}), \quad (30a)$$

$$\rho_1(\mathbf{r}) = (ie/4\kappa)(1-C)\nabla\cdot[\phi^*(\mathbf{r})\boldsymbol{\alpha}\beta\phi(\mathbf{r})], \quad (30b)$$

$$\rho_2(\mathbf{r}) = -(e/16\kappa^2)(1-C)\{[\Delta\phi^*(\mathbf{r})]\phi(\mathbf{r}) + \phi^*(\mathbf{r})\Delta\phi(\mathbf{r}) + 2[\nabla\phi^*(\mathbf{r})]\cdot\boldsymbol{\alpha}\boldsymbol{\alpha}\cdot\nabla\phi(\mathbf{r})\}. \quad (30c)$$

The neglected terms are unimportant for our purpose. Similarly, we have

$$\mathbf{j}(\mathbf{r}) = \mathbf{j}_0(\mathbf{r}) + \mathbf{j}_1(\mathbf{r}), \quad (31)$$

$$\mathbf{j}_0(\mathbf{r}) = -\frac{1}{2}ec(1-C)\phi^*(\mathbf{r})\boldsymbol{\alpha}\phi(\mathbf{r}), \quad (32a)$$

$$\mathbf{j}_1(\mathbf{r}) = (iec/4\kappa)(1-C)\{\phi^*(\mathbf{r})\beta\boldsymbol{\alpha}\boldsymbol{\alpha}\cdot\nabla\phi(\mathbf{r}) - [\nabla\phi^*(\mathbf{r})]\cdot\boldsymbol{\alpha}\boldsymbol{\alpha}\beta\phi(\mathbf{r})\}. \quad (32b)$$

Here we have retained only the terms to the order of κ^{-1} .

If we put (23) into (30a-c) and (32a, b) and rearrange the order of the multiplication of the operators using the well-known commutation rules, we obtain the expressions in which the annihilation operators come to the right of the creation operators. In this manipulation the anticommutators such as $[\phi_a(\mathbf{r}s), \phi_a^*(\mathbf{r}s)]_+$ are treated as a constant $\delta(0)$ although $\delta(0)$ is not a well-defined quantity. Then these $\delta(0)$'s cancel each other and no trouble occurs. Final results are given below. In obtaining these equations the well-known relations

$$\alpha_x\alpha_y = i \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}, \quad \text{etc.} \quad (33)$$

were used.

$$\rho_0(\mathbf{r}) = -e[\phi_a^*(\mathbf{r})\phi_a(\mathbf{r}) - \phi_b^*(\mathbf{r})\phi_b(\mathbf{r})], \quad (34a)$$

$$\rho_1(\mathbf{r}) = -(e/2\kappa)\nabla\cdot[\phi_b^*(\mathbf{r})\delta\sigma_y\phi_a^{*T}(\mathbf{r}) + \phi_a^T(\mathbf{r})\sigma_y\delta\phi_b(\mathbf{r})], \quad (34b)$$

$$\rho_2(\mathbf{r}) = -(e/8\kappa^2)\{\Delta[\phi_a^*(\mathbf{r})\phi_a(\mathbf{r}) - \phi_b^*(\mathbf{r})\phi_b(\mathbf{r})] - 2i[\nabla\phi_a^*(\mathbf{r})]\cdot[\delta\times\nabla\phi_a(\mathbf{r})] + 2i[\nabla\phi_b^*(\mathbf{r})]\cdot[\delta\times\nabla\phi_b(\mathbf{r})]\}, \quad (34c)$$

$$\mathbf{j}_0(\mathbf{r}) =iec[\phi_b^*(\mathbf{r})\delta\sigma_y\phi_a^{*T}(\mathbf{r}) - \phi_a^T(\mathbf{r})\sigma_y\delta\phi_b(\mathbf{r})], \quad (35a)$$

$$\mathbf{j}_1(\mathbf{r}) = (iec/2\kappa)\{\phi_a^*(\mathbf{r})\nabla\phi_a(\mathbf{r}) - [\nabla\phi_a^*(\mathbf{r})]\phi_a(\mathbf{r}) - \phi_b^*(\mathbf{r})\nabla\phi_b(\mathbf{r}) + [\nabla\phi_b^*(\mathbf{r})]\phi_b(\mathbf{r}) + i\nabla\times[\phi_a^*(\mathbf{r})\delta\phi_a(\mathbf{r}) - \phi_b^*(\mathbf{r})\delta\phi_b(\mathbf{r})]\}. \quad (35b)$$

5. FIRST-ORDER ENERGY

Some parts of the Hamiltonian (12) are diagonal with respect to the numbers of electrons, positrons, and photons, while other parts are nondiagonal. We can assume that the effect of the latter parts is small compared with that of the former. This assumption will be valid, provided that the cutoff mentioned in Sec. 2 is adequately made. Thus, in the first approximation, we can omit the terms which are nondiagonal with respect to the numbers of electrons, positrons, and/or photons. The resulting Hamiltonian gives the first-order energies of the states with definite numbers of electrons, positrons, and photons. In this paper we are concerned only with those states involving a certain number of electrons but no positrons or photons. In order to compute the first-order energies of these states, we need only those terms which are effective (i.e., do not give a vanishing result) when operating on state vectors involving only electrons but no positrons or photons. This part of the Hamiltonian will be called the first-order energy of the system of electrons. This first-order energy is investigated in this section.

In the first place, from (25) and (20a-d) we have

$$H_M = \sum_s \int \hbar c \kappa \phi_a^*(\mathbf{r}s) \left(1 - \frac{\Delta}{2\kappa^2} - \frac{\Delta^2}{8\kappa^4}\right) \phi_a(\mathbf{r}s) d^3r \\ + \sum_s \int \hbar c \kappa \phi_b^*(\mathbf{r}s) \left(1 - \frac{\Delta}{2\kappa^2} - \frac{\Delta^2}{8\kappa^4}\right) \phi_b(\mathbf{r}s) d^3r. \quad (36)$$

The second term in (36) is ineffective when operating on state vectors involving only electrons, so that the first-order energy due to H_M is given by

$$H_M^{(1)} = \sum_s \int \hbar c \kappa \phi_a^*(\mathbf{r}s) \left(1 - \frac{\Delta}{2\kappa^2} - \frac{\Delta^2}{8\kappa^4}\right) \phi_a(\mathbf{r}s) d^3r. \quad (37)$$

The operator in the configuration space which corresponds to $H_M^{(1)}$ is obviously (1a) plus (1b) apart from an additive constant nmc^2 , n being the number of electrons. (Note $\kappa = mc/\hbar$.) The additive constant represents the rest energy of the electrons.

The first-order energy due to H_R is zero, because H_R is ineffective when operating on state vectors involving only electrons.

Next, we consider the contribution from H_C . From (13c) and (29) we can write

$$H_C = \frac{1}{2} \int [\rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) + \rho_2(\mathbf{r})] \\ \cdot [\rho_0(\mathbf{r}') + \rho_1(\mathbf{r}') + \rho_2(\mathbf{r}')] |\mathbf{r} - \mathbf{r}'|^{-1} d^3r d^3r'. \quad (38)$$

The integrand in the right-hand side of (38) consists of the terms of the form $\rho_\mu(\mathbf{r})\rho_\nu(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1}$. Those terms with $\mu + \nu > 2$ can be neglected as small terms. Those terms with $\mu + \nu = \text{odd}$ are nondiagonal with respect to the numbers of electrons and positrons, and so do not contribute to the first-order energy. Therefore, we

have to retain only the four terms

$$\rho_0(\mathbf{r})\rho_0(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1},$$

$$\rho_1(\mathbf{r})\rho_1(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1},$$

$$\rho_0(\mathbf{r})\rho_2(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1},$$

and

$$\rho_2(\mathbf{r})\rho_0(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1}.$$

Of these four terms, $\rho_1(\mathbf{r})\rho_1(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1}$ proves to contribute a type of self energy of the electrons, and so it will be omitted. The two terms $\rho_0(\mathbf{r})\rho_2(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1}$ and $\rho_2(\mathbf{r})\rho_0(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1}$ prove to contribute equally. Using (34a) and (34c) we can write the first-order energy due to H_C as

$$H_C^{(1)} = \frac{1}{2} e^2 \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) \phi_a^*(\mathbf{r}') \phi_a(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1} d^3r d^3r' \\ + \frac{1}{8} (e/\kappa)^2 \int \{ \Delta [\phi_a^*(\mathbf{r}) \phi_a(\mathbf{r})] \} \\ \times \phi_a^*(\mathbf{r}') \phi_a(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1} d^3r d^3r' \\ - \frac{1}{4} i (e/\kappa)^2 \int [\nabla \phi_a^*(\mathbf{r})] \cdot [\delta \times \nabla \phi_a(\mathbf{r})] \\ \times \phi_a^*(\mathbf{r}') \phi_a(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1} d^3r d^3r'. \quad (39)$$

Integrating by parts and using the formula

$$\Delta |\mathbf{r} - \mathbf{r}'|^{-1} = -4\pi \delta(\mathbf{r} - \mathbf{r}'), \quad (40)$$

we obtain

$$H_C^{(1)} = \frac{1}{2} e^2 \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) \phi_a^*(\mathbf{r}') \phi_a(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1} d^3r d^3r' \\ (41a)$$

$$- \frac{1}{2} \pi (e/\kappa)^2 \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) \phi_a^*(\mathbf{r}') \phi_a(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') d^3r d^3r' \\ (41b)$$

$$+ \frac{1}{4} i (e/\kappa)^2 \int \phi_a^*(\mathbf{r}) [\nabla |\mathbf{r} - \mathbf{r}'|^{-1}] \cdot [\delta \times \nabla \phi_a(\mathbf{r})] \\ \times \phi_a^*(\mathbf{r}') \phi_a(\mathbf{r}') d^3r d^3r'. \quad (41c)$$

The operators in the configuration space corresponding to (41a), (41b), and (41c) are (2a), (2g), and (2d), respectively, apart from an additive constant of a type of self-energy.

The first-order energy due to H_I is zero, because H_I is nondiagonal with respect to the numbers of particles.

Proceeding to H_E , we can write from (13e), (29), and (31)

$$H_E = \int [\rho_0(\mathbf{r}) + \rho_1(\mathbf{r}) + \rho_2(\mathbf{r})] \phi_{\text{ex}}(\mathbf{r}) d^3r \\ - (1/c) \int [\mathbf{j}_0(\mathbf{r}) + \mathbf{j}_1(\mathbf{r})] \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}) d^3r. \quad (42)$$

The second term in the first integral and the first term in the second integral are nondiagonal with respect to the numbers of electrons and positrons, so they do not contribute to the first-order energy. Using (34a), (34c), and (35b), we can write the first-order energy due to H_E as

$$\begin{aligned} H_E^{(1)} = & -e \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) \phi_{\text{ex}}(\mathbf{r}) d^3r \\ & - (e/8\kappa^2) \int \{ \Delta[\phi_a^*(\mathbf{r}) \phi_a(\mathbf{r})] \\ & - 2i[\nabla \phi_a^*(\mathbf{r})] \cdot [\delta \times \nabla \phi_a(\mathbf{r})] \} \phi_{\text{ex}}(\mathbf{r}) d^3r \\ & - i(e/2\kappa) \int \{ \phi_a^*(\mathbf{r}) \nabla \phi_a(\mathbf{r}) - [\nabla \phi_a^*(\mathbf{r})] \phi_a(\mathbf{r}) \\ & + i \nabla \times [\phi_a^*(\mathbf{r}) \delta \phi_a(\mathbf{r})] \} \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}) d^3r. \end{aligned} \quad (43)$$

Integrating by parts and using (3a), (3b), (4), and (5) we obtain

$$H_E^{(1)} = -e \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) \phi_{\text{ex}}(\mathbf{r}) d^3r \quad (44a)$$

$$+ (\pi e/2\kappa^2) \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) \rho_{\text{ex}}(\mathbf{r}) d^3r \quad (44b)$$

$$+ (ie/4\kappa^2) \int \phi_a^*(\mathbf{r}) \mathbf{E}_{\text{ex}}(\mathbf{r}) \cdot [\delta \times \nabla \phi_a(\mathbf{r})] d^3r \quad (44c)$$

$$- i(e/\kappa) \int \phi_a^*(\mathbf{r}) [\nabla \phi_a(\mathbf{r})] \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}) d^3r \quad (44d)$$

$$+ (e/2\kappa) \int \phi_a^*(\mathbf{r}) \delta \phi_a(\mathbf{r}) \cdot \mathbf{H}_{\text{ex}}(\mathbf{r}) d^3r. \quad (44e)$$

The operators in the configuration space which correspond to (44a–e) are (1e), (1h), (1g), (1c), and (1f), respectively.

6. SECOND-ORDER EFFECT. I. VIRTUAL ELECTRON-POSITRON PAIR

Consider the first term of the second integral in (42)

$$H_E' = - (1/c) \int \mathbf{j}_0(\mathbf{r}) \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}) d^3r. \quad (45)$$

According to (35a), H_E' consists of two terms, one of which creates while the other annihilates, an electron-positron pair. Therefore, H_E' gives rise to a second-order energy. This second-order energy is investigated in this section. Since we are interested in the second-order effect on the states involving only electrons, the virtual intermediate states giving rise to the second-order effect are those states which are derived from the initial state through creation of an electron-positron pair, but not through annihilation of a pair. In the

following treatment, the virtual excitation energy for the creation of an electron-positron pair will be put equal to $2mc^2$, neglecting the kinetic energies. Justification of this neglect of the kinetic energy is given at the end of this section.

The second-order energy due to H_E' is written as

$$H_E'^{(2)} = - [H_E' H_E']^{(1)} / 2mc^2, \quad (46)$$

where the superscript (1) means that only those terms should be retained, which are diagonal with respect to the numbers of electrons and positrons, and are actually effective when operating on state vectors involving only electrons. From (46), (45), and (35a) we have

$$\begin{aligned} H_E'^{(2)} = & - (e^2/2mc^2) \int \mathbf{A}_{\text{ex}}(\mathbf{r}) \cdot \phi_a^T(\mathbf{r}) \sigma_y \delta \phi_b(\mathbf{r}) \\ & \times \phi_b^*(\mathbf{r}') \delta \sigma_y \phi_a^{*T}(\mathbf{r}') \cdot \mathbf{A}_{\text{ex}}(\mathbf{r}') d^3r d^3r'. \end{aligned} \quad (47)$$

When operating on state vectors involving only electrons, $\phi_b(\mathbf{r}s) \phi_b^*(\mathbf{r}'s')$ can be put equal to $\delta_{ss'} \delta(\mathbf{r}-\mathbf{r}')$, so that (47) becomes

$$H_E'^{(2)} = - (e^2/2mc^2) \int \phi_a^T(\mathbf{r}) \phi_a^{*T}(\mathbf{r}) [\mathbf{A}_{\text{ex}}(\mathbf{r})]^2 d^3r. \quad (48)$$

Using the commutation relation we can write (48) as

$$H_E'^{(2)} = (e^2/2mc^2) \int \phi_a^*(\mathbf{r}) \phi_a(\mathbf{r}) [\mathbf{A}_{\text{ex}}(\mathbf{r})]^2 d^3r, \quad (49)$$

apart from an additive constant. The operator in the configuration space which corresponds to (49) is obviously (1d).

We have made the assumption that the virtual excitation energy of an electron-positron pair can be put equal to $2mc^2$. This assumption is justified as follows. Consider the vector potential $\mathbf{A}_{\text{ex}}(\mathbf{r})$ in (45) decomposed to its Fourier components, and consider the creation of an electron-positron pair induced by the Fourier component of $\mathbf{A}_{\text{ex}}(\mathbf{r})$ for wave number \mathbf{k} . As mentioned in the introduction, the Fourier component of $\mathbf{A}_{\text{ex}}(\mathbf{r})$ is assumed to have an appreciable value only for those wavelengths which are sufficiently large compared with the Compton wavelength of the electron. Therefore, we can assume that $|\mathbf{k}| \ll \kappa$. If the wave numbers of the electron and the positron of the virtual pair mentioned above are \mathbf{k}' and \mathbf{k}'' , respectively, there must be a relation $\mathbf{k}' + \mathbf{k}'' = \mathbf{k}$, which means the conservation of momentum. Then, if $|\mathbf{k}'| \ll \kappa$, we can say that $|\mathbf{k}''| \ll \kappa$. In this case, the virtual excitation energy can be approximated by $2mc^2$. On the other hand, if $|\mathbf{k}'|$ is not very small compared with κ , we conclude that $|\mathbf{k}''|$ is also not very small compared with κ . In this case, the virtual excitation energy is not approximated by $2mc^2$. This latter kind of virtual excitation is never prohibited by the exclusion principle, because the wave numbers of the electrons which are present in the initial state are assumed to be very small compared with κ . Therefore, this virtual excitation

occurs irrespective of the initial state, and one can show that the contribution of this kind of virtual excitation to the second-order energy is merely an additive constant. On account of this situation we do not need to use the exact virtual excitation energy for this case, and we can put it equal to $2mc^2$ for all cases.

7. SECOND-ORDER EFFECT. II. VIRTUAL PHOTON

From (13d) and (31) we have

$$H_I = -(1/c) \int [\mathbf{j}_0(\mathbf{r}) + \mathbf{j}_1(\mathbf{r})] \cdot \mathbf{A}(\mathbf{r}) d^3r. \quad (50)$$

The first term on the right-hand side is nondiagonal with respect to each of the numbers of electrons, positrons, and photons. It gives rise to a second-order energy which is merely an additive constant. Therefore, we consider the second-order effect due to

$$H_I' = -(1/c) \int \mathbf{j}_1(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d^3r. \quad (51)$$

This operator is nondiagonal with respect to the number of photons, but it is diagonal with respect to the numbers of electrons and positrons. As can be seen from (14), the operator $\mathbf{A}(\mathbf{r})$ creates and annihilates a photon. Since the energy of the photon with wave number \mathbf{k} is $\hbar ck$, the second-order energy due to H_I' is

$$H_I'^{(2)} = -\frac{1}{4\pi^2 c^2} \sum_{\lambda} \int [\mathbf{j}_1(\mathbf{r}) \cdot \mathbf{e}(\mathbf{k}\lambda) \mathbf{e}(\mathbf{k}\lambda) \cdot \mathbf{j}_1(\mathbf{r}')]^{(1)} \times \exp[i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')] k^{-2} d^3r d^3r' d^3k, \quad (52)$$

where the meaning of the superscript (1) is the same as in the lines following (46).

We introduce the formula

$$\sum_{\lambda} \mathbf{e}(\mathbf{k}\lambda) \mathbf{e}(\mathbf{k}\lambda) = \mathbf{1} - (\mathbf{k}\mathbf{k}/k^2). \quad (53)$$

Furthermore, we use

$$\int [\mathbf{1} - (\mathbf{k}\mathbf{k}/k^2)] k^{-2} \exp(i\mathbf{k} \cdot \mathbf{r}) d^3k = \pi^2 [\mathbf{1} + (\mathbf{r}\mathbf{r}/r^2)]/r. \quad (54)$$

Then, (52) becomes

$$H_I'^{(2)} = -\frac{1}{4c^2} \int \{ \mathbf{j}_1(\mathbf{r}) \cdot [\mathbf{1} |\mathbf{r} - \mathbf{r}'|^{-1} + (\mathbf{r} - \mathbf{r}') (\mathbf{r} - \mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-3}] \cdot \mathbf{j}_1(\mathbf{r}') \}^{(1)} d^3r d^3r'. \quad (55)$$

Using (35b) we have

$$H_I'^{(2)} = -\frac{e^2}{16\kappa^2} \int \{ i\phi_a^*(\mathbf{r}) \nabla \phi_a(\mathbf{r}) - i[\nabla \phi_a^*(\mathbf{r})] \phi_a(\mathbf{r}) - \nabla \times [\phi_a^*(\mathbf{r}) \delta \phi_a(\mathbf{r})] \} \cdot [\mathbf{1} |\mathbf{r} - \mathbf{r}'|^{-1} + (\mathbf{r} - \mathbf{r}') (\mathbf{r} - \mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-3}] \cdot \{ i\phi_a^*(\mathbf{r}') \nabla' \phi_a(\mathbf{r}') - i[\nabla' \phi_a^*(\mathbf{r}')] \phi_a(\mathbf{r}') - \nabla' \times [\phi_a^*(\mathbf{r}') \delta \phi_a(\mathbf{r}')] \} d^3r d^3r'. \quad (56)$$

Integrating by parts we obtain

$$H_I'^{(2)} = \frac{e^2}{4\kappa^2} \int \phi_a^*(\mathbf{r}) [\nabla \phi_a(\mathbf{r})] \cdot \left[\frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}'|} + \frac{(\mathbf{r} - \mathbf{r}') (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \right] \cdot \phi_a^*(\mathbf{r}') \nabla' \phi_a(\mathbf{r}') d^3r d^3r' \quad (57a)$$

$$+ \frac{ie^2}{2\kappa^2} \int \left[\frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \times \phi_a^*(\mathbf{r}) \nabla \phi_a(\mathbf{r}) \right] \cdot \phi_a^*(\mathbf{r}') \delta \phi_a(\mathbf{r}') d^3r d^3r' \quad (57b)$$

$$+ \frac{e^2}{8\kappa^2} \int \phi_a^*(\mathbf{r}) \delta \phi_a(\mathbf{r}) \cdot \left[\frac{\mathbf{1}}{|\mathbf{r} - \mathbf{r}'|^3} - \frac{3(\mathbf{r} - \mathbf{r}') (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^5} \right] \cdot \phi_a^*(\mathbf{r}') \delta \phi_a(\mathbf{r}') d^3r d^3r' \quad (57c)$$

$$- \frac{\pi e^2}{3\kappa^2} \int \phi_a^*(\mathbf{r}) \delta \phi_a(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \cdot \phi_a^*(\mathbf{r}') \delta \phi_a(\mathbf{r}') d^3r d^3r'. \quad (57d)$$

The integral in (57c) is to be carried out excepting the region of $|\mathbf{r} - \mathbf{r}'| < \epsilon$, where ϵ is a small radius.

The operators in the configuration space which correspond to (57a-d) are (2b), (2c), (2e), and (2f), respectively, and thus we have derived all the terms of the Hamiltonian (1a)-(2g).