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Covariant photon interaction in atomic physics

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The covariant photon interaction between electrons is reviewed briefly. Its potential function in configuration space is obtained unambiguously in a covariant perturbation calculation. Several different forms are presented, and their applications in atomic physics are discussed. In addition, the general matrix elements of various potential functions are given in terms of radial integrals, suitable for numerical computations.

I. INTRODUCTION

The lowest-order interaction between electrons in a covariant perturbation calculation in quantum field theory is due to the exchange of four types of photons, namely, two transverse photons, one longitudinal photon, and one timelike photon. The exchange of transverse photons gives rise to the transverse interaction, which is better known in its Breit approximation form, the Breit interaction.[1] The exchange of a longitudinal photon and a timelike photon together leads to the instantaneous Coulomb interaction between charges.

In atomic physics, interaction between electrons is often described by a potential which is a function of the interelectron distance. In quantum field theory, however, there exists no potential function which depends on the coordinates of the interacting electrons taken at some instant of time, since the electrons interact not directly but via quantized electromagnetic field. Nevertheless in a covariant perturbation calculation, e.g., S-matrix expansion, it is possible to obtain a state-dependent potential function to a certain order of the expansion constant.

In this work we shall review various forms[2-5] of the lowest-order electron-electron interaction and present their potential functions in an unambiguous manner. The forms appropriate for the Dirac-Fock-Slater[6] and Dirac-Fock[7,8] formulisms are given in Secs. II and III, respectively. A brief discussion of the application is contained in Sec. IV. In the Appendix, we present the general matrix elements of various potential functions in terms of radial integrals, suitable for numerical computations.

II. COVARIANT PHOTON INTERACTION

In a formulism where the *entire* interaction between electrons is treated as a perturbation, or where the complete orthonormal set of electron states (for both the initial and final states) is generated from a *single* equation, the lowest-order interaction between electrons has a simple form. In this case, we can take all four components of the electromagnetic field potential A_μ to be four independent Hermitian Klein-Gordon fields of zero mass, subject to the usual rules of field quantization. A direct result of this treatment is the exchange of covariant photons between electrons, represented by the covariant photon propagator[9-11]

$$\langle 0\,|\,T[A_\mu(x_1)A_\nu(x_2)]\,|\,0\rangle = -\frac{i\delta_{\mu\nu}}{(2\pi)^4}\int d^4k\,\frac{e^{ik\cdot(x_1-x_2)}}{k^2-i\epsilon}\,, \tag{1}$$

where $T[\;]$ denotes the Wick time-ordered product, $|0\rangle$ stands for the vacuum state of the quantized photon field, and ϵ is a positive infinitesimal which specified unambiguously in what manner we go around the singularities. Here (1) is presented in relativistic units, or natural units. The integration of the timelike component of k in (1) will yield the energy conservation factor, and a straightforward integration of the spacelike components, $\int d^3k$, leads to a potential function when (1) is taken between the initial and final electron states. For easier use in atomic physics we present the potential function in atomic units:

$$V_{\mathrm{cov}}(r_{12}) = (1-\vec{\alpha}_1\cdot\vec{\alpha}_2)e^{i\omega r_{12}}/r_{12}\,, \tag{2}$$

where $\vec{\alpha}$ is the Dirac matrix, r_{12} the interelectron distance, and ω the exchange photon energy divided by c. This form has been used extensively in the past and may be obtained[2] from the semiclassical argument that the presence of electron 1 induces a classical four-vector potential which interacts with electron 2. This semiclassical treatment, however, has an ambiguity in choosing an appropriate boundary condition for (1), that leads to the potential function (2).

By retaining terms of order $(v/c)^2$, where v is the velocity of the electron, in (2) we obtain a state-independent potential function

$$V_B(r_{12}) = \frac{1}{r_{12}} - \frac{1}{2r_{12}}\left((\vec{\alpha}_1\cdot\vec{\alpha}_2) + \frac{(\vec{\alpha}_1\cdot\vec{r}_{12})(\vec{\alpha}_2\cdot\vec{r}_{12})}{r_{12}^2}\right), \tag{3}$$

where the first term is the Coulomb potential, and the second term the well-known Breit interaction.[1]

III. TRANSVERSE INTERACTION

In atomic physics, one often includes as large a part of the electron-electron interaction as possible to define the unperturbed electron states. This can be done, e.g., in the Dirac-Fock formulism,[7,8] at the expense of introducing a more complicated potential function than (2). Usually, the instantaneous Coulomb interaction between charges is considered in the unperturbed Hamiltonian, and therefore only the transverse part $A_i^{(t)}$ of the four-potential A_μ is treated dynamically as a perturbation. Note that although the single-electron states in a Dirac-Fock calculation are generally obtained from different differential equations, they can be made, at least in principle, orthogonal to each other by including nondiagonal Lagrangian multipliers. The rest of the complete orthonormal set of single-electron states may be obtained from a frozen-core Dirac-Fock calculation. The negative energy states may also be obtained; however, we do not need their explicit forms. With the complete orthonormal set of single-electron states, we can quantize the Dirac field in complete analogy with the quantization of the field-free Dirac field treated in many standard text books.[9-11] In a similar manner we get the transverse photon propagator, in relativistic units,

$$\langle 0|\,T[A_i^{(t)}(x_1)A_j^{(t)}(x_2)]\,|0\rangle = -\frac{i}{(2\pi)^4}\int d^4k\left(\delta_{ij} - \frac{k_i k_j}{\vec{k}^2}\right)\frac{i}{k^2 - i\epsilon}\, e^{ik\cdot(x_1-x_2)}, \tag{4}$$

where the subscripts i and j denote the spacelike components of a four-vector. Here again the integration of the timelike component of k concerns the energy conservation, and the integration of the spacelike components gives rise to a potential function which has the form, in atomic units,

$$V_{\mathrm{tr}}(r_{12}) = -\alpha_1\cdot\alpha_2\,\frac{e^{i\omega r_{12}}}{r_{12}} + \vec{\alpha}_1\cdot\vec{\nabla}_1\;\vec{\alpha}_2\cdot\vec{\nabla}_2\,\frac{e^{i\omega r_{12}}-1}{\omega^2 r_{12}}, \tag{5}$$

with $\omega \geqslant 0$. This is the so-called transverse interaction and reduces to the Breit interaction[1] in the lowest order.

Note that in (4) the positive infinitesimal ϵ comes naturally due to the properties of the Wick time-ordered product $T[\;]$, and this unambiguously specifies the treatment of the singularities encountered in the integration of the spacelike components. To demonstrate that an ambiguity in choosing the appropriate boundary condition may otherwise arise, we shall derive the transverse interaction by the noncovariant second-order perturbation theory[3] based on energy denominator, rather than on relativistically invariant denominator which treates the energy and momentum on the same footing as in the covariant perturbation theory.

In the semiclassical treatment, the emission or absorption of a photon by an electron may be considered as an interaction of the electron with an equivalent unquantized vector potential. Regarding this vector potential as a perturbation, we can easily write down the second-order transition matrix element,[3] in atomic units,

$$\langle f|V_{\mathrm{tr}}(r_{12})|i\rangle = -\frac{c}{4\pi^2}\sum_{\vec{\epsilon}}\sum_n\int\frac{d^3k}{|\vec{k}|}\left(\frac{\langle f|\vec{\alpha}_1\cdot\vec{\epsilon}\,e^{i\vec{k}\cdot\vec{r}_1}|n\rangle\langle n|\vec{\alpha}_2\cdot\vec{\epsilon}\,e^{-i\vec{k}\cdot\vec{r}_2}|i\rangle}{|\vec{k}|c + E_n - E_i} + \frac{\langle f|\vec{\alpha}_2\cdot\vec{\epsilon}\,e^{i\vec{k}\cdot\vec{r}_2}|n\rangle\langle n|\vec{\alpha}_1\cdot\vec{\epsilon}\,e^{-i\vec{k}\cdot\vec{r}_1}|i\rangle}{|\vec{k}|c + E_n - E_i}\right). \tag{6}$$

Here $|i\rangle$ and $\langle f|$ denote the two-electron initial and final states, respectively, the first summation is over the two polarization states perpendicular to the momentum vector $\vec{k}$, E_i is the total energy of the two-electron initial state and E_n that of the intermediate state $|n\rangle$, and the n summation is over all possible eigenstates of the two-electron system, including energy-conserving and energy-nonconserving intermediate states. Physically, the first term of (6) corresponds to the process in which a virtual photon is emitted by electron 2 and subsequently absorbed by electron 1, and the second term corresponds to the reverse process. A straightforward calculation of (6) yields the potential function $V_{\mathrm{tr}}(r_{12})$ in an integral form,[3]

$$V_{\mathrm{tr}}(r_{12}) = \frac{1}{2\pi^2}\int d^3k\left(\vec{\alpha}_1\cdot\vec{\alpha}_2 - \frac{\vec{\alpha}_1\cdot\vec{k}\,\vec{\alpha}_2\cdot\vec{k}}{\vec{k}^2}\right)\frac{e^{i\vec{k}\cdot\vec{r}_{12}}}{\vec{k}^2-\omega^2}. \tag{7}$$

To obtain the appropriate potential function in configuration space, we must determine the integration contour in the complex k plane with respect to the poles at $\pm\omega$. We find, however, that a sensible choice of the contour may not generally be obtained in this ansatz. Note that the replacement $\omega \rightarrow \omega - i\epsilon$ $(\omega > 0,\ \epsilon > 0)$, suggested[3] by the physical model of decaying states with finite level width, gives rise to an effective potential which differs from (5) in that ω is replaced by $-\omega$.

IV. DISCUSSION

The covariant photon interaction presented in (2) can be used in the Dirac-Fock-Slater[6] formulism or in cases where the unperturbed electron states are free-electron states or are obtained in a single effective potential. The transverse interaction in (5) should be used in the Dirac-Fock formulism or in cases where the unperturbed electron states are obtained from different differential equations. The general matrix elements of these interactions are presented in the Appendix.

It is worth noting that both potentials (2) and (5) are not Hermitian. Because they are obtained from the S-matrix expansion defined in terms of the time-evolution operator, the matrix elements of (2) and (5) are to be considered as transition amplitudes. The appropriate physical meaning of the diagonal S-matrix element, when evaluated to all orders, is the probability amplitude that the system under consideration remains unchanged. Therefore, the nonunity of (or the nonvanishing of the imaginary part of) the diagonal S-matrix element of the zero-order ground state indicates simply that it is not the true ground state. Since the amplitude is not physically measureable, the imaginary part needs no further interpretation.

On the other hand, in the usual first-order pertrubation theory the diagonal matrix element of the interaction Hamiltonian *in configuration space* is always real and corresponds physically to the energy shift. This may seem disturbing. We note, however, that in quantum field theory although the interaction Hamiltonian *in terms of field operators* is itself Hermitian, the S matrix derived from it is unitary. In fact, it is the Hermiticity of the interaction Hamiltonian which proves the unitarity of the S matrix. Nevertheless, the interaction Hamiltonian in configuration space is certainly required to be Hermitian in order to satisfy the probability conservation in the quantum theory. Therefore, the potential forms (2) and (5) are not to be considered as the interaction Hamiltonian in configuration space in the usual sense. Although it should be possible to extract unambiguously a configuration-space Hamiltonian from the S-matrix expansion via a Rayleigh-Ritz variatonal procedure, it requires further investigation. Alternatively, a configuration-space Hamiltonian can be obtained[12] by defining a Fock-space wave function which contains only a single (no electron-positron pair) amplitude function and by successive contact transformations to decouple the radiation and matter fields to some order in α.

In bound-state energy calculations, the real part of the matrix element represents the energy shift of the atomic level while the imaginary part concerns the level width. Using Dirac-Fock wave functions, Mann and Johnson[5] have taken the real part of (5) to calculate binding energies of inner-shell electrons in heavy atoms with good agreement with the experimental results. We have used both form (2) (Ref. 13) and form (3) (Ref. 14) to perform the binding-energy calculation in the Dirac-Fock-Slater formulism. The difference between energy shifts obtained from the Dirac-Fock and Dirac-Fock-Slater calculations is insignificant when state-dependent forms are used in both cases.

A few Auger transition calculations have been carried out by using form (2);[15] however, we expect that a Dirac-Fock calculation using form (5) would give significantly different results because Auger transitions are more sensitive to the electron correlation.[16] Also we expect form (5) of the transverse interaction could play an important role in atomic collision processes for the same reason. In configuration interaction or multiconfiguration calculations, only the real part of the covariant photon interaction has been treated.[17,18] Although in principle the imaginary part could contribute, it is of no interest at the present stage of the multiconfiguration formulation. In addition, we note that the present forms (2) and (5) are strictly applicable only to cases where the total energy is conserved. Mittleman[12] however has obtained a form of electron-electron interaction valid when the total energies of the initial and final states are not the same.

APPENDIX: GENERAL MATRIX ELEMENTS

A more complete relativistic formulation is necessary in the calculations of atomic collisions, transitions, correlations, binding energies, level widths, and others. In most cases, matrix elements of the electron-electron interaction between many-electron configurations are needed. Because these matrix elements can always be expressed as linear combinations of matrix elements in corresponding two-electron configurations,[19,20] we shall deal only with the general matrix of the electron-electron interaction between two-electron configurations in the jm scheme, i.e.,

$$\langle ab\,|\,V(r_{12})\,|\,cd\rangle = \int d^3r_1 \int d^3r_2\, U_a^\dagger(1) U_b^\dagger(2) \times V(r_{12}) U_c(1) U_d(2)\,, \quad \text{(A1)}$$

where a, b, c, and d denote generally different Dirac orbitals. These orbitals are assumed to have the form[7]

$$U_{n\kappa m}(\vec{r}) = \frac{1}{r}\begin{pmatrix} iG_{n\kappa}(r)\Omega_{\kappa m} \\ F_{n\kappa}(r)\Omega_{-\kappa m}\end{pmatrix}, \quad \text{(A2)}$$

where the radial functions $G_{n\kappa}$ and $F_{n\kappa}$ are the large and small components, respectively; the $\Omega_{\kappa m}$ are normalized two-component Dirac spinors. Here the orbitals are completely specified by the quantum numbers n, κ, and m, which have their usual meanings. By using the techniques of the vector-spherical-harmonics expansion,[21,22] first employed by Mann and Johnson[5] in this connection, we have obtained the general matrix elements as linear combinations of radial integrals, suitable for numerical computations.

The general matrix elements (A1) can be calculated with the result

$$\langle ab\,|\,V(r_{12})\,|\,cd\rangle = \sum_j G_j(ab;cd) X_j(ab;cd)\,, \quad \text{(A3)}$$

where the coefficient $G_j(ab;cd)$ concerns the angular-momentum recoupling and is defined in terms of Wigner's $3j$ symbols[21] as

$$G_j(ab;cd) = (-)^{j_b - m_b + j_c + m_c}\begin{pmatrix} j_a & j & j_c \\ m_a & -m_a+m_c & -m_c\end{pmatrix} \times \begin{pmatrix} j_b & j & j_d \\ m_b & m_a - m_c & -m_d\end{pmatrix}. \quad \text{(A4)}$$

The expression $X_j(ab;cd)$ in (A3) is called *the interaction strength*, having the form

$$X_j(ab;cd) = (-)^{j_b+j_c} \times [(2j_a+1)(2j_b+1)(2j_c+1)(2j_d+1)]^{1/2} \times \begin{pmatrix} j_a & j_c & j \\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix}\begin{pmatrix} j_b & j_d & j \\ \frac{1}{2} & -\frac{1}{2} & 0\end{pmatrix} I_j(ab;cd)\,, \quad \text{(A5)}$$

where $I_j(ab;cd)$ is defined in terms of radial integrals, depending on the specific form of $V(r_{12})$.

We summarize the results[16,18,23] for various commonly used potential functions as follows.

(*i*) *Coulomb potential.*

$$I_j(ab;cd) = \langle W_{ac} R_j W_{bd}\rangle^{\text{even}}\,, \quad \text{(A6)}$$

which has the explicit form

$$\langle W_{ac} R_j W_{bd}\rangle^{\text{even}} = \int_0^\infty dr_1 \int_0^\infty dr_2\, W_{ac}(r_1) \times R_j(r_1 r_2) W_{bd}(r_2) \quad \text{(A7)}$$

with

$$W_{ac}(r) = G_a(r)G_c(r) + F_a(r)F_c(r)\,,$$

$$R_j(r_1 r_2) = r_<^j / r_>^{j+1}\,.$$

Here the notation $\langle\,\rangle^{\text{even (odd)}}$ denotes that the integral is to be replaced by zero unless both (l_a+j+l_c) and (l_b+j+l_d) are even (odd).

(*ii*) *Covariant photon interaction as defined by (2).*

$$\begin{aligned} I_j(ab;cd) = {} & (2j+1)\langle W_{ac} g_j W_{bd}\rangle^{\text{even}} \\ & -(1-\delta_{j0})(\kappa_a+\kappa_c)(\kappa_b+\kappa_d)\,\frac{2j+1}{j(j+1)} \\ & \times \langle V_{ac} g_j V_{bd}\rangle^{\text{odd}} + j\langle P_{ac} g_{j-1} P_{bd}\rangle^{\text{even}} \\ & + (j+1)\langle Q_{ac} g_{j+1} Q_{bd}\rangle^{\text{even}}\,, \end{aligned} \quad \text{(A8)}$$

where

$$g_j(r_1 r_2) = i\omega\, j_j(\omega r_<) h_j(\omega r_>) \quad \text{(A9)}$$

with j_j and h_j being the spherical Bessel and Hankel functions, respectively. In (A8) the different combinations of radial functions are defined as

$$\begin{aligned} V_{ac}(r) &= G_a(r)F_c(r) + F_a(r)G_c(r)\,, \\ P_{ac}(r) &= G_a(r)F_c(r) - F_a(r)G_c(r) + V_{ac}(r)(\kappa_c-\kappa_a)/j\,, \\ Q_{ac}(r) &= -G_a(r)F_c(r) + F_a(r)G_c(r) \\ &\quad + V_{ac}(r)(\kappa_c-\kappa_a)/(j+1)\,. \end{aligned} \quad \text{(A10)}$$

(*iii*) *Transverse photon interaction as defined by (5).*

$$\begin{aligned} I_j(ab;cd) = {} & -(1-\delta_{j0})(\kappa_a+\kappa_c)(\kappa_b+\kappa_d) \\ & \times [(2j+1)/j(j+1)]\langle V_{ac} g_j V_{bd}\rangle^{\text{odd}} \\ & + (\kappa_c-\kappa_a)[\langle V_{ac} g_{j-1} P_{bd}\rangle^{\text{even}} + \langle V_{ac} g_{j+1} Q_{bd}\rangle^{\text{even}}] \\ & + j(j+1)[\langle P_{ac} s_j Q_{bd}\rangle^{\text{even}} + \langle Q_{ac} t_j P_{bd}\rangle^{\text{even}}]\,, \end{aligned}$$

where

$$s_j = \begin{cases} -(i/r_1) j_{j+1}(\omega r_2) h_j(\omega r_1)\,, & r_1 > r_2 \\ r_1^{j-1}/\omega^2 r_2^{j+2} - (i/r_1) j_j(\omega r_1) h_{j+1}(\omega r_2)\,, & r_1 < r_2\,, \end{cases}$$

$$t_j = \begin{cases} r_2^{j-1}/\omega^2 r_1^{j+2} - (i/r_1) j_{j-1}(\omega r_2) h_j(\omega r_1)\,, & r_1 > r_2 \\ -(i/r_1) j_j(\omega r_1) h_{j-1}(\omega r_2)\,, & r_1 < r_2\,. \end{cases} \quad \text{(A12)}$$

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