Natural spectral-line broadening in multiply-charged ions and the problem of surface divergences

R. Kh. Gaĭnutdinov

Kazan State University, 420008 Kazan, Russia
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The difficulties, associated with surface divergences, of a consistent QED theory in describing the natural broadening of spectral line profiles of atoms are studied. In the case of heavy multiply-charged ions, when levels with the same values of the total angular momentum J, its projection J_z, and parity may overlap, these difficulties are shown to manifest themselves in QED calculations of the respective spectral line profiles even in the lowest approximation. The possibility is discussed of using the equation for the relativistic T matrix to cope with these difficulties. Finally, it is shown that the boundary condition for this equation can be chosen in such a way that no difficulties involving surface divergences arise in the description of the temporal evolution of QED systems, with the solution of this equation by perturbation techniques leading to the ordinary renormalized expression for the S matrix. © *1995 American Institute of Physics.*

1. INTRODUCTION

It is well known that in quantum electrodynamics (QED) the ultraviolet divergences can be removed from the S matrix and in the Green's functions, but cannot be removed from quantities characterizing the temporal evolution of the processes, since regularization of the scattering matrix leads to a situation in which divergent terms automatically appear in the Schrödinger equation and the Tomonaga–Schwinger equation.[1] For this reason these equations are of only formal importance to quantum field theory.

Thus, the description of temporal evolution of QED systems, which determines the energy and other characteristics of bound states, encounters unregularizable surface ultraviolet divergences. This leads, in particular, to difficulties in finding a consistent QED description of natural broadening of spectral line profiles in atomic systems. This problem, however, has only minor importance for most applications. The reasons are twofold. First, in most problems related to the description of atomic spectra the QED effects contribute little in comparison to other factors determining the broadening of spectral lines. Second, most excited states of atomic systems satisfy the condition of quasistationarity, so that the decay law is close to an exponential one. Here the spectral line is Lorentzian and is characterized by the energy and width of the corresponding energy levels, which can be calculated by standard QED methods.

Recent progress in heavy-ion beam techniques, however, has made it possible to begin experimental studies of multiply-charged heavy ions, whose interaction with their own radiation field can no longer be considered a small perturbation and, accordingly, the radiative broadening of spectral lines may be much greater than other types of broadening. In the case of multiply-charged heavy ions there may, for example, be an overlap of energy levels with the same total angular momentum J, its projection J_z, and parity. The decay law for such states may differ dramatically from the exponential one and, accordingly, the natural broadening of spectral lines differs from that of a Lorentzian line. The problems associated with describing such states are described in Refs. 2–10. The difficulties that a researcher encounters in describing the radiative broadening of spectral lines and that are associated with surface divergences were discussed in Ref. 3. These difficulties arise in describing the natural broadening of spectral line profiles. In Ref. 3 it was noted, however, that at least in calculating with an accuracy of α^2 these difficulties do not arise.

In this paper we will see that when energy levels with the same J, J_z, and parity overlap, the situation with surface divergences is much more complicated than it was assumed to be. Already in calculating the corresponding line profiles in the lowest approximation such divergences come into play. This fact, on the one hand, stimulates the development of quantum electrodynamics to resolve the situation with surface divergences and, on the other, shows that the line profiles of multiply-charged heavy ions can supply new information about the fundamental laws governing the QED interaction. We will examine the possibility of using the equation for the relativistic T matrix (see Refs. 5 and 11–14) to solve this problem. We will also show that the boundary condition for this equation can be formulated in such a way that no difficulties associated with surface divergences arise. Finally, we will show that the S matrix built via this equation coincides with the ordinary renormalized S matrix.

2. THE METHOD OF THE RELATIVISTIC *T*-MATRIX

A method for building a scattering matrix was developed in Refs. 5 and 11–14. Its main idea is to use the Feynman superposition principle[15,16] in conjunction with the most general principles of axiomatic quantum field theory.[17] As is known, two postulates lie at the base of the Feynman approach to building quantum field theory. The first is the superposition principle applied to the probability amplitudes, according to which the probability amplitude of an event occurring is the sum of the amplitudes of the various alter-

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native possibilities for this event to occur. In the Feynman approach this principle is used in the following way: the probability amplitude of a particle traveling from point q_a, where it was at time t_a, to a point q_b, at which it arrives at time t_b, is the sum of contributions of the motion of a classical particle along all conceivable paths connecting these points. In the case of quantum field theory the integral over all the paths is replaced by an integral over all field configurations.

The second postulate states that the contribution of each path to the probability amplitude is $\exp\{iS_{ba}[g(t)]/\hbar\}$, where $S_{ba}[g(t)]$ is the classical action integral calculated for the path $g(t)$. The first postulate determines the general scheme that must be used in quantum mechanics to calculate probabilities. The second invests this scheme with specific content, indicating a way of determining the amplitude corresponding to a definite way in which this event occurs. Essentially, this postulate is the quantum generalization of the classical principle of least action.

On the other hand, principles have been formulated within the framework of axiomatic quantum field theory that are mandatory for any feasible quantum theory.[18] Among these are the causality principle, the unitarity of the S matrix, and the assumptions of relativistic quantum theory about the properties of free states, assumptions that constitute what is known as the zeroth axiom of quantum field theory. As shown in Refs. 11–14, in building the scattering matrix these "mandatory" physical principles can be used instead of Feynman's second principle.

Let us examine the scattering S matrix. It describes scattering processes in which measurements in the system are conducted only as $t\to-\infty$ and $t\to+\infty$ and, accordingly, no attempts are made to determine the beginning and end of the interaction in the system. According to the basic Feynman postulate, the scattering amplitude can be represented as the sum of contributions of possible ways in which the given scattering process can be realized. Since no attempts are made to determine the beginning or end of the interaction in the system, we can assign any values to these times. Each specific pair of time values t_1 and t_2 of the beginning and end of the interaction correspond to definite ways of implementing the events described by the scattering matrix.

According to Feynman, each of these ways contribute to the scattering amplitude, which is simply the sum of these contributions:

$$\langle\varphi_2|S|\varphi_1\rangle=\langle\varphi_2|\varphi_1\rangle+\int_{-\infty}^{\infty}dt_2\int_{-\infty}^{\infty}dt_1\langle\varphi_2|\tilde{S}(t_2,t_1)|\varphi_1\rangle, \quad (1)$$

where $\langle\varphi_2|\tilde{S}(t_2,t_1)|\varphi_1\rangle$ is the probability amplitude that if at $t\to-\infty$ the state of the system was $|\text{in},\varphi_1\rangle$, then the interaction in the system begins at time t_2 and at $t\to+\infty$ the system is found in the state $|\text{out},\varphi_2\rangle$. The first term on the right-hand side of Eq. (1) corresponds to the situation in which the system's particles do not interact at any time. The following relationship is the Lorentz-invariant generalization of (1):

$$\langle\varphi_2|S|\varphi_1\rangle=\langle\varphi_2|\varphi_1\rangle+\int_{-\infty}^{\infty}d\sigma_2\int_{-\infty}^{\sigma_2}d\sigma_1\langle\varphi_2|\tilde{S}(\sigma_2,\sigma_1)|\varphi_1\rangle, \quad (2)$$

where $\langle\varphi_2|\tilde{S}(\sigma_2,\sigma_1)|\varphi_1\rangle$ is the amplitude corresponding to the variant of the evolution in which the interaction occurs in the space–time region between the hypersurfaces σ_1 and σ_2. Here σ stands for the hypersurface $xq=\sigma$, where q is the unit time-like vector pointing to the future. The amplitude $\langle|\varphi_2\tilde{S}(t_2,t_1)|\varphi_1\rangle$ can itself be represented by the sum of amplitudes corresponding to the alternative realizations of the event represented by this amplitude. For instance, in nonrelativistic quantum mechanics the amplitude $\langle\varphi_2|\tilde{S}(t_2,t_1)|\varphi_1\rangle$ can be written in the form of integrals along all conceivable paths corresponding to processes in which the interaction begins at t_1 and ends at t_2. If, following the second postulate of the Feynman method, we assume that each path provides a contribution proportional to the exponential function of the respective action integral and substitute the expression obtained in this manner into Eq. (1), we arrive at the ordinary expression for the Feynman amplitude.

In Refs. 11–14 it was found that building the scattering matrix does not require using the second postulate of the Feynman method, i.e., we need not assume that the amplitudes $\langle\varphi_2|\tilde{S}(t_2,t_1)|\varphi_1\rangle$ and $\langle\varphi_2|\tilde{S}(\sigma_2,\sigma_1)|\varphi_1\rangle$ are specified by exponential functions of the action integral, which in quantum mechanics corresponds to each path and in quantum field theory to each field configuration. At the same time this approach uses the main idea of the Feynman formalism, namely, that such amplitudes as $\langle\varphi_2|\tilde{S}(t_2,t_1)|\varphi_1\rangle$ and $\langle\varphi_2|\tilde{S}(\sigma_2,\sigma_1)|\varphi_1\rangle$, which correspond to the various possibilities of an event occurring, have physical meaning. It appears that by combining these amplitudes with the most general principles of axiomatic quantum field theory we can define a relativistic T matrix and derive a dynamic equation for it.

The T matrix is defined as follows:

$$\langle n_2,q|T(z,q)|n_1,q\rangle=i\int_0^{\infty}d\tau\exp(iz\tau)\langle n_2,q|\tilde{T}(\tau)|n_1,q\rangle,$$

$$\langle n_2,q|\tilde{T}(\sigma_2-\sigma_1)|n_1,q\rangle=\exp(-ip_{n_2}q\sigma_2)\times\langle n_2,q|\tilde{S}(\sigma_2,\sigma_1)|n_1,q\rangle\times\exp(ip_{n_1}q\sigma_2), \quad (3)$$

where $|n,q\rangle$ is the state vector in the interaction picture related to vector q, i.e.,

$$|n,\sigma\rangle=\exp(-ip_nq\sigma)|n,q\rangle.$$

Here $|n,\sigma\rangle$ are the eigenvectors of the total 4-momentum p_n that describe the free states of the system on the hypersurface σ, and n stands for the entire set of discrete and continuous variables that characterize the system in full. The relativistic T matrix defined in this way is related to the S matrix by

$$\langle n_2,q|S|n_1,q\rangle=\langle n_2,q|n_1,q\rangle-2\pi i\delta(p_{n_2}q-p_{n_1}q)\times\langle n_2,q|T(p_{n_1}q,q)|n_1,q\rangle, \quad (4)$$

and satisfies the following relationship:

$$\langle n_2,q|T(z_1,q)|n_1,q\rangle-\langle n_2,q|T(z_2,q)|n_1,q\rangle=(z_2-z_1)\langle n_2,q|T(z_2,q)G_0(z_2,q)\times G_0(z_1,q)T(z_1,q)|n_1,q\rangle,$$

$$G_0(z,q)=\sum_n\frac{|n,q\rangle\langle n,q|}{z-p_nq+i0}. \quad (5)$$

Note that Eq. (5) was derived as a corollary of the most general physical principles: the Feynman superposition principle, the unitarity of the S matrix, and the assumptions of relativistic quantum theory about the properties of free states. If a boundary condition for $\langle\varphi_2|T(z,q)|\varphi_1\rangle$ is specified, we can think of (5) as being a difference equation. In Ref. 12 it was found that the boundary condition at which the dynamics determined by this equation proves to be equivalent to the Hamiltonian dynamics has the following form:

$$\langle\varphi_2|T(z,q)|\varphi_1\rangle\underset{z\to i\infty}{\to}\langle\varphi_2|B(q)|\varphi_1\rangle, \quad (6)$$

$$\langle\varphi_2|B(q)|\varphi_1\rangle=\int d^4x\langle\varphi_2|\mathscr{H}_1(x)|\varphi_1\rangle\delta(qx), \quad (7)$$

where $\mathscr{H}_1(x)$ is the interaction Hamiltonian density. With such a boundary condition applied in nonrelativistic quantum mechanics, Eq. (5) yields the Lippmann–Schwinger[11] and Schrödinger[19] equations. In quantum field theory the solution of Eq. (5) with the boundary condition (6) leads to the ordinary representation of the S matrix in the form of a T exponential function.

Note that only in nonrelativistic quantum mechanics is the definition of the T matrix via (3) equivalent to the definition of the T matrix in formal scattering theory. Indeed, as is well known, quantum field theory does not allow using the standard definition of the scattering matrix in quantum mechanics—it must be modified because in quantum field theory bare particles, described by the free Hamiltonian, do not coincide with physical particles, described by the total Hamiltonian.

What is important is that the T matrix determined by (5) describes the self-action of particles. The presence of the corresponding matrix elements leads to a situation in which Eq. (5) proves to be essentially singular in the physical region. This difficulty, however, can be overcome by reduction,[5,13] which amounts to the propagator $G_0(z,q)$ describing the evolution of free particles being replaced by the propagator $G(z,q)$ describing the evolution of particles interacting with the vacuum and, accordingly, $T(z,q)$ being replaced by $M(z,q)$, which describes particle interactions proper. These operators are related as follows:

$$G_0(z,q)+G_0(z,q)T(z,q)G_0(z,q)=G(z,q)+G(z,q)M(z,q)G(z,q).$$

As a result of such reduction, equations were obtained[5,13] that made it possible to find $M(z,q)$ and the propagator $G(z,q)$ that determines the kinematics of real particles interacting with the vacuum. In the process it proved more convenient to set up equations not for the propagator $G(z,q)$ but for the amplitude $C(z,q;n)$ specified by the following relationship:

$$\langle n_2,q|G(z,q)|n_1,q\rangle=\frac{\langle n_2,q|n_1,q\rangle}{z-p_{n_1}q-C(z,q;n_1)}.$$

The poles of $\langle n_2,q|G(z,q)|n_1,q\rangle$ determine the physical masses of the particles.

3. ELECTRODYNAMICS IN THE FIELD OF THE NUCLEUS AND NATURAL BROADENING IN THAT FIELD

In Refs. 2 and 5 a theory of unstable states of atomic systems was built that enabled describing these states without resorting to the quasistationary approximation and perturbation theory. The gist of the theory is as follows. "Bare" bound states of electrons in the field of the nucleus are defined for the case where all the interaction in the system reduces to that of an electron and the field of the nucleus, which can be interpreted as an externa, unquantized field. Real states can be obtained from such states by allowing for the interaction of the electrons with their radiation field and with each other. Here for the space of free states one uses the space $\mathscr{H}_{as}$ constructed on the basis of the bound states of electrons in the field of the nucleus and the free states of electrons and positrons. However, it is more convenient to take for the free states the states of electrons in the field of the nucleus belonging to the discrete and continuous spectra. In this case the interaction of electrons and positrons with the Coulomb field of the nucleus has already been accounted for in these states. With such a choice of the "free" states, Eq. (5) describes the interaction of electrons and positrons with each other and with their radiation field.

The interaction of the particles in the system with their radiation field and with each other can be described by the equations for the operators $M(z)$ and $G(z)$ mentioned earlier. Here and in what follows we employ a system of coordinates in which vector q is directed along the time axis. In this case the matrix elements

$$\langle m_2|G(z)|m_1\rangle=\frac{\langle m_2|m_1\rangle}{z-E_{m_1}-C(z,m_1)},$$

where $|m\rangle$ corresponds to the discrete part of the spectrum, characterize the interaction of atoms with their radiation and the interaction of the electrons of an atom with each other. While for the ground state this interaction results in a shift in the energy level, for the excited states $\langle m_2|G(z)|m_1\rangle$ has no poles, with the result that no definite energy can be associated with these states. Such states are characterized by a certain energy distribution defined by the functions $C(z,m)$. The elements of the M-matrix describe the emission and absorption of photons in the atomic system, various scattering processes in the system, and transitions between the various states of the electron–positron field.

The natural broadening of spectral line profiles is determined by the probability of a photon being emitted with energy ω as the atomic system goes from the ith excited state to the ground state:[2,5]

$$\frac{dW_i(\omega)}{d\omega}=A\omega\sum_{\lambda}\int d\Omega_k\left|\frac{\langle 1,\mathbf{k},\varepsilon_\lambda|M(E_1+\omega)|i\rangle}{E_1+\omega-E_i-C(E_1+\omega)}\right|^2, \tag{8}$$

where A is a normalization factor, and $\mathbf{k}$ and ε_λ are, respectively, the photon's momentum and polarization. The ground-state energy E_1 already incorporates the correction due to the interaction of the atom in the ground state with the vacuum. Equation (8) holds when the contribution of interference terms can be ignored. If within the limits of the spectral line profile we can ignore the z-dependence of $C_j(z)$, we can put

$$C_j(z)=C_j(E_j)=\Delta E_j-\frac{i}{2}\Gamma_j. \tag{9}$$

Equation (8) implies that ΔE_j and Γ_j can be interpreted, accordingly, as a shift in energy caused by the interaction of the atom with the vacuum and the width of the energy level.

4. SPECTRAL LINE PROFILE AND SURFACE DIVERGENCES

The equations used in the method under discussion can be solved iteratively when the coupling constant is fairly small. This approach was used in Refs. 5 and 7 to find the solutions that determine the natural broadening of spectral line profiles. For instance, in the first order of the iterative solution we have

$$\langle n_2|M^{(1)}(z)|n_1\rangle=\langle n_2|H_1|n_1\rangle. \tag{10}$$

In the next order, for $C_i(z)$ and $\langle i|M(z)|j\rangle$ we have

$$C_i^{(2)}(z)=\langle i|\Sigma(z)|i\rangle-\lim_{z_2\to i\infty}\langle i|H_1G_0(z_2)H_1|i\rangle+C_i(i\infty), \tag{11}$$

$$\langle i|M^{(2)}(z)|j\rangle=\langle i|\Sigma(z)|j\rangle-\lim_{z_2\to i\infty}\langle i|H_1G_0(z_2)H_1|j\rangle+\langle i|M(i\infty)|j\rangle, \tag{12}$$

where

$$\langle i|\Sigma(z)|i\rangle=\langle i|H_1G_0(z)H_1|i\rangle, \tag{13}$$

$$\langle i|\Sigma(z)|j\rangle=\langle i|H_1G_0(z)H_1|j\rangle, \tag{14}$$

and $|i\rangle$ is the state vector describing the ith state of the atom. If the distance between the energy levels with the same values of J, J_z, and parity is much larger than the widths of these levels, in solving the problem to within α^2 we can ignore the radiative transitions between different states of the atom, which are described by $\langle i|M(z)|j\rangle$, with (9) providing $C_i(z)$ to the given accuracy.

At $z=E_i$ the right-hand side of (9) can be reduced to a form coinciding with the ordinary QED expression for the radiative shift of an atomic energy level. If, however, energy levels with the same values of J, J_z, and parity overlap, we allow for transitions between these states, which means we cannot limit ourselves to the second-order iterative solution in determining $C_i(z)$.

In the next order we arrive at the following expression[7] for the spectral line profile, defined by (8), for a three-level atomic system:

$$\frac{dW_{12}(\omega)}{d\omega}=A\omega\sum_{\lambda}\int d\Omega_k\left|\frac{\langle 1,\mathbf{k},\varepsilon_\lambda|H_{\rm int}|2\rangle+\dfrac{\langle 1,\mathbf{k},\varepsilon_\lambda|H_{\rm int}|3\rangle\langle 3|\Sigma^{(2)}(z)|2\rangle}{E_1+\omega-E_3-C_3^{(2)}(z)}}{E_1+\omega-E_2-C_2^{(2)}(z)-\dfrac{\langle 2|\Sigma^{(2)}(z)|3\rangle\langle 3|\Sigma^{(2)}(z)|2\rangle}{E_1+\omega-E_3-C_3^{(2)}(z)}}\right|^2, \tag{15}$$

where $z=E_1+\omega$. If we ignore the z-dependence of $\langle i|\Sigma(z)|j\rangle$ and $\langle i|\Sigma(z)|i\rangle$ within the line profile and set $\langle j|\Sigma(z)|j\rangle=\Delta E_j-(i/2)\Gamma_j$, the above expression coincides in form with the expression for the emission probability obtained in Ref. 1 as a result of summing an infinite perturbation series.

Note that the solution as a result of which we obtained (15) is of a formal nature and does not take into account the problem of ultraviolet divergences mentioned earlier. When energy levels with the same values of J, J_z, and parity do not overlap, these problems are solved by a standard method if we assume that the line is Lorentzian. In this case the line profile is determined by the quantity $C_i(z=E_i)$, which coincides with $\langle i|\Sigma(z=E_i)|i\rangle$ (we ignore the second and third terms on the right-hand side of (12), which can be incorporated into the renormalization constants). The quantity $\langle i|\Sigma(z=E_i)|i\rangle$ can be calculated via the ordinary renormalization method.

But the situation changes drastically when the energy levels of such states do overlap. In this case the spectral line profiles strongly depend on the law by which the system evolves. It is, therefore, natural to assume that difficulties associated with surface divergences must be encountered here. For (15) this becomes apparent in calculations of $\langle j|\Sigma(z)|i\rangle$, which describes transitions between states $|i\rangle$ and $|j\rangle$ with different energies, i.e., $\langle j|\Sigma(z)|i\rangle$ is obviously a quantity whose calculation involves dealing with surface divergences.

We now discuss this question in greater detail. For the sake of simplicity we examine the case of a one-electron atom.

At $z=E_i$ the expression (14) for $\langle j|\Sigma(z)|i\rangle$ can be represented in the form

$$\langle j|\Sigma(z=E_i)|i\rangle=-ie^2\int \bar{\psi}_j^0(\mathbf{r})[\Sigma_{E_i}^A(\mathbf{r},\mathbf{r}')+\Sigma_{E_j}^B(\mathbf{r},\mathbf{r}')]\psi_i^0(\mathbf{r}')d^3xd^3x', \quad (16)$$

where

$$\Sigma_{E_i}^A(\mathbf{r},\mathbf{r}')=\int_0^\infty \exp\{iE_i(t-t')\}\Sigma(x,x')d(t-t'), \quad (17)$$

$$\Sigma_{E_j}^B(\mathbf{r},\mathbf{r}')=\int_{-\infty}^0 \exp[iE_j(t-t')]\Sigma(x,x')d(t-t'), \quad (18)$$

$\Sigma(x,x')$ is the mass operator, and the $\psi_i^0(\mathbf{r})$ are the time-independent electron wave functions. Using the representation

$$\Sigma(x,x')=(1/2\pi)\int dE\ \exp\{-iE(t-t')\}\Sigma_E(\mathbf{r},\mathbf{r}'),$$

we can rewrite Eqs. (17) and (18) as

$$\Sigma_{E_i}^A(\mathbf{r},\mathbf{r}')=\frac{1}{2\pi i}\int dE\frac{\Sigma_E(\mathbf{r},\mathbf{r}')}{E_i-E+i0}, \quad (19)$$

$$\Sigma_{E_j}^B(\mathbf{r},\mathbf{r}')=-\frac{1}{2\pi i}\int dE\frac{\Sigma_E(\mathbf{r},\mathbf{r}')}{E_j-E-i0}. \quad (20)$$

The necessary regularization here reduces to replacing $\Sigma_E(\mathbf{r},\mathbf{r}')$ by the renormalized mass operator $\Sigma_E^{(r)}(\mathbf{r},\mathbf{r}')$. But since $\Sigma_E^{(r)}(\mathbf{r},\mathbf{r}')$ behaves like $E\ln E$ as $E\to\infty$, the integrals in (19) and (20) diverge at large values of E, which is the manifestation of the surface divergences mentioned above.

At $E_i=E_j$ this difficulty is not present because in this case the sum of integrals (19) and (20) is equal to $\Sigma_{E_i}^{(r)}\times(\mathbf{r},\mathbf{r}')$, and (16) reduces to

$$\langle j|\Sigma(z=E_i)|i\rangle=ie^2\int \bar{\psi}_j^0(\mathbf{r})\Sigma_{E_i}^{(r)}(\mathbf{r},\mathbf{r}')\psi_i^0(\mathbf{r}')d^3xd^3x'.$$

But E_i is not equal to E_j. Otherwise, the state $|i\rangle$ would coincide with $|j\rangle$, in which case Eq. (16) would be an expression for the self-energy shift $C_i^{(2)}(E_i)$. As for the off-diagonal elements $\langle j|\Sigma(z)|i\rangle$, this expression cannot be used even as the first approximation, since the sum of the integrals (19) and (20) diverges for an arbitrarily small value of E_i-E_j.

Thus, $\langle j|\Sigma(z)|i\rangle$ remains divergent even after renormalization, and hence Eq. (16) is meaningless. The fact that difficulties associated with surface divergences emerge in the given problem, which is related to the description of temporal evolution, is quite natural. But it must be stressed that, as noted earlier, when energy levels with the same values of J, J_z, and parity overlap, these difficulties cannot be ignored even in the lowest approximation. In this case the ultraviolet divergences cannot be removed by standard QED methods.

In studying the natural broadening of spectral line profiles,[7] when levels with the same value of J, J_z, and parity overlapped, the equation for $\langle i|M(z)|j\rangle$ was dropped from the system of equations, because of the difficulties discussed above. In the process it was assumed that

$$\langle i|M(z)|j\rangle=\langle i|M(z)G(z)M(z)|j\rangle.$$

Such a model made it possible to investigate how strongly the natural broadening of line profiles depends on the overlap of energy levels. However, in a consistent QED calculation of the line profiles the problem under consideration cannot be ignored.

5. ULTRAVIOLET DIVERGENCES AND THE *T*-MATRIX EQUATION

As is known, removing ultraviolet divergences does not settle the difficulties of quantum field theory since the infinities go from the matrix elements to the interaction Hamiltonian. The problem under discussion is a perfect illustration of this. On the other hand, solving the problem in full requires a thorough modification of the theory. Since ultraviolet divergences are related to the local nature of the theory, it seems natural to resolve the problem through a nonlocality in the theory. But nonlocal quantum field theory has its own difficulties, which have proved to be more serious than the difficulties of the local theory associated with ultraviolet divergences.

For instance, an attempt to introduce a nonlocal form factor into the interaction Hamiltonian density $\mathscr{H}_1(x)$ fails because it violates the integrability condition

$$[\mathscr{H}_1(x),\mathscr{H}_1(x')]=0, \quad (x-x')^2<0, \quad (21)$$

which is the compatibility condition of the Tomonaga–Schwinger equation.

We now examine Eq. (5) with the boundary condition (6). In Ref. 13 it was found that for Eq. (5) to be compatible with the boundary condition (6), $\mathscr{H}_1(x)$ in Eq. (7) must satisfy condition (21). This means that a nonlocal form factor cannot be introduced into (6).

In Refs. 13 and 14 a more general boundary condition for Eq. (5) was formulated. This condition is specified not for the T matrix but for an operator $\tilde{S}(x_2,x_1)$ (see Refs. 13 and 14) related to the operator $\tilde{S}(\sigma_2,\sigma_1)$ through the following expression:

$$\langle n_2|\tilde{S}(\sigma_2,\sigma_1)|n_1\rangle=\int d^4x_2\int d^4x_1\delta(qx_2-\sigma_2)\times\delta(qx_1-\sigma_1)\langle n_2|\tilde{S}(x_2,x_1)|n_1\rangle. \quad (22)$$

The meaning of introducing the operator $\tilde{S}(x_2,x_1)$, an operator-valued function of the two points x_2 and x_1, arises from its difference from $\tilde{S}(\sigma_2,\sigma_1)$, which is a function of the surfaces σ_2 and σ_1. The covariance of expressions becomes more evident. For instance, the expression (2) for the S matrix can be written as

$$\langle n_2|S|n_1\rangle=\langle n_2|n_1\rangle+\int d^4x_2\int d^4x_1\langle n_2|\tilde{S}\times(x_2,x_1)|n_1\rangle\theta(x_2q-x_1q), \quad (23)$$

where

$$\theta(y)=\begin{cases}1, & \text{if } y\geq 0,\\ 0, & \text{if } y<0.\end{cases}$$

In Refs. 13 and 14 the boundary condition for $\tilde{S}(x_2,x_1)$ is given as

$$\langle n_2|\tilde{S}(x_2,x_1)|n_1\rangle \xrightarrow[x_2\to x_1]{} \langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle, \tag{24}$$

with $\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle$ describing an "elementary" interaction with the system. If $\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle$ is specified in the form

$$\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle = -2i\langle n_2|.\mathscr{H}_1(x_1)|n_1\rangle\delta^4(x_2-x_1) + \langle n_2|\tilde{S}'_N(x_2,x_1)|n_1\rangle, \tag{25}$$

where the amplitude $\langle n_2|\tilde{S}'_N(x_2,x_1)|n_1\rangle$ has no singularity at the point $x_2=x_1$, then the boundary condition (24) proves to be equivalent to the boundary condition (6).

The boundary condition (24) opens up new possibilities for solving the problem of ultraviolet divergences. Indeed, the integrability condition (21), which actually allows only for local interaction, limits the development of the theory when the boundary condition (6) is employed. Equation (25) demonstrates this clearly since $\mathscr{H}_1(x)$ is a local characteristic.

On the other hand, $\langle n_2|\tilde{S}'_N(x_2,x_1)|n_1\rangle$ in (24) is essentially nonlocal, since it describes a process in which the interaction takes place in a finite space–time region determined by the points x_2 and x_1. This means that the amplitudes $\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle$ can be specified by form factors that determine the behavior of the amplitudes as functions of particle momenta.

In QED the operator $\tilde{S}_N(x_2,x_1)$, which specifies the elementary interaction in the system, must generally have the following form:

$$\tilde{S}_N(x_2,x_1)=\int d^4y_1\int d^4y_2 F(x_2-x_1,y_1-x_1,y_2-x_1)j_\mu(y_1)A^\mu(y_2),$$
$$(x_2-x_1)^2>0,\quad x_2>x_1, \tag{26}$$

where $F(x_2-x_1,y_1-x_1,y_2-x_1)$ is a Lorentz-invariant form factor, $j_\mu(x)$ is the current density operator, and $A^\mu(x)$ is the electromagnetic field potential. The compatibility condition for $\tilde{S}(x_2,x_1)$, which is a generalization of the condition on $\mathscr{H}(x)$, has the form

$$\tilde{S}(x_4,x_3)\tilde{S}(x_2,x_1)=\tilde{S}(x_2,x_1)\tilde{S}(x_4,x_3) \tag{27}$$

when x_4 and x_3 are spatially similar to the points x_2 and x_1. For $\tilde{S}_N(x_2,x_1)$ defined by (26) to satisfy (27), the form factor $F(x_2-x_1,y_1-x_1,y_2-x_1)$ must be nonzero only if y_1 and y_2 lie within the space–time region limited by two light cones with their vertices at points x_2 and x_1:

$$(x_1-y_{1,2})^2>0,\ (x_2-y_{1,2})^2>0,\ x_2>y_{1,2}>x_1.$$

Obviously, $F(x_2-x_1,y_1-x_1,y_2-x_1)$ can be chosen in such a way that the amplitudes $\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle$ as functions of particle momenta will have the "right" properties. However, according to (24), as $x_2\to x_1$ the behavior of $\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle$ is important only when the region in which $F(x_2-x_1,y_1-x_1,y_2-x_1)$ is nonzero collapses to a point.

Obviously, for all $|n_1\rangle$ and $|n_2\rangle$, we can write the following relationship for $\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle$ in a small enough neighborhood of the point $x_2=x_1$:

$$\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle = \langle n_2|.\mathscr{H}_1(x_1)|n_1\rangle\int d^4y_1\int d^4y_2 F(x_2-x_1,y_1-x_1,y_2-x_1), \tag{28}$$

where

$$.\mathscr{H}_1(x)=j_\mu(x)A^\mu(x).$$

From this it follows that for all $|n_1\rangle$ and $|n_2\rangle$ we can select a z such that

$$\langle n_2|T(z,q)|n_1\rangle = g(z,q)\int d^4x\langle n_2|.\mathscr{H}_1(x)|n_1\rangle\delta(qx), \tag{29}$$

$$g(z,q)=\int_0^\infty d\sigma\int d^4x\int d^4y_1\int d^4y_2\ \exp\{iz\tau\}\times F(x,y_1,y_2)\delta(qx-\sigma). \tag{30}$$

If $F(x_2-x_1,y_1-x_1,y_2-x_1)$ has no singularity at $x_2-x_1=0$ similar to the one in (25), the function $g(z,q)$, according to (30), must tend to zero as $z\to i\infty$.

But does Eq. (5) have a nontrivial solution when

$$\lim_{z\to\infty}\langle n_2|T(z,q)|n_1\rangle=0$$

Sending z_2 to $i\infty$ in Eq. (5) and then interchanging the order of integration and taking the limit on the right-hand side of the equation, which cannot be done in general, we find that

$$\langle n_2|T(z,q)|n_1\rangle=0$$

for all values of z. This situation resembles the "zero-charge" problem in QED.

But the reason for the current difficulty is obvious and lies in the fact that generally one cannot employ the above method for solving Eq. (5). Indeed, to be able to interchange the integration and the limit we must make sure that the respective integrals converge. But in view of ultraviolet divergences, this is obviously not the case. On the other hand, z_2 in Eq. (5) can be chosen as large as one wishes, which means that Eq. (5) can be solved perturbatively, assuming that the operator $T(z_2,q)$ is known.

Thus, we arrive at the following expression:

$$\langle n_2|S(z_2)|n_1\rangle = \langle n_2|n_1\rangle - 2\pi i\delta(p_{n_2}q-p_{n_1}q)\times\langle n_2|T'(z_1;z_2)|n_1\rangle = \langle n_2|T\exp\left\{-i\int_{-\infty}^{+\infty}d\sigma H_1(\sigma;z_2)\right\}|n_1\rangle, \tag{31}$$

where

$$\langle n_2|T'(z;z_2)|n_1\rangle=\frac{(z_2-z)^{1/2}}{(z_2-E_{n_2})^{1/2}}\langle n_2|T(z;q)|n_1\rangle\frac{(z_2-z)^{1/2}}{(z-E_{n_1})^{1/2}},$$

$$\langle n_2|H_1(\sigma;z_2)|n_1\rangle=\exp(ip_{n_2}q\sigma)\langle n_2|T(z_2;q)|n_1\rangle \times\exp\{-ip_{n_1}q\sigma\}.$$

Obviously, the S matrix is related to $\langle n_2|S(z_2)|n_1\rangle$ via the formula

$$\langle n_2|S|n_1\rangle=\lim_{z_2\to i\infty}\langle n_2|S(z_2)|n_1\rangle. \tag{32}$$

If a certain cutoff momentum is introduced, then according to Eq. (29) we can choose a z such that for all states $|n\rangle$ in which the particle momenta are smaller than the cutoff momentum, the matrix element $\langle n_2|H_1(\sigma;z_2)|n_1\rangle$ coincides with the respective matrix elements of the ordinary local interaction Hamiltonian.

Thus, the expression for the S matrix determined by (31) and (32) essentially coincides with the ordinary expression for the S matrix regularized by introducing a "cutoff" form factor. If in (31) we renormalize by going over to physical masses and charge and then sending z_2 to $i\infty$, we arrive at the ordinary expression for the renormalized S matrix. Since all parameters used to build the S matrix are reduced in the process to physical masses and charge, the expression for the S matrix is clearly independent of the type of form factor in (26). This is obviously a reflection of the law as a consequence of which in ordinary theory the renormalized S matrix is independent of the way in which intermediate regularization is performed. Thus, the theory according to which the dynamics is determined by the boundary conditions (24) and (26) manifests itself as an ordinary theory in describing the scattering matrix.

On the other hand, using such a boundary condition offers the possibility of describing processes whose depiction in ordinary theory involves surface divergences. In such processes the dependence on a specific type of form factor in (26) may have some effect.

For this reason there is a need to establish what class of form factors in (26) is admissible in principle. To this end, using the integro-differential form of Eq. (3) (see Ref. 12) and the representation (3), we can derive the following equation:

$$(\sigma_2-\sigma_1)\langle n_2|\tilde{T}(\sigma_2-\sigma_1)|n_1\rangle = \sum_n\int_{\sigma_1}^{\sigma_2}d\sigma_4\int_{\sigma_1}^{\sigma_4}d\sigma_3(\sigma_4-\sigma_3)\exp[ip_nq(\sigma_4-\sigma_3)] \times\langle n_2|\tilde{T}(\sigma_2-\sigma_4)|n\rangle\langle n|\tilde{T}(\sigma_3-\sigma_1)|n_1\rangle. \tag{33}$$

Combining this with (24), we see that when $\sigma_2\to\sigma_1$, the following relationship holds:

$$(\sigma_2-\sigma_1)\langle n_2|\tilde{T}_N(\sigma_2-\sigma_1)|n_1\rangle = \sum_n\int_{\sigma_1}^{\sigma_2}d\sigma_4\int_{\sigma_1}^{\sigma_4}d\sigma_3(\sigma_4-\sigma_3)\exp[ip_nq(\sigma_4 -\sigma_3)]\langle n_2|\tilde{T}_N(\sigma_2-\sigma_4)|n\rangle\langle n|\tilde{T}_N(\sigma_3-\sigma_1)|n_1\rangle, \tag{34}$$

where

$$\langle n_2|\tilde{T}_N(\sigma_2-\sigma_1)|n_1\rangle = \int d^4x_2\int d^4x_1\,\delta(qx_2-\sigma_2)\,\delta(qx_1-\sigma_1) \times\exp[i(p_{n_2}q)\sigma_2]\langle n_2|\tilde{S}_N(x_2,x_1)|n_1\rangle \times\exp[-i(p_{n_1}q)\sigma_1].$$

The form factors in (24) must be such that (34) holds for all values of q. Thus, Eq. (34) determines the class of admissible form factors. Such form factors (for which (34) holds) can be shown to exist. This problem, however, requires a separate discussion and is not considered here.

6. CONCLUSION

We have shown that calculating $\langle j|\Sigma(z)|i\rangle$ encounters difficulties related to surface divergences. On the other hand, as Eq. (15) implies, the natural broadening of line profiles strongly depends on $\langle j|\Sigma(z)|i\rangle$ if its value is comparable to the distances between the corresponding energy levels. Such a situation can occur only in multiply-charged heavy ions, in which the interaction of an ion with its own field cannot be considered a small perturbation. This means that such ions have states for which calculations of the respective line profiles cannot be done by standard QED methods even in the lowest approximation.

We also found that the boundary condition for Eq. (24) can be formulated in such a way that no difficulties with surface divergences arise in describing the temporal evolution of QED systems; solution of the equation by perturbative techniques leads to the ordinary renormalized expression for the S matrix. For this the boundary condition must be such that the physical electron mass and charge, which in this case are found by solving the equations of the method, coincide with the respective experimental values.

Such a statement of the problem in which the boundary condition is chosen on the basis of the values of the physical electron mass and charge is entirely in keeping with the renormalization scheme common in QED. But in our case such renormalization is finite, which opens up the possibility for calculations of the natural broadening of spectral line profiles free of surface divergences. This proves important in describing the spectra of multiply-charged heavy ions, in which the natural broadening plays a dominant role and one cannot ignore corrections whose description with standard methods involves surface divergences.

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