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1989 J. Phys. A: Math. Gen. 22 269

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The decay and energy distribution of unstable bound states

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Received 4 January 1988, in final form 26 July 1988

Abstract. An approach to the theory of unstable bound states of electrons in the nuclear field is suggested. This approach permits the determination of unstable bound states when a quasistationary approximation is unjustified and, therefore, methods normally used for this purpose in the atomic theory cannot be applied. The equations employed in our approach make it possible, without resorting to perturbation theory, to determine the energy distribution of excited states, the shape of the natural broadening of spectral lines, the amplitudes of the resonance scattering of photons and electrons over atomic systems, and to describe spontaneous radiation and autoionisation decay. Calculated results are given of the shape of the natural broadening of spectral lines in a three-level atomic system when energy levels overlap. In the quasistationary approximation standard expressions of the relativistic atomic theory for level energy shifts and radiation widths follow from the equations.

1. Introduction

The quantum theory of unstable systems has been an object of intensive study for a number of years. A fairly comprehensive review of the extensive literature on the subject can be found in Fonda *et al* (1978). An important variety of unstable states is that of bound complexes, e.g. excited atomic and nuclear states. The description of atomic-system unstable states is based on the concept of their quasistationarity, which makes it possible to attribute certain complex energy values to these states. In the general case the decay law is fully determined by the setting of the unstable state vector $|\psi_i, t\rangle$ at the moment of time $t=0$ (Fock and Krylov 1948)

$$|\psi_i, t=0\rangle = \int a_i(E) |\varphi_i, E\rangle dE \quad (1)$$

where $|\varphi_i, E\rangle$ is the eigenvector of the energy operator. In the case of atomic systems, given an unstable state at the moment of time $t=0$, the attenuation theory (Heitler 1954) permits an exact determination of the law of finite-state probability distribution. This theory, however, gives no exact determination of an excited state bound with a finite lifetime (Heitler 1954). Therefore, 'unperturbed' bound states are used as initial states (in this case perturbation is the interaction between the atomic system and the radiation field). This is justified, however, only in the quasistationary approximation. As concerns the basic difference between the determination of unstable excited states and that of the basic ground state, it should be noted that in the stationary state the system has a definite energy; hence the determination of the excited state is reduced

to the determination of the energy operator eigenvector. No definite energy can be related to unstable states, and for this reason they cannot be determined by equations for obtaining energy operator eigenvalues, except for quasistationary approximations, where a certain complex energy is attributed to the unstable state. In this case quasistationary states can also be determined by an equation in complex energy eigenvalues (the Schwinger equation).

For the quasistationary approximation to hold for a certain state, it is necessary that the width of the corresponding energy level Γ should be small compared with the characteristic interval of the irregularities of the state's decay. From this it follows that the distances between the energy levels of states with the same total moment \mathcal{J} , its projection on axis z and parity must be much greater than the width of these levels. However, in the case of multicharge ions the energy levels of certain states with identical \mathcal{J} , \mathcal{J}_z and parity can overlap. Thus, in the multicharge-ion case certain bound states cannot be regarded as quasistationary and for this reason, when describing such states, one should transcend the bounds of the quasistationary approach.

Gainutdinov (1983) suggested an approach to a non-relativistic quantum theory of scattering, based on Feynman's principle of amplitude superposition and the more general principles of relativistic quantum theory. This approach was further generalised (Gainutdinov 1987) to the case of the relativistic theory. It was shown by Gainutdinov (1986) that using this approach one could determine the unstable states of an electron in the nuclear field without resorting to the notion of their quasistationarity. Equations were obtained for the operator $C(z)$, determining the energy distribution of excited bound states, and for the operator $M(z)$, describing the emission and absorption of photons by hydrogen-like ions. In the present paper this approach is extended to the atomic-system case with an arbitrary number of electrons.

2. *T*-matrix formalism

2.1. Basic physical principles

Feynman's formulation of quantum mechanics (Feynman 1948, Feynman and Hibbs 1965) is based on two principles. According to the principle of amplitude superposition the probability amplitude of each event is the sum of the probability amplitudes of different alternative realisations of that event. In Feynman's formalism the use of this principle consists of the fact that the probability amplitude of particle transition from point X_1 , at the moment of time t_1 , to point X_2 , at moment t_2 , is written as a sum of the contributions of classical movements over all possible trajectories. The second postulate of Feynman's formalism is that the contribution of each trajectory to the amplitude is equal to $\exp(i/\hbar S_{21}[x(t)])$ where $S_{21}[x(t)]$ is the classic action, calculated for the trajectory $x(t)$. It was demonstrated by Gainutdinov (1983) that instead of Feynman's second postulate, which has a rather artificial character, one can use, together with the amplitude superposition principle, the more general principles of relativistic quantum theory, constituting the so-called 'zero' axiom of the axiomatic field quantum theory (Streater and Wightman 1964). In Gainutdinov (1983, 1987) the use of Feynman's superposition principle involved scattering amplitudes corresponding to certain temporal versions of the scattering process

$$\langle \varphi_2 | S | \varphi_1 \rangle = \langle \varphi_2 | \varphi_1 \rangle + \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{t_2} dt_1 \langle \varphi_2 | \tilde{S}(t_2, t_1) | \varphi_1 \rangle \quad (2)$$

where $\langle \varphi_2 | \tilde{S}(t_2, t_1) | \varphi_1 \rangle$ determines the amplitude of probability that, whereas at $t \rightarrow -\infty$ the state of the system was $|\text{in}, \varphi_1\rangle$, the interaction of the system particles will occur within the time interval (t_1, t_2) and at $t \rightarrow \infty$ the system will be determined in the state $|\text{out}, \varphi_2\rangle$. The first term on the right-hand side of (2) corresponds to the evolution variant in which the system particles do not interact at any time. Note that in the present paper we use a non-covariant version of the formalism. To explain the meaning of (2), we shall point out the following. In keeping with Feynman's approach, something may be represented in the form of an integral over all the classic trajectories, for which interaction begins at time t_1 and ends at t_2 . Obviously, in this case (2) coincides with the standard expression for a scattering amplitude in the shape of path integrals.

2.2. T-matrix equation

The principal object of our approach—the T matrix—is introduced as follows:

$$\langle n_2 | T(z) | n_1 \rangle = i \int_0^\infty d\tau \exp(iz\tau) \langle n_2 | \tilde{T}(\tau) | n_1 \rangle \tag{3}$$

$$\langle n_2 | \tilde{T}(t_2 - t_1) | n_1 \rangle = \exp(-iE_{n_2}t_2) \langle n_2 | \tilde{S}(t_2, t_1) | n_1 \rangle \exp(iE_{n_1}t_1).$$

Here the vector $|n\rangle$ describes the state of the system with the energy E_n , n denoting the entire set of discrete and continuous parameters which characterise this state. It was shown by Gainutdinov (1983, 1987) that the T matrix satisfies the following relationships:

$$\langle n_2 | T(z_1) | n_1 \rangle - \langle n_2 | \overset{\dagger}{T}(z_2) | n_1 \rangle = (z_2 - z_1) \langle n_2 | \overset{\dagger}{T}(z_2) \overset{\dagger}{G}_0(z_2) G_0(z_1) T(z_1) | n_1 \rangle \tag{4}$$

$$\langle n_2 | T(z_1) | n_1 \rangle - \langle n_2 | \overset{\dagger}{T}(z_2) | n_1 \rangle = (z_2 - z_1) \langle n_2 | T(z_1) G_0(z_1) \overset{\dagger}{G}_0(z_2) \overset{\dagger}{T}(z_2) | n_1 \rangle \tag{5}$$

$$G_0(z) = \sum_n \frac{|n\rangle\langle n|}{z - E_n + i0}.$$

These equations were derived as off-shell generalisations of the relationships for the T matrix:

$$\langle n_2 | T(E_{n_1}) | n_1 \rangle - \langle n_2 | \overset{\dagger}{T}(E_{n_2}) | n_1 \rangle = (E_{n_2} - E_{n_1}) \langle n_2 | \overset{\dagger}{T}(E_{n_2}) \overset{\dagger}{G}_0(E_{n_2}) G_0(E_{n_1}) T(E_{n_1}) | n_1 \rangle \tag{6}$$

$$\langle n_2 | T(E_{n_2}) | n_1 \rangle - \langle n_2 | \overset{\dagger}{T}(E_{n_1}) | n_1 \rangle = (E_{n_1} - E_{n_2}) \langle n_2 | T(E_{n_2}) G_0(E_{n_2}) \overset{\dagger}{G}_0(E_{n_1}) \overset{\dagger}{T}(E_{n_1}) | n_1 \rangle \tag{7}$$

which follow directly from the unitarity conditions introduced by Gainutdinov (1983, 1987) of the operators $S(t_K)$ and $S(t_H)$. For example, the operator $S(t_K)$ is an operator whose matrix elements determine the probability that if no interaction was present in the system at $t \rightarrow -\infty$ and the system state was $|\text{in}, \varphi\rangle$ and the system particles do not interact at the moment t , then the system will be found in the state $|\text{out}, \psi\rangle$ at this moment of time. The operator $S(t_K)$ satisfies the unitarity condition

$$\overset{\dagger}{S}(t_K) S(t_K) = 1. \tag{8}$$

In keeping with the superposition principle for $\langle n_2 | S(t_K) | n_1 \rangle$ the following expression can be written:

$$\begin{aligned} \langle n_2 | S(t_K) | n_1 \rangle &= \langle n_2 | n_1 \rangle + \int_{-\infty}^t dt_2 \int_{-\infty}^{t_2} dt_1 \langle n_2 | \tilde{S}(t_2, t_1) | n_1 \rangle \\ &= \langle n_2 | n_1 \rangle + \frac{\exp[-i(E_{n_1} - E_{n_2})t_K]}{E_{n_1} - E_{n_2} + i0} \langle n_2 | T(E_{n_1}) | n_1 \rangle. \end{aligned} \tag{9}$$

Substituting this expression into the unitarity condition (8) one can see the validity of expression (6). It should be noted that, if relationships (4) and (5) are considered separately, it appears that their choice as off-shell continuations of relationships (4) and (5) is somewhat arbitrary. Taken as a set, however, they eliminate this arbitrariness. A proof of this assertion is given in the appendix since this question has not been discussed before. Note that this proof is important for the development of the approach in question and for the rigorous justification of its equations.

Now, using (4) and (5), it can be shown that if some boundary-value condition were set for $T(z)$ then the equation

$$T(z_1) - T(z_2) = (z_2 - z_1)T(z_2)G_0(z_2)G_0(z_1)T(z_1) \quad (10)$$

could be used to determine this operator over the whole complex plane z . Using (3) it can be shown that

$$\langle n_2 | T(z) | n_1 \rangle \xrightarrow{z \rightarrow i\infty} \langle n_2 | B | n_1 \rangle \quad (11)$$

where $\langle n_2 | B | n_1 \rangle$ can be interpreted as an interaction Hamiltonian. In fact, in keeping with the superposition principle $\langle n_2 | \tilde{T}(\tau) | n_1 \rangle$ can be written in the form

$$\langle n_2 | \tilde{T}(\tau) | n_1 \rangle = \langle n_2 | B | n_1 \rangle \delta(\tau) + \langle n_2 | \tilde{T}'(\tau) | n_1 \rangle.$$

Here $\langle n_2 | B | n_1 \rangle \delta(\tau)$ describes a momentary interaction, $\langle n_2 | \tilde{T}'(\tau) | n_1 \rangle$ being the superposition of amplitudes, corresponding to the processes in which interaction lasts a finite time. Therefore, the amplitude $\langle n_2 | \tilde{T}'(0) | n_1 \rangle$ is equal to zero. Hence, the uniform Fourier transform (3) for $\langle n_2 | \tilde{T}'(\tau) | n_1 \rangle$ at $z \rightarrow i\infty$ tends to zero. From this expression (11) obviously follows.

2.3. Physical meaning of the T -matrix equation

Concerning the physical meaning of (10) it should be pointed out that in the case of non-relativistic potential scattering this relationship coincides in form with Hilbert's identity for the T matrix of the standard non-relativistic quantum theory of scattering, based on Hamiltonian formalism. In this connection we note the following. In terms of non-relativistic quantum theory, based on Hamiltonian formalism, this relationship follows from the determination of the T matrix with the help of the energy operator resolvent. In our approach the T matrix has a different definition, expressing the principles of causality and superposition (3), while (10), following from the general physical principles, has an entirely new physical content, as compared with Hilbert's identity. Then the interaction potential satisfies normal requirements of the Schrödinger theory, the Lippman-Schwinger (Gainutdinov 1983) and Schrödinger (Gainutdinov 1984) equations follow from (10) and the boundary-value condition. The T matrix, determined by (3), proves to be equivalent to the T matrix of the standard potential theory. However, in the general case, (10) may be valid even when the Schrödinger equation does not hold true. For example, describing scattering at a certain potential we can use as initial information the value $T(z)$ at arbitrary point $z = a$ of the complex plane z rather than the potential operator $V = T(i\infty)$. Obviously, $\langle q_2 | T(a) | q_1 \rangle$ as a function of the particle impulses q_1 and q_2 can be chosen in such a way (Gainutdinov 1983) that (10) with $z_2 = a$ will have a meaning and will permit both the calculation of $T(z)$ at all physical z values and the determination of bound states (Gainutdinov 1984), but no Lippman-Schwinger or Schrödinger equations will follow from it. In this case the T matrix bound with the S matrix cannot be determined with the help of the energy operator resolvent. Thus, the approach described in this paper permits

the consideration of models which have no analogues within the framework of Hamiltonian formalism.

3. Unstable bound states

3.1. Determination of an 'undressed' bound state

Let us consider the question of bound states of electrons in the nuclear field. We shall consider a system which contains a nucleus with a charge Z , electrons, positrons and photons. If the interaction with the radiation field is ignored, the T matrix on the negative real half-axis will have a number of poles corresponding to the principal one and to excited ionic states. However, owing to the fact that an electron in an excited state may radiate a photon while changing over into another state, all excited states prove to be unstable. What then is an unstable state in this case? Obviously, this is a bound state of the electrons with the nucleus which, in the absence of interaction of the electron with the radiation field, possesses all the properties of a stable particle. In the temporal translations $t \rightarrow t + a$ the vector describing this state will be transformed in the following way $|i, \mathbf{p}\rangle \rightarrow \exp[-i(E_p + E_i)a]|i, \mathbf{p}\rangle$. Here \mathbf{p} is the ion impulse and E_i is the energy of the i th bound state. A question arises as to how to determine E_i and $|i, \mathbf{p}\rangle$ if, in contrast to the stable bound state, the T -matrix poles do not correspond to the given state. However, an operator can be determined whose poles will correspond to unstable bound states. As has already been pointed out, $\langle \varphi_2 | S(t) | \varphi_1 \rangle$ is the superposition of amplitudes corresponding of all alternative probabilities of the event described by the amplitude $\langle \varphi_2 | S(t) | \varphi_1 \rangle$. One such possible process is that in which all the interaction within a system is confined to the Coulomb interaction of a certain electron with a nucleus. Let us determine the operator $S_K(t)$ as an operator whose matrix elements determine the amplitude of the probability that, if at $t \rightarrow -\infty$ the system state is $|\text{in}, \varphi_1\rangle$ and if all interaction in the system is confined to Coulomb interaction between the electrons and the nucleus and is over by the moment t , then at this moment t the system is found in the state $|t, \varphi_2\rangle$. Obviously, the operator $S_K(t)$ must satisfy the unitarity condition $\int_{\xi}^{\dagger} S_K(t) S_K(t) = 1$.

The operators $\tilde{T}_K(\tau)$ and $T_K(z)$ are determined accordingly. Similarly to the derivation of (10) the following relationship can be derived:

$$T_K(z_1) - T_K(z_2) = (z_2 - z_1) \times \sum_{\xi} \int \int \frac{T_K(z_2) | \mathbf{q}_1, \mathbf{q}_2, \xi \rangle \langle \mathbf{q}_1, \mathbf{q}_2, \xi | T_K(z_1) d^3 q_1 d^3 q_2}{(z_1 - \sqrt{q_1^2 + M^2} - \sqrt{q_2^2 + m^2} + i0)(z_2 - \sqrt{q_1^2 + M^2} - \sqrt{q_2^2 + m^2} + i0)} \quad (12)$$

where M and m are the nuclear and electron mass, respectively, q_1 is the nuclear impulse, q_2 is the electron impulse and ξ describes the nuclear and electron spin states. Obviously the boundary value for $\langle \varphi_2 | T_K(z) | \varphi_1 \rangle$ is the potential of the Coulomb interaction between the nucleus and an electron. A peculiarity of the operator $T_K(z)$ is the fact that it has poles corresponding not only to the ground state but also to the unstable excited bound states. Note that in their physical meaning the bound states $|i, \mathbf{p}\rangle$ are 'undressed' bound states.

3.2. Equation for bound states

The fact that the operator $T_K(z)$ has poles corresponding to bound states makes it possible to derive from (12) an equation determining both the stable ground and unstable excited states. The following equation may be derived in the same way as the T -matrix equation for bound states (Gainutdinov 1984)

$$(E_i - \sqrt{k^2 + M^2} - \sqrt{k^2 + m^2})\psi_i(\mathbf{k}, \xi_1) = (a - E_i) \sum_{\xi} \int d^3q \frac{R(a, \mathbf{k}, \mathbf{q}, \xi_1, \xi)\psi_i(\mathbf{q}, \xi)}{a - \sqrt{q^2 + M^2} - \sqrt{q^2 + m^2}} \quad (13)$$

$$\delta(\mathbf{k}'_1 + \mathbf{k}'_2)R(a; \mathbf{k}, \mathbf{q}, \xi_2, \xi_1) = \langle \mathbf{k}'_1, \mathbf{k}'_2, \xi_2 | T(a) | \mathbf{k}_1, \mathbf{k}_2, \xi_1 \rangle$$

$$\mathbf{k}_1 = -\mathbf{k}_2 = \mathbf{q} \quad \mathbf{k}'_1 = -\mathbf{k}'_2 = \mathbf{k}$$

where $\psi_i(\mathbf{k}, \xi)$ and E_i are the wavefunction and energies of the i th bound state, respectively. Equation (13) is virtually identical to the quasipotential Logunov-Tavkhelidze equation, describing a two-particle bound system (Logunov and Tavkhelidze 1963, Faustov 1970). So far we have considered bound states of one electron in the nuclear field, but one can also determine bound states of several electrons, interacting in the Coulomb manner with the nucleus and not interacting with one another. The vectors describing such states shall also be denoted $|i, \mathbf{p}\rangle$. In the non-relativistic approximations at $a \rightarrow i\infty$, the Schrödinger stationary equation follows from (13).

It should be pointed out that in the general case it is more convenient to redefine the states $|i, \mathbf{p}\rangle$ in such a way as to use Dirac's equation for their calculation. For this purpose $S_K(t_K)$ should be redefined so that it could describe, apart from the above-mentioned processes, also the processes of birth of electron-positron pairs in the Coulomb nuclear field.

3.3. Bound states and Coulomb interaction

As concerns the fact that $T_K(z)$ describes a Coulomb interaction, which does not meet the requirements of the standard quantum scattering theory, note that the long-ranging character of Coulomb interaction does not contradict defining $T_K(z)$ with the help of (3). Furthermore, this operator must satisfy relationship (10), which follows from fundamental physical principles. But at $z_2 \rightarrow i\infty$ the Lippman-Schwinger equation no longer follows from this relationship, since the Coulomb potential is not 'good' enough for this. In this case the boundary-value condition (11) does not seem to permit the introduction of all the data necessary for the determination of the T matrix with the help of (10). On the other hand, the stationary Schrödinger equation follows from (13) and from the boundary-value condition (11), allowing for the precise determination of the state vectors $|i, \mathbf{p}\rangle$, i.e. we obtain exactly what we need in this particular case. As to the description of scattering in the Coulomb interaction case, our approach may view it from a new standpoint. This question, however, has not yet been investigated.

Note also that the states $|i, \mathbf{p}\rangle$ coincide with the eigenstates of the Hamiltonian \mathcal{H}_0 when \mathcal{H}_1 in the expression

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

describes the interaction between the electrons and the radiation field and among themselves. Here \mathcal{H} is the complete Hamiltonian of the system. Formally, 'undressed' bound states could be thus defined, but then we would have to employ a rather artificial notion of turning off the interaction described by the Hamiltonian \mathcal{H}_1 .

4. The dynamics of unstable bound complexes

4.1. Equations describing the dynamics of unstable bound complexes

The bound states determined above are 'undressed' bound states. In order to determine the properties of real 'dressed' bound states, let us consider the interaction of the 'undressed' bound complexes with a vacuum. For this purpose let us in the first place redefine the notion of free states and consider the states described by the vectors $|i, \mathbf{p}\rangle$ to be free, although in this case the particles constituting an ion certainly interact. Accordingly, the notion of interaction in a system is also redefined. To describe such 'free' states the Hilbert space

$$\mathcal{H}_R = \mathcal{H} \oplus \mathcal{H}_U$$

is introduced, where \mathcal{H} is the Hilbert space whose elements describe the free states of the nucleus, electrons, positrons and photons, \mathcal{H}_U is the space whose elements describe the states containing, together with the atomic system, electrons, positrons and photons. Note that the operators $S(t)$ and $T(z)$ were determined in the space \mathcal{H} . In the space \mathcal{H}_R the operation $S_R(t)$ and the corresponding operator $T_R(z)$ may be determined in a similar manner. This operator satisfies the following relationship, which is the generalisation of (10) for this space:

$$\begin{aligned} T_R(z_1) - T_R(z_2) &= (z_2 - z_1) T_R(z_2) G_0(z_2) G_0(z_1) T_R(z_1) \\ G_0(z) &= \sum_n \sum_i \int d^3p \frac{|i, \mathbf{p}, n\rangle \langle i, \mathbf{p}, n|}{z - E_i - E_p - E_n + i0} + \sum_m \frac{|m\rangle \langle m|}{z - E_m + i0}. \end{aligned} \quad (14)$$

Here the $|m\rangle$ form an orthonormal basis in \mathcal{H} , and n denotes a set of discrete and continuous parameters, fully determining the states of the electrons, positrons and photons. Note that (14) includes the matrix elements $\langle i, \mathbf{p}_2 | T_R(z) | i, \mathbf{p}_1 \rangle$. Since the intermediate single-particle unstable states are in the continuous spectrum region, the nucleus of (14) is basically singular at physical z values. Therefore, one should go from (14) to another equation following from it. For this purpose let us rewrite (14) in the form

$$\begin{aligned} F(z_1) - F(z_2) &= (z_2 - z_1) F(z_2) F(z_1) \\ F(z) &= G_0(z) + G_0(z) T_R(z) G_0(z). \end{aligned} \quad (15)$$

The operator $G(z)$ is determined as follows:

$$\begin{aligned} \langle j, \mathbf{p}_2, n_2 | G(z) | i, \mathbf{p}_1, n_1 \rangle &= \langle j, \mathbf{p}_2, n_2 | G_0(z) | i, \mathbf{p}_1, n_1 \rangle + \delta_{ij} \langle n_2 | n_1 \rangle \\ &\quad \times \langle i, \mathbf{p}_2 | G_0(z - E_{n_1}) T_R(z - E_{n_1}) G_0(z - E_{n_1}) | i, \mathbf{p}_1 \rangle \end{aligned} \quad (16)$$

$$\begin{aligned} \langle m_2 | G(z) | m_1 \rangle &= \langle m_2 | G_0^F(z) | m_1 \rangle \\ &\equiv \langle m_2 | G_0(z) | m_1 \rangle + \langle m_2 | G_0(z) T_K(z) G_0(z) | m_1 \rangle. \end{aligned} \quad (17)$$

From this it follows that the matrix elements $\langle i, \mathbf{p}_2, n_2 | G(z) | i, \mathbf{p}_1, n_1 \rangle$ describe the system evolution when interaction in the system is reduced to the interaction of the bound complex with a vacuum. The matrix elements $\langle m_2 | G(z) | m_1 \rangle$ describe the system evolution when interaction in the system is reduced to the Coulomb interaction between the electrons and positrons and the nucleus, and for this reason coincides with the

corresponding matrix elements of the 'free' propagator in the Furry representation. The operator $F(z)$ can be represented in the form

$$F(z) = G(z) + G(z)M(z)G(z).$$

It follows from (15) that $G(z)$ satisfies the equation

$$\langle i, \mathbf{p}_2 | \{ G(z_1) - G(z_2) - (z_2 - z_1) \times [G(z_2)G(z_1) + G(z_2)M(z_2)G(z_2)G(z_1)M(z_1)G(z_1)] \} | i, \mathbf{p}_1 \rangle = 0. \quad (18)$$

In the general case $G(z)$ can be represented in the following form:

$$\langle i, \mathbf{p}_2, n_2 | G(z) | i, \mathbf{p}_1, n_1 \rangle = \frac{\delta(\mathbf{p}_2 - \mathbf{p}_1) \langle n_2 | n_1 \rangle}{z - E_i - E_{p_1} - E_{n_1} - \langle i, \mathbf{p}_1 | C(z - E_{n_1}) | i, \mathbf{p}_1 \rangle} \quad (19)$$

where $C(z)$, in keeping with (15), satisfies the equation

$$\begin{aligned} \langle i, \mathbf{p} | \{ C(z_1) - C(z_2) - (z_2 - z_1) M_\tau(z_2, z_1) \} | i, \mathbf{p} \rangle &= 0 \\ \delta(\mathbf{p}_2 - \mathbf{p}_1) \langle i, \mathbf{p}_2 | M_\tau(z_2, z_1) | i, \mathbf{p}_1 \rangle &= \langle i, \mathbf{p}_2 | M(z_2, z_1) | i, \mathbf{p}_1 \rangle. \end{aligned} \quad (20)$$

Here the operation $M(z_2, z_1)$ is determined as follows:

$$\begin{aligned} \langle i, \mathbf{p}_2, n_2 | M(z_2, z_1) | i, \mathbf{p}_1, n_1 \rangle \\ = \langle n_2 | n_1 \rangle \langle i, \mathbf{p}_2 | M(z_2 - E_{n_2}) G(z_2 - E_{n_2}) G(z_1 - E_{n_1}) M(z_1 - E_{n_1}) | i, \mathbf{p}_1 \rangle \\ \langle m | M(z_2, z_1) | \varphi \rangle = 0 \quad \langle \varphi | M(z_2, z_1) | m \rangle = 0 \end{aligned}$$

where $|\varphi\rangle \in \mathcal{H}_R$, $|m\rangle \in \mathcal{H}$. Taking into account (18) we obtain from (15) for $M(z)$ the following equation:

$$\begin{aligned} M(z_1) - M(z_2) - (z_2 - z_1) [M(z_2) G(z_2) G(z_1) M(z_1) \\ - M(z_2, z_1) G(z_1) M(z_1) - M(z_2) G(z_2) M(z_2, z_1)] = 0. \end{aligned} \quad (21)$$

It can be demonstrated that $M(z)$ and $C(z)$ satisfy the following boundary-value condition:

$$\lim_{z \rightarrow i\infty} \langle \psi_2 | M(z) | \psi_1 \rangle = \langle \psi_2 | H_1 | \psi_1 \rangle \quad (22)$$

$$\begin{aligned} \lim_{z \rightarrow i\infty} \delta(\mathbf{p}_2 - \mathbf{p}_1) \langle i, \mathbf{p}_2 | C(z) | i, \mathbf{p}_1 \rangle &= \lim_{z \rightarrow i\infty} \langle i, \mathbf{p}_2 | T(z) | i, \mathbf{p}_1 \rangle \\ &= \langle i, \mathbf{p}_2 | B | i, \mathbf{p}_1 \rangle \end{aligned} \quad (23)$$

where H_1 can be interpreted as the Hamiltonian of the electromagnetic interaction in the system, while $\langle i, \mathbf{p}_2 | B | i, \mathbf{p}_1 \rangle$ describes an instantaneous interaction of an ion with a vacuum. To calculate the matrix elements of the interaction Hamiltonian, the wavefunctions of bound states should be determined in the first place. For this purpose one can use (13). If the nucleus is viewed as the scattering centre, one can use the Dirac equation for the determination of the wavefunctions and E_i . The values of $\langle i, \mathbf{p}_2 | B | i, \mathbf{p}_1 \rangle$ are fully determined by the boundary value of the operator $C(z)$ describing interaction of the free electron with a vacuum. At the same time, as will be shown below, one can do without the determination of $\langle i, \mathbf{p}_2 | B | i, \mathbf{p}_1 \rangle$ in the approximate solution of (20) and (21).

4.2. Physical meaning of the operators $M(z)$ and $C(z)$

Let us now consider the questions concerning the physical meaning of the operators $C(z)$ and $M(z)$ and with the methods of solving (20) and (21). We shall view the nucleus as the scattering centre and the vectors describing the ion states will be designated $|i\rangle$. The matrix elements $\langle i|C(z)|i\rangle$ will be designated $C_i(z)$.

The matrix element $C_i(z)$ corresponding to the ion ground state determines the radiation shift of the lower level. If $|\text{Im } C_i(E_i)|$ is much less than the distance between this level and the closest level with the same \mathcal{J} , \mathcal{J}_z and parity, then the energy distribution of the corresponding excited state can be described by means of two-parameter representation. In this case $\text{Re } C_i(E_i)$ and $-\text{Im } C_i(z)$ can be interpreted as radiation shift and excited-level shift respectively. In the more general case no specific energy (not even a complex one) can be assigned to excited states and for this reason these states must be characterised by energy distributions, which define $C_i(z)$ as functions of z .

Let us consider ways of solving (20) and (21). In our first approach of the perturbation theory for $M(z)$ we get

$$M'(z) = H_1.$$

Substituting $M'(z)$ into (20) and taking into account the fact that $G(z)$ coincides with $G_0^F(z)$ in a zero approximation for the interaction constant in the Furry representation, for $C(z)$ to the second order, we get

$$C_i^{(2)}(z_1) - C_i^{(2)}(z_2) = \mathcal{A}_i(z_1) - \mathcal{A}_i(z_2) \tag{24}$$

$$\mathcal{H}_i(z) = \langle i|H_1 G_0^F(z) H_1|i\rangle - \langle 0|H_1 G_0^F(z - E_i) H_1|0\rangle. \tag{25}$$

The presence of the second term on the right-hand side of (25) is due to the fact that $C_i(z)$ describes the interaction of an ion with the vacuum and, therefore, it cannot be due to the vacuum-vacuum transitions, which should formally be accounted for in the first term of the right-hand side of (25). Letting z_2 tend to $i\infty$ in (24), we obtain for $C_i^{(2)}(E_i)$ in the case of a single-electron bound state

$$C_i^{(2)}(E_i) = \mathcal{A}_i(E_i) - \lim_{z \rightarrow i\infty} (\mathcal{A}_i(z) - C_i^{(2)}(z)). \tag{26}$$

This expression can be rewritten in the form

$$C_i^{(2)}(E_i) = -i\pi\alpha \int d(t_2 - t_1) d^3x_2 d^3x_1 \bar{\psi}_i(\mathbf{x}_2) \gamma_\mu S_F^e(\mathbf{x}_2, \mathbf{x}_1) \gamma^\mu \psi_i(\mathbf{x}_1) \mathcal{D}_F(\mathbf{x}_2 - \mathbf{x}_1) - B_i \tag{27}$$

$$B_i = \lim_{z \rightarrow i\infty} (\mathcal{A}_i(z) - C_i(z))$$

where $\mathcal{D}_F(\mathbf{x}_2 - \mathbf{x}_1)$ and $S_F^e(\mathbf{x}_2, \mathbf{x}_1)$ are, respectively, the photon and electron propagators in the Coulomb nuclear field and $\psi_i(\mathbf{x})$ is the Dirac wavefunction of the i th bound state in the coordinate representation. Equation (27) coincides with the normal expression for the radiation energy shift of quantum electrodynamics (Morh 1974) if B_i is interpreted as a counter term of renormalisation. Therefore, to calculate $C_i^{(2)}(E_i)$ one can use standard methods and the values obtained can subsequently be used as boundary-value conditions in (24), which enables one to obtain $C_i^{(2)}(z)$ at any z value. For bound states containing more than one electron, $C_i^{(2)}(E_i)$ apart from the self-energy

terms, contains members describing interaction between the electrons due to one-photon exchange. This results from the fact that in this case $\mathcal{A}_i(E_i)$ contains the terms describing the instantaneous Coulomb interaction between the electrons.

5. Spontaneous atomic system radiation

5.1. Non-perturbative methods of solution

First of all we would like to note that (20) and (21) make it possible to derive $C_i(z)$ and $M(z)$ without resorting to perturbation theory. An approximate solution of these equations may be obtained in the manner of Tamm–Dankov, cutting off the series over the number of particles in an infinite set of equations with a subsequent exact solution of this approximate set. For instance, if we confine ourselves to the accuracy of the order of α^2 , then in (20) and (21) the intermediate states containing more than one photon may be neglected. When the nuclear charge is sufficiently large, the autoionisation decay may also be neglected. For simplicity we shall also consider as intermediate states only the bound electron states and neglect the possibility of the appearance of electron-positron pairs. In this case (20) and (21) will no longer describe the energy level shift owing to the vacuum polarisation. Therefore, when going over to the simplified set, one must redefine E_i and include in them the energy shifts due to the vacuum polarisation which can be calculated using standard methods. Besides, E_i may include corrections allowing for the finite dimensions of the nucleus. It can be seen that within the framework of this model $\langle j; \mathbf{k}_2, \boldsymbol{\varepsilon}_{\lambda_2} | M(z) | i; \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1} \rangle$ and $\langle j | M(z) | i \rangle$ ($j \neq i$) which are solutions of (21) may be written in the form

$$\langle j; \mathbf{k}_2, \boldsymbol{\varepsilon}_{\lambda_2} | M(z) | i; \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1} \rangle = \sum_n \frac{M_{jn}^{(+)}(z, \mathbf{k}_2, \boldsymbol{\varepsilon}_{\lambda_2}) M_{ni}^{(-)}(z, \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1})}{z - E_n - C_n(z)} \quad (28)$$

$$\langle j | M(z) | i \rangle = \sum_n \sum_{\lambda} \int \frac{d^3 k}{2|k|} \frac{M_{jn}^{(-)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda}) M_{ni}^{(+)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda})}{z - E_n - |k| - C_n(z - |k|)} \quad (29)$$

$$M_{ij}^{(+)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda}) \equiv \langle i; \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda} | M(z) | j \rangle \quad M_{ij}^{(-)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda}) \equiv \langle i | M(z) | j, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda} \rangle$$

where \mathbf{k} and $\boldsymbol{\varepsilon}_{\lambda}$ are the photon impulse and polarisation vectors, respectively. It should be noted that (28) is the generalisation of the Breit–Wigner formula for the photon resonance scattering amplitude of the bound electron. Substituting (28) and (29) in (21) we obtain within the framework of this model the following equation for $M_{ji}^{(+)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda})$:

$$\begin{aligned} & M_{ij}^{(+)}(z_1, \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1}) - M_{ij}^{(+)}(z_2, \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1}) \\ &= (z_2 - z_1) \sum_l \sum_{n \neq j} \int \frac{d^3 k}{2|k|} [M_{in}^{(+)}(z_2, \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1}) G_n(z_2) M_{nl}^{(-)}(z_2, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda}) \\ &\quad \times G_l(z_2 - |k|) G_l(z_1 - |k|) M_{ij}^{(+)}(z_1, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda}) \\ &\quad + M_{in}^{(+)}(z_2, \mathbf{k}_1, \boldsymbol{\varepsilon}_{\lambda_1}) G_n(z_2) G_n(z_1) M_{nl}^{(-)}(z_1, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda}) \\ &\quad \times G_l(z_1 - |k|) M_{ij}^{(+)}(z_1, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda})] \end{aligned} \quad (30)$$

where $G_n(z) \equiv \langle n | G(z) | n \rangle$.

Similarly an equation may be written for $M_{ij}^{(-)}(z, \mathbf{k}, \epsilon_\lambda)$. These equations together with the equation

$$\begin{aligned} \tilde{C}_i(z_1) - \tilde{C}_i(z_2) = & (z_2 - z_1) \left[\sum_{j \neq i} \langle i | M(z_2) G(z_2) | j \rangle \langle j | G(z_1) M(z_1) | i \rangle \right. \\ & + \sum_j \sum_\lambda \int \frac{d^3 k}{2|\mathbf{k}|} (M_{ij}^{(-)}(z_2, \mathbf{k}, \epsilon_\lambda) G_j(z_2 - |\mathbf{k}|) G_j(z_1 - |\mathbf{k}|) M_{ji}^{(+)}(z_1, \mathbf{k}, \epsilon_\lambda) \\ & \left. - \langle i | H_1 G(z_2) | j; \mathbf{k}, \epsilon_\lambda \rangle \langle j; \mathbf{k}, \epsilon_\lambda | G(z_1) H_1 | i \rangle \right] \end{aligned} \quad (31)$$

where $\tilde{C}_i(z) \equiv C_i(z) - \langle i | C^{(2)}(z) | i \rangle$, form a closed set of difference equations, which allows the determination of $M_{ij}^{(+)}(z, \mathbf{k}, \epsilon_\lambda)$, $M_{ij}^{(-)}(z, \mathbf{k}, \epsilon_\lambda)$ and $C_i(z)$. The following boundary-value condition must be used together with (22) for this model:

$$\tilde{C}_i(z) \xrightarrow{z \rightarrow i\infty} 0. \quad (32)$$

Hence, it follows that at large $\text{Im } z$ values the perturbation theory in the solution of (20) and (21) proves to be also valid, and for sufficiently large $\text{Im } z$ values, with an accuracy of α^2 , the function $C_i(z)$ equals $C_i^{(2)}(z)$. It is from this that the boundary-value condition (32) follows.

It should be noted that the reason for writing (31) for $\tilde{C}_i(z)$ rather than for $C_i(z)$ is the fact that only in this case can we neglect the intermediate states containing electron-positron pairs and use the boundary-value condition (32). In fact, (31) describes the low-energy resonance part $C(z)$, while the high-energy relativistic contribution with a given accuracy is defined by $C_i^{(2)}(z)$.

5.2. Shape of a spontaneous radiation spectral line

As a result of interaction with vacuum the energy levels of bound states are 'spread out', which is expressed by the fact that the Green function $\langle i | G(z) | i \rangle$ of the 'dressed' bound state differs from $\langle i | G_0(z) | i \rangle$ in E_i being replaced by $E_i + C_i(z)$. Therefore, instead of the poles, $|\langle i | G(z) | i \rangle|$, corresponding to the excited states, have resonance maxima at z_i determining the energy-level centres. The energy levels themselves may be defined as z_i environments, in which $\langle i | G(z) | i \rangle$ have resonance behaviour. Note that $\langle i | G(z) | i \rangle$ together with the apical functions $M_{ji}^{(+)}(z, \mathbf{k}, \epsilon_\lambda)$ and $M_{ji}^{(-)}(z, \mathbf{k}, \epsilon_\lambda)$ provide all information on bound states, both stable and unstable. For example, they define the forms of spontaneous radiation spectral lines and their relative intensities. In order to show this, let us write an expression for the amplitude corresponding to a process during which an atomic system, as a result of interaction with a certain particle, becomes excited, passing from the ground state to the i th excited one, after which it emits a photon, passing into the ground state $|1\rangle$

$$\langle 1; \mathbf{k}, \epsilon_\lambda; \mathbf{p}' | S_i | 1; \mathbf{p} \rangle = -2\pi i \delta(E_k - z') \frac{\langle 1; \mathbf{k}, \epsilon_\lambda | M(z') | i \rangle \langle i; \mathbf{p}' | M(z) | 1; \mathbf{p} \rangle}{z' - E_i - C_i(z')} \quad (33)$$

$$z = E_p + E_1 \quad z' = z - E_{p'}.$$

Here $|\mathbf{p}\rangle$ describes the state of the particle which interacts with the atomic system. In keeping with the superposition principle the S matrix, corresponding to interaction between the atomic system and the exciting particle, may be written in the form

$$\langle \varphi_2 | S | \varphi_1 \rangle = \langle \varphi_2 | S_i | \varphi_1 \rangle + \langle \varphi_2 | \tilde{S}_i | \varphi_1 \rangle \quad (34)$$

where \tilde{S}_i describes all the processes during which at no moment of time is the atomic system in the i th bound state. It follows from (33) and (34) that the photon birth amplitude will have a resonance maximum at the photon energy value close to $E_i - E_1$. Note that in (33) the S -matrix element is already 'renormalised' and E_1 includes a radiation correction. When the width of this resonance is less than the characteristic interval of variations in the interaction of the atomic system with the exciting particle, then $\langle i; \mathbf{p}' | M(z) | 1, \mathbf{p} \rangle$ in (33) may be considered independent of z . In this case, one can write the following for the probability of a photon with an energy ω being emitted as a result of the system transition from the i th state into ground state:

$$\frac{dW_i(\omega)}{d\omega} = \mathcal{A} \omega \sum_{\lambda} \int d\Omega_{\kappa} \left| \frac{\langle 1, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda} | M(E_1 + \omega) | i \rangle}{E_1 + \omega - E_i - C_i(E_1 + \omega)} \right|^2 \quad (35)$$

where \mathcal{A} is the normalising constant. When the profile width is small enough, $M_{ji}^{(+)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda})$ and $C_i(z)$ can be also considered independent of z , and a normal Lorentzian radiation profile will be obtained. $\text{Re } C_i(E_i)$ defines the shift and $\text{Im } C_i(E_i)$ the spectral linewidth. But in the general case, when the quasistationary approximation is unjustified, the shape of a spontaneous radiation spectral line, according to (35), may differ significantly from the Lorentzian one and is determined in the resonance region by the dependence of $M_{ji}^{(+)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda})$ and $C_i(z)$ on z . As for the necessity to transcend the quasistationary approximation and perturbation theory, it appears when the energy levels with an identical set of quantum numbers overlap. This follows from the fact that according to (21) and (31) $M_{ji}^{(+)}(z, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda})$ and $C_i(z)$ have resonance behaviour at z corresponding to the centres of neighbouring levels with an identical set of quantum numbers.

To investigate the dependence of the spontaneous radiation of atomic systems on the overlapping of energy levels with the same set of quantum numbers, we carried out (Gainutdinov and Salakhov 1987) a numerical solution of (30) and (31) for the model three-level system with a Hamiltonian

$$\begin{aligned} \langle 1, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda} | H_1 | i \rangle &= -i l (2\pi)^{-3/2} \mathbf{k} \boldsymbol{\varepsilon}_{\lambda}(\mathbf{k}) \langle 1 | \tau | i \rangle f(\omega) & i = 2, 3 \\ f(\omega) &= 1 \text{ at } \omega < k_0 & f(\omega) = k_0^2 / \omega^2 \text{ at } \omega \geq k_0 & \omega = |\mathbf{k}|. \end{aligned} \quad (36)$$

Here $\langle 1, \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda} | H_1 | i \rangle$ describe transitions between two excited states, with the same quantum numbers, and the ground state. The following values were used as initial information:

$$\Gamma_i = -2 \text{Im } C_i(E_i) = 2\pi \int |\langle 1; \mathbf{k}, \boldsymbol{\varepsilon}_{\lambda} | H_1 | i \rangle|^2 \delta(E_i - E_1 - |\mathbf{k}|) \frac{d^3 k}{2|\mathbf{k}|}$$

$\text{Re } C_i^{(2)}(E_i)$ being included in the E_2 and E_3 excited-level energies. The solution of (30) and (31) was carried out in non-dimensional units ($c = \hbar = 1$, $\alpha = 1/137$, $E_1 = 0$, $E_2 = 100$, $E_3 = E_2 + \Delta E_{23}$, $|\langle 1 | \tau | i \rangle| = 0.001$). The value of ΔE_{23} was varied in the units Γ_2 : $\Delta E_{23} = \beta \Gamma_2$. A material difference of $dW_i(\omega)/d\omega$ profile shapes from the Lorentzian one was observed at $\beta \leq 3$. In this case one must go beyond not only the quasistationary approximation but also beyond perturbation theory. Figure 1 shows the variation of $dW_i(\omega)/d\omega$ profile shapes depending on the parameter β when $k_0 = 101$.

Note that shape of a natural spectral line broadening in the case of overlapping energy levels was also investigated in the theory of the adiabatic S matrix (Labazovsky 1983, Labazovsky and Sultanaev 1986). To investigate the decay of unstable bound states in the adiabatic theory as well as in Heitler's theory 'unperturbed' bound states

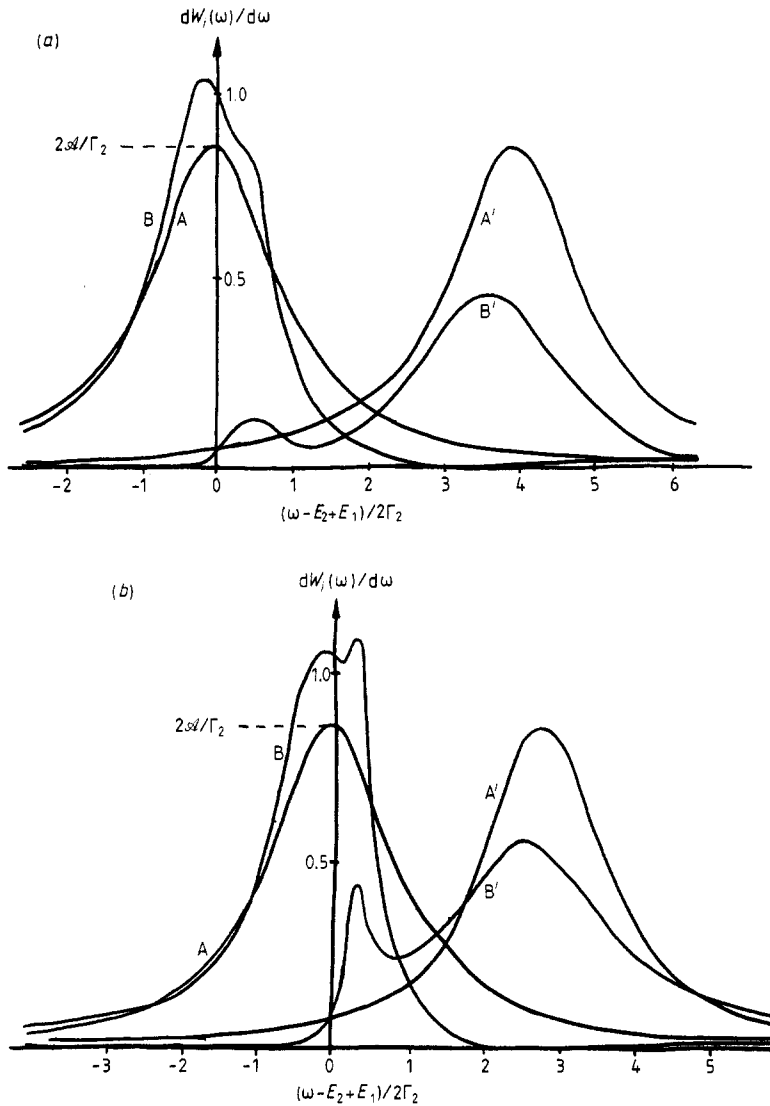


Figure 1. The dependence of profile shapes during the variation of level overlapping for (a) $\beta = 2.0$ and (b) $\beta = 1.5$. Curves A and A' are Lorentzian profiles; curves B and B' are computed profiles at $k_0 = 101$.

are used as initial states $|\psi_i, t = 0\rangle$. Therefore, the results of this theory are valid only in the case when the overlapping is not strong.

5.3. Ultraviolet divergences and their elimination

The most serious difficulty that has to be overcome in using this formalism is caused by the ultraviolet divergences. In terms of the relativistic theory of atoms in calculating by perturbation theory the problem of divergence elimination is solved for each order of perturbation theory. In the non-perturbative solution of equations (20) and (21) the problem of ultraviolet divergences has to be solved for each approximation

individually. Let us consider, e.g., an approximation to which equations (30) and (31) correspond. These equations contain no divergences. This is due to the fact that (30) makes no allowance for intermediate states containing free electrons, and equation (31) is written for $\tilde{C}_i(z)$. We encounter ultraviolet divergences only when calculating $C_i^{(2)}(z)$. One method of overcoming this difficulty has already been mentioned. One may ignore the dependences of $C_i^{(2)}(z)$ on z and use the value $C_i^{(2)}(E_i)$, which can be calculated by standard methods. However, $C_i^{(2)}(z)$ can be determined more precisely. One can write

$$C_i^{(2)}(z) \equiv C_{Ri}^{(2)}(z) + \langle i | \Sigma^{(2)}(z) | i \rangle$$

where $\Sigma^{(2)}(z)$ is self-energy operator (in second-order perturbation theory) of the free electrons and positrons. This operator satisfies the equation

$$\langle i | \Sigma^{(2)}(z_1) | i \rangle - \langle i | \Sigma^{(2)}(z_2) | i \rangle = (z_2 - z_1) \sum_m \frac{\langle i | H_1 | m \rangle \langle m | H_1 | i \rangle}{(z_2 - E_m + i0)(z_1 - E_m + i0)} \quad |m\rangle \in \mathcal{H}.$$

Using this relationship, (24) may be rewritten in the form

$$\begin{aligned} C_{Ri}^{(2)}(z_1) - C_{Ri}^{(2)}(z_2) &= (z_2 - z_1) \left(\langle i | H_1 G_0^F(z_0) G_0^F(z_1) H_1 | i \rangle \right. \\ &\quad \left. - \sum_m \frac{\langle i | H_1 | m \rangle \langle m | H_1 | i \rangle}{(z_2 - E_m + i0)(z_1 - E_m + i0)} - \langle 0 | H_1 G_0^F(z_2 - E_i) G_0^F(z_1 - E_i) H_1 | 0 \rangle \right). \end{aligned} \quad (37)$$

This equation no longer contains any divergences and $C_i^{(2)}(E_i)$ may be used as a boundary-value condition at $z = E_i$. It remains to determine $\langle i | \Sigma^{(2)}(z) | i \rangle$. The standard methods of quantum electrodynamics determine $\langle i | \Sigma^{(2)}(z) | i \rangle$ only at $z = E_i$. Thus for a one-electron state we get

$$\langle i | \Sigma^{(2)}(E_i) | i \rangle = i \int \bar{\varphi}_i(\mathbf{p}) \Sigma_R(\mathbf{p}) \varphi_i(\mathbf{p}) d^3p$$

where $\varphi_i(\mathbf{p})$ is the bound-state wavefunction in impulse space and $\Sigma_R(\mathbf{p})$ is the regularised part of the self-energy operator. Note that in a more exact approximation, when equation (20) allows for states containing free electrons, this equation will contain ultraviolet divergences. These divergences may be eliminated by the above method. One can make sure of this if it is borne in mind that a solution of equation (20) $\langle i | M(z) | \varphi \rangle$ may be sought in the following form:

$$\langle i | M(z) | \varphi \rangle = \sum_j \langle i | \tilde{M}(z) | j \rangle \langle j | H_1 | \varphi \rangle \quad | \varphi \rangle \in \mathcal{H}_R.$$

Substituting this expression into (20), one can obtain an equation for a $\langle i | \tilde{M}(z) | j \rangle$. The divergences in this equation, just as in equation (31), are due to the expression

$$\langle i | H_1 G_0^F(z_2) G_0^F(z_1) H_1 | j \rangle$$

that it incorporates.

6. Conclusion

Now let us summarise. Unstable bound states are defined as follows. The concept of 'undressed' bound states of electrons in a nuclear field is introduced. These states are

determined by the position and deduction of the poles of the $\langle \varphi_2 | S_K | \varphi \rangle$ matrix corresponding to the alternative variant of electron scattering in the nucleus, during which the electrons interact with the nucleus only and do not interact with one another or with their own radiation field. Thus defined 'undressed' states prove to be equivalent to the stationary states defined by the Dirac and Schrödinger equations, with an interaction Hamiltonian describing only the interaction between electrons and the nucleus. In order to determine 'dressed' bound complexes, the interaction between 'undressed' bound complexes and a vacuum is considered. Equations have been obtained enabling the determination of the operator $C(z)$, characterising the energy distributions of unstable bound states, and of the operator $M(z)$, describing spontaneous radiation, the autoionisation decay of unstable states and various collision processes.

Equations (20) and (21) are a generalisation of the normal equations of the Green function method. Indeed, from (19) it follows that

$$\langle i | G(z) | i \rangle = \langle i | G_0(z) | i \rangle + \langle i | G_0(z) C(z) G(z) | i \rangle. \quad (38)$$

In the case of a one-electron atomic system this coincides with Dyson's equation, whereas in the two-electron case it coincides with the Bethe-Salpeter equation for Green functions. These equations make possible the determination of Green function of an atomic system when the mass operator can be calculated with the help of the perturbation theory, e.g. by formula (27). When the energy levels overlap, the apical functions $M_{ij}^{(+)}(z, \mathbf{k}, \epsilon_\lambda)$, in keeping with (30), have resonance maxima at z , corresponding to the neighbouring levels. In this case $M_{ij}^{(+)}(z, \mathbf{k}, \epsilon_\lambda)$ and accordingly $C_i^{(2)}(z)$ cannot be determined with the help of the perturbation theory, and the Dyson and Bethe-Salpeter equations, unlike (20) and (21), are unclosed.

In this approach both unstable and stable bound states are considered from the same point of view. The difference between them is reduced to the fact that the propagator of the 'dressed' ground state $\langle 1 | G(z) | 1 \rangle$ has a pole in the physical field. The operators $G(z)$ and $M(z)$ describing unstable bound states provide the same information as vector (1). In fact the Green function of state (1) may be written as

$$\langle \varphi_i | G(z) | \varphi_i \rangle = \int \frac{a_i^*(E) a_i(E)}{(z - E + i0)} dE.$$

Thus, knowing $G(z)$ one can determine the density of the energy distribution $\omega_i(E) = a_i^*(E) a_i(E)$, the data on $|\psi_i, E\rangle$ being contained in the apical functions $M_{ij}^{(+)}(z, \mathbf{k}, \epsilon_\lambda)$. In a quasistationary limit, when $\text{Im } C_i(z) = -\Gamma_i/2$ can be set for the energy distribution density, we get

$$\omega_i(E) = 2\Gamma_i / [4(E - E_i)^2 + \Gamma_i^2].$$

As for the application of this approach, it is in the first place a multicharge-ion theory. For example, it can be used to determine the exact shape of the natural widening of the spectral lines corresponding to the doubly excited states of ions with very large charges (in this case the energy levels with the same \mathcal{J} , \mathcal{J}_z and parity may overlap).

Note in this connection the great importance of theoretical and experimental investigations of doubly excited states of heavy multicharge ions. Interaction of atomic systems in these states with a vacuum may be strong. Therefore, the data on the shape of the spectral lines corresponding to transitions from these states may contain information on unperturbed quantum electrodynamic effects.

This approach may also be used for the investigation of the autoionisation states of atoms. Besides, it enables one to calculate the amplitudes of resonance scattering of photons in bound electrons (28) when the Breit-Wigner formula cannot be used and one must go beyond perturbation theory. This situation may arise in the case of the autoionisation states of ions with a small charge and in the case of ions with a very large charge, when overlapping of energy levels with an identical set of principal quantum numbers takes place. It should be noted that when the quasistationary condition is fulfilled, equations (20) and (21) appear to be non-competitive in comparison with the standard methods and yield the same results.

One may hope that this approach could be used in the investigation of vacuum restructuring in the vicinity of nuclei with a supercritical charge ($z > 170$), but it is not clear what difficulties may arise in the process.

Acknowledgments

The author would like to express his gratitude to Professors L N Labozovsky, R N Faustov and V Ya Fainberg for their discussions and helpful remarks.

Appendix

From equation (19), taken from Gainutdinov (1987), it follows that

$$\begin{aligned} \mathcal{A}_1^+(z_2, z_1) T(z_1) G_0(z_1) - \mathring{G}_0^+(z_2) \mathring{T}^+(z_2) \mathcal{A}_1^+(z_1, z_2) \\ - \mathring{G}_0^+(z_2) \mathring{T}^+(z_2) \mathring{G}^+(z_2, z_1) T(z_1) G_0(z_1) = 0 \end{aligned} \quad (\text{A1})$$

$$\mathring{G}^+(z_2, z_1) = G_0(z_1) - \mathring{G}_0^+(z_2).$$

Similarly, proceeding from (7), it can be shown that the relationship

$$\begin{aligned} G_0(z_1) T(z_1) \mathcal{A}_2^+(z_2, z_1) - \mathcal{A}_2^+(z_1, z_2) \mathring{T}^+(z_2) \mathring{G}_0^+(z_2) \\ - G_0(z_1) T(z_1) \mathring{G}^+(z_2, z_1) \mathring{T}^+(z_2) \mathring{G}_0^+(z_2) = 0 \end{aligned} \quad (\text{A2})$$

is also valid. In relationships (A1) and (A2) $\mathcal{A}_1(z_1, z_2)$ and $\mathcal{A}_2(z_1, z_2)$ are the arbitrary operators, satisfying the conditions

$$\mathcal{A}_1(z_1, z_2) - \mathcal{A}_1^+(z_2, z_1) = \mathcal{A}_2(z_1, z_2) - \mathcal{A}_2^+(z_2, z_1) = \mathring{G}^+(z_2, z_1) \quad (\text{A3})$$

$$\langle n_2 | \mathcal{A}_1(E_{n_1}, z) | n_1 \rangle = \langle n_2 | G_0(E_{n_1}) | n_1 \rangle \quad (\text{A4})$$

$$\langle n_2 | \mathcal{A}_2(E_{n_2}, z) | n_1 \rangle = \langle n_2 | G_0(E_{n_2}) | n_1 \rangle. \quad (\text{A5})$$

However, it follows from the compatibility condition of (A1) and (A2) that

$$\mathcal{A}_1(z_2, z_1) = \mathcal{A}_2(z_2, z_1) = G_0(z_2). \quad (\text{A6})$$

In order to demonstrate this, let us assume that interaction in the system is weak enough and $T(z)$ can be expanded into a series of terms of the interaction constant

$$T_1(z, \lambda) = \lambda B_1(z) + \lambda^2 B_2(z) + \dots + \lambda^n B_n(z) + \dots \quad (\text{A7})$$

Substituting (A7) into (A1) and (A2) to first order in terms of λ we get

$$\langle n_2 | \{ \mathring{F}_1^+(z_2, z_1) B_1(z_1) - \mathring{B}_1^+(z_2) F_1(z_1, z_2) \} | n_1 \rangle = 0 \quad (\text{A8})$$

$$\langle n_2 | \{ B_1(z_1) \mathring{F}_2^+(z_2, z_1) - F_2(z_1, z_2) \mathring{B}_1^+(z_2) \} | n_1 \rangle = 0$$

$$F_1(z_1, z_2) \equiv \mathcal{A}_1(z_1, z_2) G_0^{-1}(z_1) \quad (A9)$$

$$F_2(z_1, z_2) \equiv G_0^{-1}(z_1) \mathcal{A}_2(z_1, z_2).$$

This follows from the fact that equations (A8) and (A9) must be fulfilled at any values of z_1 and z_2 that

$$\langle n_2 | F_1(z_1, z_2) | n_1 \rangle = \varphi_1(z_1, z_2) \langle n_2 | F_1(z_1) | n_1 \rangle$$

$$\langle n_2 | F_2(z_1, z_2) | n_1 \rangle = \varphi_2(z_1, z_2) \langle n_2 | F_2(z_1) | n_1 \rangle$$

where $\varphi_1(z_1, z_2)$ and $\varphi_2(z_1, z_2)$ are the arbitrary functions z_1 and z_2 , satisfying the condition

$$\varphi_{1,2}(z_1, z_2) = \varphi_{1,2}^*(z_2, z_1).$$

From relation (A3) it follows that

$$\langle n_2 | F_{1,2}(z_1) G_0(z_1) | n_1 \rangle = \langle n_2 | \overset{\dagger}{F}_{1,2}(z_2) \overset{\dagger}{G}_0(z_2) | n_1 \rangle \quad n_2 \neq n_1$$

$$\langle n | R_{1,2}(z_1, z_2) G_0(z_1) | n \rangle = \langle n | \overset{\dagger}{R}_{1,2}(z_2, z_1) \overset{\dagger}{G}_0(z_2) | n \rangle$$

$$F_{1,2}(z_1, z_2) \equiv 1 + R_{1,2}(z_1, z_2).$$

Hence

$$\langle n_2 | F_{1,2}(z_1) G_0(z_1) | n_1 \rangle = \langle n_2 | \overset{\dagger}{F}_{1,2}(E_{n_2}) \overset{\dagger}{G}_0(E_{n_2}) | n_1 \rangle = 0 \quad n_1 \neq n_2$$

$$\langle n | R_{1,2}(z_1, z_2) | n \rangle = \langle n | \overset{\dagger}{R}_{1,2}(z_1, z_2) | n \rangle.$$

Thus

$$\text{Im} \langle n | R_{1,2}(z) | n \rangle = 0$$

$$\langle n_2 | F_{1,2}(z) | n_1 \rangle = 0 \quad n_2 \neq n_1$$

and equations (A8) and (A9) can be rewritten in the form

$$\psi_1(z_2, E_{n_2}) \langle n_2 | B_1(z_1) | n_1 \rangle - \psi_1(z_1, E_{n_1}) \langle n_2 | \overset{\dagger}{B}_1(z_2) | n_1 \rangle = 0$$

$$\psi_2(z_2, E_{n_1}) \langle n_2 | B_1(z_1) | n_1 \rangle - \psi_2(z_1, E_{n_2}) \langle n_2 | \overset{\dagger}{B}_1(z_2) | n_1 \rangle = 0$$

$$\psi_{1,2}(z, E_{n_1}) \langle n_2 | n_1 \rangle \equiv \langle n_2 | F_{1,2}(z) | n_1 \rangle \quad \psi_{1,2}(z, z) = 1.$$

Hence it follows that

$$\psi_1(z_2, E_{n_2}) / \psi_1(z_1, E_{n_1}) = \psi_2(z_2, E_{n_1}) / \psi_2(z_1, E_{n_2}).$$

If (A4) and (A5) are taken into account, then it can be easily seen that (A6) follows from this expression. Therefore, equations (A1) and (A2) may be rewritten in the form of expressions (4) and (5).

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