# Energy level splitting of multicharged ions due to interaction of the ion with its own radiation field

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The overlapping of the energy levels of He-like uranium states with identical principal quantum numbers is investigated. Results are presented of a numerical calculation of the states produced as a result of mixing of the $2s_{1/2}\,8p_{1/2}$ and $2p_{1/2}\,8s_{1/2}$ states and of the respective spectral lines. It is shown that the interaction between the ion and its own radiation field splits each of the overlapping energy levels into several sublevels. The sublevels are isolated from each other to such an extent that interference effects become insignificant. The shapes of the spectral lines differ substantially from the Lorentz shape and many of the lines are anomalously narrow.

## 1. INTRODUCTION

Recently quantum-electrodynamic effects in the fields of superheavy, multiply charged ions have been the object of intense interest. In such fields certain features of the electrodynamic interactions can be manifested which are not manifested in fields created by relatively small charges. Thus, in the case of superheavy multicharged ions overlapping of the energy levels having identical total angular momentum $J$, projection $J_z$, and parity can take place. For such states the quasistationary condition is violated. In this case the shape of the natural broadening of the spectral lines corresponding to transitions to such states can differ substantially from the Lorentzian. Questions concerning the shape of natural broadening of the spectral lines and problems associated with the overlapping of energy levels were investigated in Refs. 1–5.

In the present work we have carried out an investigation of doubly excited states of He-like uranium and the shape of natural broadening of the corresponding spectral lines. We have used the method for describing unstable states developed in Refs. 4 and 5. It will be shown that in the case of overlap of energy levels with identical quantum numbers the interaction of the ion with its own radiation field splits them into several quite well isolated sublevels. In light of the fact that the theory of overlapping energy levels of atomic systems has been developed only recently and much here is still unclear, we have attempted here to clarify some aspects of this problem which are important for understanding the results obtained in this work.

## 2. UNSTABLE STATES OF ATOMIC SYSTEMS AND METHODS FOR THEIR DESCRIPTION

Let us consider the question of the existence of unstable electron bound states in the field of the nucleus and how their properties are manifested through observable quantities. In contrast to the case of stable states, a definite energy (in general this energy can even be complex) cannot be assigned to the unstable states, and the problem of their determination no longer reduces to the determination of the eigenvalues of the energy. In general, an unstable state must be characterized by some energy distribution[6]

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

where $|\varphi,E\rangle$ is an eigenvector of the energy operator. The Green's function of such a state is given by

$$\langle\psi_i|G(z)|\psi_i\rangle = \int \frac{a_i^*(E)\,a_i(E)}{z-E+i0}\,dE. \qquad (2)$$

Thus, an unstable state can be characterized by an energy distribution or the corresponding Green's function. So there arises the problem of determining such energy distributions. The Schrödinger, Dirac, and Schwinger equations, obviously, are not suitable for this purpose. Because of the difficulties associated with a consistent description of unstable states, the question can be raised whether there is any sense in a general consideration of such states, since in principle the description of any physical process can be reduced to the calculation of the $S$-matrix of the initial and final states, which contain only stable particles. But, in the first place, the lifetime of such states can be even greater than those of ordinary quasistationary states, wherefore their properties are no less important than those of any of the excited states of an atomic system. Second, the calculation of the elements of the $S$-matrix which describe the resonant scattering itself requires a knowledge of the properties of the unstable state to which the given resonance corresponds.

Let us consider, for example, the scattering of a photon by an atomic system. For simplicity we take a hydrogen-like ion. We denote by $E_i$ the energies of the bound states of the ion, determined without taking account of their interaction with the self radiation field of the ion. For photon energies $\omega$ near $E_i - E_1$ the scattering amplitude has a resonance (here $E_1$ in the energy of the ground state), and if we do not take into account the interaction with the radiation field, then this amplitude becomes infinite. Obviously, in the resonance region it is necessary in the calculation of such matrix elements to depart from the framework of perturbation theory. Even though nonperturbative methods have been developed in quantum electrodynamics, calculating these amplitudes in the resonance region without using the idea of the unstable intermediate state to which the given resonance corresponds runs into enormous difficulties since in this case it becomes necessary to consider the interaction of the electrons with the radiation field in addition to their interaction with the nucleus.

The usual way of overcoming this difficulty is the fol-

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lowing. In the calculation of the scattering amplitude, for the basis set one usually uses the wave functions of the electron in the field of the nucleus (the Furry representation), which already contains this interaction within itself. To calculate the photon scattering amplitude in such a basis, a perturbation theory is constructed which describes the interaction of the atomic system with the radiation field.

To second order in the perturbation theory, in this case we obtain a formula accurate to $\alpha^2$ which describes the scattering of a photon by a bound electron

$$\langle n_2|S^{(2)}|n_1\rangle=-2\pi i\delta(E_{n_2}-E_{n_1})\sum_n\frac{\langle n_2|H_{\text{int}}|n\rangle\langle n|H_{\text{int}}|n_1\rangle}{E_{n_1}-E_n+i0}. \tag{3}$$

Here $H_{\text{int}}$ is the Hamiltonian of the electrodynamic interaction in the system, the vectors $|n\rangle$ form an orthonormal set of eigenvectors of the Hamiltonian $H'=H_0+H'_{\text{int}}$, where $H'_{\text{int}}$ describes the Coulomb interaction of the electrons with the nucleus, and $n$ is the entire set of discrete and continuous parameters which characterize the state $|n\rangle$.

In the description of resonant scattering from all the intermediate states it is sufficient to take into account only the bound state to which the given resonance corresponds (let this be the $i$th state). True, in this case the amplitude becomes infinite at $\omega=E_i-E_1$, but this difficulty is easily overcome by taking account of the fact that the system in the $i$th state interacts continuously with the vacuum.

There are various ways to take this interaction into account. In the method proposed in Ref. 7, Eq. (3) is modified by introducing the exact Green's function of the electron, as a result of which the matrix element becomes finite at $\omega=E_i-E_1$. Another method, leading to the same results, consists in summing an infinite series of graphs which describe the interaction of the bound electron with the vacuum.[1,8]

When the distance between the energy levels of two states with identical total angular momentum $J$, projection $J_z$, and parity is not large in comparison with the widths of the levels, it is necessary in the resonance approximation to take both intermediate states into account. In the description of the interaction of such states with the photon field it is also necessary to allow for the presence of a neighboring intermediate state and to sum over not only the terms of the perturbation theory series describing the interaction of the atomic system with the vacuum, but also those terms which describe transitions between these states due to the interaction of the ion with its own radiation field.[1,2]

At first glance it would appear that such an approach allows one to determine the amplitude of the scattering of the photon by the bound electron exactly. However, this is not the case. The reason is that the eigenvectors of the Hamiltonian $H'$ used as the basis set do not form a complete set of vectors in the Hilbert space of states of the given problem, since $H'$ differs from the true Hamiltonian $H$ by the absence of those terms which describe the interaction with the radiation field. The physical essence of the given approximation is that it assumes that the interaction of the bound electron with the self radiation field does not alter the wave functions of the given electron in the Coulomb field of the nucleus.

Since the eigenvectors of the Hamiltonian $H'$ do not form a complete set of vectors in the Hilbert state space $\mathscr{H}$, we must supplement this set with vectors from $\mathscr{H}$ orthogonal to the eigenvectors of the Hamiltonian $H'$. In the case in which the energy levels of states with identical principal quantum numbers overlap, as will be shown below, it is no longer possible to neglect such vectors. In this case, to calculate the resonance scattering it is necessary to use as the intermediate states the unstable states determined without resorting to the quasistationary approximation.

In Refs. 4 and 5 an approach to the theory of unstable states of atomic systems was proposed which allows one to describe these states without resorting to the quasistationary approximation or to perturbation theory. This approach makes use of the formalism of the relativistic $T$-matrix developed in Refs. 5, 9, and 10. The essence of the method consists in the following. The "undressed" bound states are defined as the bound states of the electrons in the field of the nucleus in the case in which all the interactions in the system reduce to the Coulomb interaction of the electrons with the nucleus. The real unstable states are obtained from these states by taking account of the interaction of the atomic system with the vacuum, i.e., the interaction of the electrons with the radiation self-field and vice versa. In Refs. 4 and 5 equations were obtained which describe the interaction of the atomic system with the vacuum and which allow one to determine the Green's function of the unstable states. These equations are difference equations in the operators $M(z)$, which describes spontaneous emission, autoionization decay, and various collisional processes, and $C(z)$, which characterizes the energy distribution and is associated with the Green's function, and have the following form:[5]

$$\begin{aligned}&M(z_1)-M(z_2)-(z_2-z_1)[M(z_2)G(z_2)G(z_1)M(z_1)\\&-M(z_2,z_1)G(z_1)M(z_1)-M(z_2)G(z_2)M(z_2,z_1)]=0,\end{aligned} \tag{4}$$

$$\langle i,\mathbf{p}|\{C(z_1)-C(z_2)-(z_2-z_1)M_\tau(z_2,z_1)\}|i,\mathbf{p}\rangle=0. \tag{5}$$

Here we have introduced the following notation:

$$\begin{aligned}&\langle i,\mathbf{p}_2,n_2|M(z_2,z_1)|i,\mathbf{p}_1,n_1\rangle\\&\quad=\langle n_2|n_1\rangle\langle i,\mathbf{p}_2|M(z_2-E_{n_2})G(z_2-E_{n_2})\\&\quad\times G(z_1-E_{n_1})M(z_1-E_{n_1})|i,\mathbf{p}_1\rangle,\\&\qquad\langle m_2|G(z)|m_1\rangle=\langle m_2|G^F(z)|m_1\rangle,\ |m\rangle\in\mathscr{H},\\&\quad\langle\varphi|M(z_2,z_1)|m\rangle=0,\ \langle m|M(z_2,z_1)|\varphi\rangle=0,\ |\varphi\rangle\in\mathscr{H}_u,\\&\delta(\mathbf{p}_2-\mathbf{p}_1)\langle i,\mathbf{p}_2|M_\tau(z_2,z_1)|i,\mathbf{p}_1\rangle=\langle i,\mathbf{p}_2|M(z_2,z_1)|i,\mathbf{p}_1\rangle,\end{aligned}$$

$\mathscr{H}_u$ is the Hilbert space whose elements describe the states which contain along with the atomic system the electrons, positrons, and photons. The operator $G^F(z)$ is a "free" propagator in the Furry representation. The space $\mathscr{H}_R$, in which the operators $M(z)$, $G(z)$, and $C(z)$ are defined, is the space of asymptotic states:[5]

$$\mathscr{H}_R=\mathscr{H}_u\oplus\mathscr{H}.$$

In this space the bound complexes correspond to vectors orthogonal to the vectors from the space of free particles $\mathscr{H}$. The boundary conditions for Eqs. (4) and (5) have the form

$$\lim_{z\to i\infty}\langle\psi_2|M(z)|\psi_1\rangle=\langle\psi_2|H_{\text{int}}|\psi_1\rangle. \tag{6}$$

Note that the problem of describing the interaction of the atomic system with the vacuum does not differ in any essential way from the quantum-electrodynamic problem of describing the process of "dressing" the electron due to the interaction of the "undressed" electron with the vacuum. In connection with this, note that Eqs. (4) and (5) are a particular case of the equations obtained in Ref. 10, which describe the interaction of elementary particles with the vacuum. An important feature of the equations of this method is that they allow one to determine the operators $M(z)$ and $C(z)$ without resorting to perturbation theory.

As for the fact that this system of equations is in general infinite, an approximate solution can be found by a method analogous to the Tamm-Dankov method, by truncating the number of particles. For example, if we limit ourselves to accuracy of the order of $\alpha^2$ and ignore the possibility of ionization and the creation of electron-positron pairs, then for

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

$$M_{ij}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)=\langle i|M(z)|j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda\rangle,\qquad C_i(z)=\langle i|C(z)|i\rangle$$

it is possible to obtain a closed system of equations[5]

$$\begin{aligned}
&M_{ij}^{(+)}(z_1,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)-M_{ij}^{(+)}(z_2,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)\\
&\quad=(z_2-z_1)\sum_{n\neq j}\sum_{l}\int\frac{d^3k}{2|\mathbf{k}|}[M_{in}^{(+)}(z_2,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)\\
&\quad\times G_n(z_2)M_{nl}^{(-)}(z_2,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)G_l(z_2\\
&\quad-|\mathbf{k}|)G_l(z_1-|\mathbf{k}|)M_{lj}^{(+)}(z_1,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)\\
&\quad+M_{in}^{(+)}(z_2,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)G_n(z_2)G_n(z_1)M_{nl}^{(-)}\\
&\quad\times(z_1,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)G_l(z_1-|\mathbf{k}|)M_{lj}^{(+)}(z_1,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)],
\end{aligned}\tag{7}$$

$$\begin{aligned}
&C_i(z_1)-C_i(z_2)=(z_2-z_1)\\
&\qquad\times\Big[\sum_{j\neq i}\langle i|M(z_2)G(z_2)|j\rangle\langle j|G(z_1)M(z_1)|i\rangle\\
&\qquad+\sum_{j}\int\frac{d^3k}{2|\mathbf{k}|}M_{ij}^{(-)}(z_2,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)G_j(z_2-|\mathbf{k}|)\\
&\qquad\times G_j(z_1-|\mathbf{k}|)M_{ji}^{(+)}(z_1,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)\Big].
\end{aligned}\tag{8}$$

Here $|i\rangle$ describes a state of the atomic system which is taken to be the scattering center, and the vector $|j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda\rangle$ describes a state of the photon with momentum $\mathbf{k}$ and a polarization $\boldsymbol{\varepsilon}_\lambda$.

Physically, Eqs. (7) and (8) represent a generalization of the equations of the Green's-function method, and are, like these equations, highly nonlinear.

But, while as a result of their nonlinearity the equations of the Green's function method are not closed, in the case of Eqs. (7) and (8) nonlinearity does not imply nonclosure. This is because these equations are difference equations. In this connection, note that from the equations for $\langle j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda|M(z)|i\rangle$, $\langle i|M(z)|j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda\rangle$, and $\langle i|C(z)|i\rangle$ it is possible to obtain a system of ordinary differential equations

$$\frac{dM_{ij}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)}{dz}=F_1(M_{kl}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda),M_{kl}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda),C_k(z)),\tag{9}$$

$$\frac{dM_{ij}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)}{dz}=F_2(M_{kl}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda),M_{kl}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda),C_k(z)),\tag{10}$$

$$\frac{dC_i(z)}{dz}=F_3(M_{kl}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda),M_{kl}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda),C_k(z)).\tag{11}$$

This system of equations has a unique solution if boundary conditions are prescribed for $M_{ij}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$, $M_{ij}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$, and $C(z)$. Representation of these equations in differential form permits a better understanding of their nature and shows that the obtained system is closed and that to solve them one need not resort to perturbation theory. In addition, in their numerical solution it is more convenient to use the equations in difference form since in the calculations it is necessary one way or another to go over to approximate finite-difference formulas.

### 3. NATURAL BROADENING OF THE SPECTRAL LINES

The matrix elements of the operators $M(z)$ and $C(z)$ carry within themselves all the information of the unstable bound states and elementary processes in which the atomic system participates when it is in these states. The functions $M_{ij}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$, $M_{ij}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$, and $C(z)$ determine the formula of natural broadening of the spectral lines and their relative intensities and describe the processes of emission and absorption of photons by atomic systems.[4,5] Using these functions, one can construct the resonant scattering amplitudes without resorting to the quasistationary approximation. Thus, for resonant scattering of a photon by the atomic system in the case of overlap of the energy levels of the intermediate states the amplitude can be written accurate to $\alpha^2$ as

$$\begin{aligned}
&\langle\mathbf{k}_2\,\boldsymbol{\varepsilon}_\lambda,1|S|\mathbf{k}_1,\boldsymbol{\varepsilon}_\lambda,1\rangle\\
&\quad-2\pi i\delta(E_{k_2}-E_{k_1})[M_{1i}^{(+)}(\mathbf{k},\boldsymbol{\varepsilon}_\lambda,1)G_i(z)M_{i1}^{(-)}(\mathbf{k},\boldsymbol{\varepsilon}_\lambda,1)\\
&\quad+M_{1j}^{(+)}(\mathbf{k},\boldsymbol{\varepsilon}_\lambda,1)G_j(z)M_{j1}^{(-)}(\mathbf{k},\boldsymbol{\varepsilon}_\lambda,1)],
\end{aligned}$$

$$G_i(z)=\frac{1}{z-E_i-C_i(z)},\qquad z=|\mathbf{k}_1|+E_1.\tag{12}$$

Here we assume that the initial and final states of the system are stable, or that their instability can be neglected.

Now let us consider the question of the shape of the natural broadening of the spectral lines corresponding to transitions from the states with overlapping energy levels. In principle, in the description of the process of radiation of the atomic system it is necessary to consider the element of the $S$-matrix which describes the process of excitation and subsequent radiation of the ion. We assume that the excitation of the ion is due to collision with an electron whose state with momentum $\mathbf{p}$ and spin $s$ we will describe by the vector $|\mathbf{p},s\rangle$.

The amplitude of such a process coincides with the resonant part of the scattering amplitude which describes the scattering of the electron by the atomic system, and can be written in the following form:

$$\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_R|l_1, \mathbf{p}_1, s_1\rangle=\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_i|l_1, \mathbf{p}_1, s_1\rangle +\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_j|l_1, \mathbf{p}_1, s_1\rangle, \quad (13)$$

$$\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_i|l_1, \mathbf{p}_1, s_1\rangle=\delta(E_{l_2}+E_{p_2}+|\mathbf{k}|-E_{l_1}-E_{p_1}) \times\frac{\langle l_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|M(z)|i\rangle\langle i, \mathbf{p}_2, s_2|M(z')|l_1, \mathbf{p}_1, s_1\rangle}{z-E_i-C_i(z)}$$

$$z=E_{l_1}+E_{p_1}-E_{p_2},\quad z'=E_{l_1}+E_{p_1}. \quad (14)$$

For the probability (density) that as a result of collision of an electron with momentum **p** and spin $s$ a photon will be emitted with momentum **k** and polarization $\boldsymbol{\varepsilon}_\lambda$ we can write

$$\begin{aligned} &|\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_R|l_1, \mathbf{p}_1, s_1\rangle|^2 \\ &=|\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_i|l_1, \mathbf{p}_1, s_1\rangle|^2 \\ &\quad+|\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_j|l_1, \mathbf{p}_1, s_1\rangle|^2 \\ &\quad+\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_i^*|l_1, \mathbf{p}_1, s_1\rangle\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_j|l_1, \mathbf{p}_1, s_1\rangle \\ &\quad+\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_j^*|l_1, \mathbf{p}_1, s_1\rangle\langle l_2, \mathbf{p}_2, s_2, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|S_i|l_1, \mathbf{p}_1, s_1\rangle. \end{aligned} \quad (15)$$

It can be seen that this expression contains interference terms. Questions associated with such interference effects were considered in Ref. 11. If interference is neglected, then the probability defined by Eq. (15) becomes equal to a sum of probabilities corresponding to transitions from the *i*th and the *j*th excited states. In this case the notion commonly used in spectroscopy of contours of spectral lines corresponding to transitions from definite excited states was justified. Thus, for the probability of emission of a photon with energy $\omega$ during a transition of the atomic system from the *i*th state to the ground state we obtain the following expression:

$$\frac{dW_i(\omega)}{d\omega}=\mathscr{A}\omega\sum_\lambda\int d\Omega_k\left|\frac{\langle 1, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|M(E_1+\omega)|i\rangle}{E_1+\omega-E_i-C_i(E_1+\omega)}\right|^2 \quad (16)$$

where $\mathscr{A}$ is a normalizing factor. Here we have made use of the fact that the matrix element

$$\langle i, \mathbf{p}_2, s_2|M(z)|l_1, \mathbf{p}_1, s_1\rangle$$

in Eq. (14), which describes the process of excitation of the atomic system, can be assumed to be independent of $z$ in the resonance region since the dimensions of this region are generally much smaller than the interval of irregularities of the excitation process. As a result, the profile of the corresponding spectral line does not depend on the excitation process. For ordinary processes the contribution of the interference term is negligibly small. In the case of close levels, which is the case that we are considering, the contribution of the interference terms, generally speaking, can be substantial. Then the contour of the natural broadening of the spectral lines will depend not only on $M_{kl}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$ and $C_k(z)$, which characterize the given unstable states, but also on the value of the matrix element

$$\langle i, \mathbf{p}_2, s_2|M(z)|l_1, \mathbf{p}_1, s_1\rangle,$$

which describes the process of excitation of the atomic system. In addition, in order to calculate the experimentally observed profile of the emission contour, we must carry out a statistical average over all factors leading to excitation of the ion. An exception is the case of coherent excitation of the ion, considered in Refs. 2 and 11. On the other hand, statistical averaging will obviously give rise to a decrease in the contribution of the interference terms. Also, the nearness of the levels in general no longer implies that they overlap significantly. The reason for this is that when one speaks of overlap of closely spaced energy levels, one usually assumes that the spectral line shapes are Lorentzian. In general, the line shapes can depart significantly from a Lorentzian shape and it may turn out that the nearness of the energy levels causes such a deformation of the contours that overlap and the corresponding interference effects become insignificant.

Let us now consider the case in which the overlap of energy levels is small and perturbation theory can be applied to the solution of Eqs. (4) and (5). To first order for $\langle j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda|M(z)|i\rangle$ we obtain

$$\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|M^{(1)}(z)|i\rangle=\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|H_{\mathrm{int}}|i\rangle. \quad (17)$$

Allowing $z_2$ in Eqs. (4) and (5) to approach $i\infty$ and noting that according to Eq. (6) $\langle j|M(i\infty)|i\rangle$ and $\langle i|C(i\infty)|i\rangle$ are equal to zero, to second order for $\langle j|M(z)|i\rangle$ and $C_i(z)$ we obtain

$$\langle j|\Sigma^{(2)}(z)|i\rangle=\langle j|H_{\mathrm{int}}G(z)H_{\mathrm{int}}|i\rangle, \quad (18)$$

$$\begin{aligned} &C_i^{(2)}(z)=\langle i|H_{\mathrm{int}}G(z)H_{\mathrm{int}}|i\rangle, \\ &\langle j|\Sigma(z)|i\rangle=\langle j|M(z)|i\rangle. \end{aligned} \quad (19)$$

Here we ignore the fact that Eqs. (18) and (19) contain ultraviolet divergences. Thus, Eqs. (18) and (19) are to be understood in a formal sense, and the renormalization counterterms must be included in these expressions in the calculations. To second order in the perturbation theory the other matrix elements of the operator $M(z)$ are equal to zero. To third order for $\langle j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda|M(z)|i\rangle$ we can write

$$\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|M^{(3)}(z)|i\rangle=\sum_{l\neq i}\frac{\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|H_{\mathrm{int}}|l\rangle\langle l|\Sigma^{(2)}(z)|i\rangle}{z-E_l-C_l^{(2)}(z)}. \quad (20)$$

Finally, to fourth order for $C_i(z)$ we obtain

$$C_i^{(4)}(z)=\sum_{j\neq i}\frac{\langle i|\Sigma^{(2)}(z)|j\rangle\langle j|\Sigma^{(2)}(z)|i\rangle}{z-E_j-C_j^{(2)}(z)}. \quad (21)$$

If we restrict ourselves to these terms of the perturbation theory series, then for $\langle j,\mathbf{k},\boldsymbol{\varepsilon}_\lambda|M(z)|i\rangle$ and $C_i(z)$ we obtain the following expressions:

$$\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|M(z)|i\rangle=\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|H_{\mathrm{int}}|i\rangle +\sum_{l\neq i}\frac{\langle j, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda|H_{\mathrm{int}}|l\rangle\langle l|\Sigma^{(2)}(z)|i\rangle}{z-E_l-C_l^{(2)}(z)}, \quad (22)$$

$$C_i(z)=C_i^{(2)}(z)+\sum_{j\neq i}\frac{\langle i|\Sigma^{(2)}(z)|j\rangle\langle j|\Sigma^{(2)}(z)|i\rangle}{z-E_j-C_j^{(2)}(z)}. \quad (23)$$

Substituting expressions (22) and (23) into Eq. (16), we obtain for a three-level atomic system

$$\frac{dW_{12}(\omega)}{d\omega} = \mathcal{A}\omega \sum_{\lambda} \int d\Omega_{\mathbf{k}} \left| \frac{\langle 1, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda | H_{\text{B3}} | 2 \rangle + \dfrac{\langle 1, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda | H_{\text{int}} | 3 \rangle \langle 3 | \Sigma^{(2)}(z) | 2 \rangle}{E_1 + \omega - E_3 - C_3^{(2)}(z)}}{E_1 + \omega - E_2 - C_2^{(2)}(z) - \dfrac{\langle 2 | \Sigma^{(2)}(z) | 3 \rangle \langle 3 | \Sigma^{(2)}(z) | 2 \rangle}{z - E_3 - C_3^{(2)}(z)}} \right|^2 . \tag{24}$$

If we note that $\langle j | \Sigma(z) | j \rangle$ is a nondiagonal matrix element of the eigenenergy operator and that $C_i(z) = \Delta E_i - (1/2)\Gamma_i$, then it is easy to see that Eq. (24) coincides with the corresponding expression for the probability of emission obtained in Ref. 1. But, whereas in Ref. 1 expression (24) was obtained by summing an infinite series of perturbation theory, in the iterative solution of Eqs. (4) and (5) this result is obtained by summing only the first few terms of the iteration series. Taking the subsequent terms of the series into account leads to an expression for the probability of emission, determined with the help of Eqs. (4) and (5), that differs from expression (24). And this difference can be significant, since for a strong enough overlap the perturbation-theory series for the solutions of Eqs. (4) and (5) begins to diverge. This result shows what a significant contribution those intermediate states whose vectors are not elements of the Hilbert space $\mathscr{H}$ can make.

## 4. SPECTRAL LINE SHAPES OF TRANSITIONS IN DOUBLY EXCITED He-LIKE URANIUM

In order to examine the influence of the interaction of the ion with its own radiation field on the shape of the natural broadening of the spectral lines, we have chosen states which are formed from the $2s_{1/2}8p_{1/2}$ and $2p_{1/2}8s_{1/2}$ states as a result of mixing due to the Coulomb interaction between the electrons. Such a choice is motivated by the fact that for the given configuration of He-like uranium the interaction with the radiation field is comparable with the Coulomb interaction between the electrons, and the distance between the energy levels of such states is not great in comparison with the width of these levels. We have used Eqs. (7) and (8) to calculate the atomic characteristics of these states and the shapes of the corresponding spectral lines, i.e., we have limited ourselves to accuracy of order $\alpha^2$ and not taken into account intermediate states containing free electrons or positrons in addition to the atomic system or nucleus.

Note that the numerical solution of Eq. (8) in the vicinity of certain points on the real axis becomes unstable. Therefore, along with Eqs. (7) and (8) we also use the following equation for Im $C_i(z)$:

$$\operatorname{Im} C_i(z) = -\operatorname{Im} z \left( \sum_{j \neq i} \left| \frac{\langle j | M(z) | i \rangle}{z - E_j - C_j(z)} \right|^2 + \sum_{l} \sum_{\lambda} \int d^3k \left| \frac{\langle l, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda | M(z) | i \rangle}{z - E_l - |\mathbf{k}| - C_l(z)} \right|^2 \right). \tag{25}$$

To obtain this equation, it is necessary to set $z_1 = z$ and $z_2 = z^*$ in Eq. (8) and to note that

$$M(z) = M^+(z^*), \quad C(z) = C^+(z^*).$$

Equation (8) can be used to calculate Re $C_i(z)$, and Eq. (25) can be used to calculate Im $C_i(z)$. And whereas we have already calculated the values of $\langle l, \mathbf{k}, \boldsymbol{\varepsilon}_\lambda | M(z) | i \rangle$ and Re $C_i(z)$ for certain $z$, for arbitrary $z$ Eq. (25) is efficiently solved by iteration. Taking proper account of Eq. (25), which is in fact a particular case of Eq. (8), allows one to overcome the difficulties associated with the use of Eq. (8) in its difference equation form.

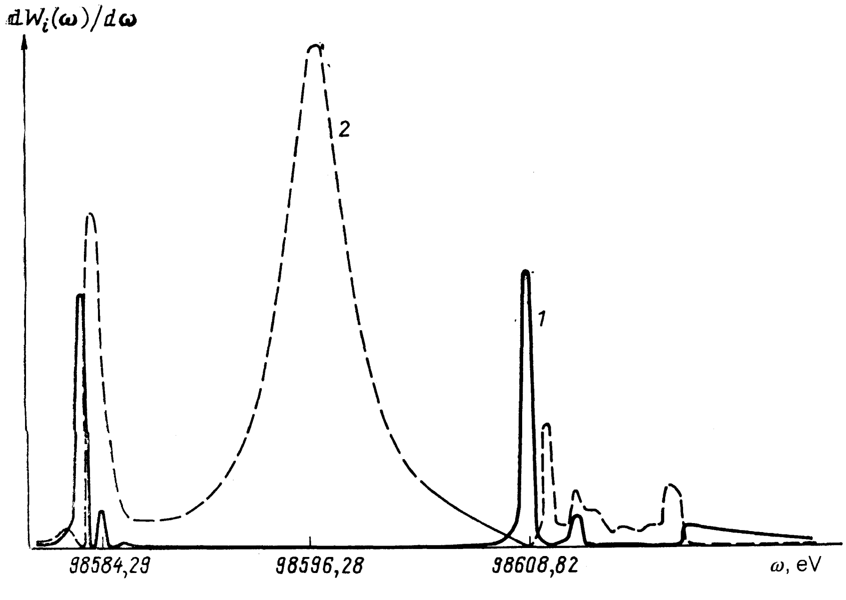

FIG. 1. General form of the spectral picture of the transitions to the $1s_{1/2}8s_{1/2}$ state from the $A$ state (solid line) and the $B$ state (dashed line).

With the help of Eqs. (7), (8), and (25) we have calculated $M_{ij}^{(+)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$,$M_{ij}^{(-)}(z,\mathbf{k},\boldsymbol{\varepsilon}_\lambda)$, and $C_i(z)$ for the states $(2s_{1/2}8p_{1/2}+2p_{1/2}8s_{1/2})_A$ $[J=0]$ and $(2s_{1/2}8p_{1/2}+2p_{1/2}8s_{1/2})_B$ $[J=0]$ and have constructed the spectral line shapes of the transitions from these states to the state $1s_{1/2}8s_{1/2}$ $[J=1]$. State $A$ differs from state $B$ in that the "undressed" energy of the first state is less than the "undressed" energy of the second. Curve 1 in Fig. 1 depicts the line shape corresponding to the transition $B\rightarrow 1s_{1/2}2s_{1/2}$ $[J=1]$. As follows from the form of the profiles, the interaction of the ion with its own radiation field deforms them in such a way that there is practically no overlap. Thus, for example, in the region of the central peak of profile $B$ the following estimate is valid:

$$\frac{dW_B(\omega)/d\omega}{dW_A(\omega)/d\omega}\sim 10^{18}.$$

The profile of line $A$ consists of two anomalously narrow peaks. The profile of line $B$ consists of a relatively wide central peak and two narrow peaks which lie near the peaks of profile $B$. The profiles of the spectral lines corresponding to the transitions from states $A$ and $B$ to any other state have the same form. In essence, the effect is that of splitting of the energy levels. And this splitting is caused by the interaction of the ion with its own radiation field, which in this case has a strong effect; the absence of overlap of the spectral lines also plays a part.

Physically, this phenomenon arises because the probability of emission of a photon with energy $\omega$ during a transition from the $A$ state tends to zero for those values of $\omega$ at which the probability of emission during a transition from the $B$ state has a resonance maximum. At the same time, the probability of emission during a transition from the $B$ state tends to zero for those $\omega$ at which there is a resonance maximum of the probability of emission during a transition from the $A$ state. All of this has a quite simple explanation. As we noted above, emission here is part of a more general process, including within itself also the excitation of the ion, for example, as a result of collision with the electron. There are two resonance channels for such a process: through the intermediate state $A$ and through the intermediate state $B$. If the probability that the process will proceed through one channel at some given energy is large, then the probability that the process will go through the other channel is quite small. This is because the unitary condition must be fulfilled. Thus, interference effects are practically absent in this case.

Line shapes $A$ and $B$ can be interpreted as a set of spectral lines corresponding to energy levels formed as a result of the splitting of "undressed" levels. Figures 2 and 3 show the spectral lines respectively in the right and left wings of the $A$ and $B$ profiles at a scale which shows the structure of these lines. Here it should be noted that anomalous narrowness (e.g., the width of the left line in Fig. 2 is of the order of 0.1 eV) does not mean that the corresponding states are long-lived. Such an interpretation is valid only in the case of quasi-stationary states and is inapplicable in the present case.

Note also that in the calculations we have neglected a number of important factors, such as the corrections associated with the finite size of the nucleus and the polarization of the vacuum. They can be taken into account in the usual way. In fact this leads only to a shift of the energy levels and of the entire spectral shape depicted in Fig. 1. Besides, as was mentioned above, system of equations (7) and (8) takes account only of those intermediate states containing ions and photons. To obtain a more accurate result, it is necessary to take into account intermediate states which contain free electrons and electron-positron pairs in addition to the ion (nucleus) and photons. For some states corrections which take the contribution of such states into account can be substantial.

## 5. CONCLUSION

For the case of doubly excited states of He-like uranium we have shown that when the distance between the energy levels of states with identical principal quantum numbers is not large in comparison with the widths of these levels, the interaction with the radiation self-field leads to such a defor-

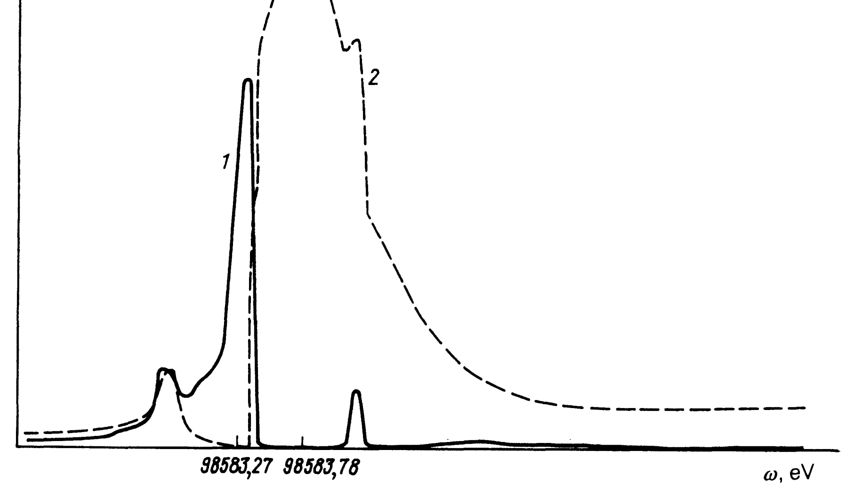

FIG. 2. Left wing of the spectral picture.

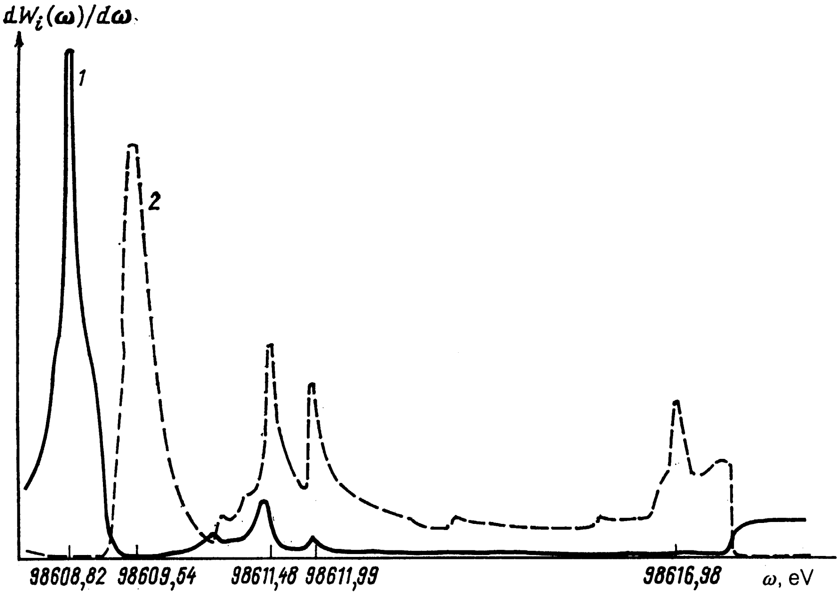

FIG. 3. Right wing of the spectral picture.

mation of the emission profiles that we obtain a complete set of spectral lines. In essence, the interaction with the radiation self-field gives rise to a splitting of these energy levels. It is important that overlap is practically absent, and interference effects are therefore insignificant. Thus, intersection of the energy levels leads to splitting into several sublevels which are quite well isolated from one another. One may hope that these effects will obtain experimental confirmation. But in order that the calculations of the emission spectra may be compared with experimental data, it is necessary to take all of the above-mentioned corrections into account. Some of the corrections can be made with the help of ordinary methods of atomic theory. The remaining corrections can be introduced with the help of a corresponding modification of system of equations (7), (8), and (25).

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