Stark effect in multiply charged two-electron ions

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A calculation is made of the energy levels of multiply charged two-electron ions in the $1s2s+1s2p$ configuration with a nuclear charge in the range $10 \leq Z \leq 50$, subjected to an external electric field which is either weak or strong compared with the Coulomb interaction of electrons. It is shown that the crossing of levels (as a function of Z), which occurs in the absence of the field, changes to pseudocrossing when the field is applied. However, new crossings of levels appear in the field.

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1. Recently there have been many experimental and theoretical investigations of the spectra of multiply charged ions. This is due to the fact that such ions are important in the processes occurring in the sun and other stars and also because of practical applications. The principal experimental methods for generating multiply charged ions in the laboratory are the transmission of a beam of ions through a foil (the beam–foil method) and the action of laser radiation on matter. In the latter case, multiply charged ions are created in a strong electric field: the electric field intensity in the laser beam may reach 10^9 V/cm, which is comparable with the internal atomic fields. Therefore, it would be interesting to investigate theoretically the spectra of multiply charged ions in strong electric fields.

Such an investigation should have another useful result. In recent years a considerable effort has been made to search for possible effects of parity nonconservation in atomic spectra. In particular, it has been pointed out that such effects may be observed in the spectra of multiply charged two electron ions.[1] Theoretical calculations of the spectra[2] have led to the prediction of crossing of levels of different parity when the nuclear charge Z is varied. It is clear from the results given below that a strong electric field produces new crossings and, in principle, this also can be used for detection of parity nonconservation effects.

2. As in[2], we shall consider here two electron ions in the $1s2s+1s2p$ configuration with an arbitrary nuclear charge Z. We shall assume that the external electric field is homogeneous. If this field is sufficiently weak compared with the Coulomb interaction of electrons, we can calculate the splitting and shift of the energy levels by the external field ignoring the interaction of states of different parity. Then, the matrix elements in the first order perturbation theory in the external field vanish, i. e., the quadratic Stark effect is observed.

When the field intensity is increased, the splitting becomes comparable with the separation between the terms and mixing of states with different parities is considerable. If the external field is stronger than the Coulomb interaction, the linear Stark effect should be observed. One of the present authors considered this situation in the case of two-electron multiply charged ions.[3] In the present paper we shall discuss a more general situation, which is the splitting and shift of the energy levels of two-electron ions with an arbitrary nuclear charge Z in arbitrary electric fields, which can be weak or strong compared with the Coulomb interaction of electrons. However, we shall assume that the energy of the interaction with the external field is still much less than the binding energy of electrons. This assumption is justified particularly for multiply charged ions because the binding energy is Z times higher than the Coulomb interaction of electrons with one another.

The problem can be solved, subject to the above assumption, by diagonalizing the Hamiltonian which includes the interaction with the external field and is based on wave functions of states of just one configuration. This assumption means that the levels of other configurations are located sufficiently far away and in the first approximation their influence can be ignored. The Hamiltonian is

$$H(12)=h(1)+h(2)+\alpha/r_{12}+\alpha^{1/2}F(z_1+z_2), \tag{1}$$

where $h(i)$ is the relativistic one-electron Dirac Hamiltonian for an electron in the field of a nucleus; r_{12} is the distance between electrons; $z_{1,2}$ are the Cartesian coordinates of electrons in the direction of the field; F is the field intensity; α is the fine-structure constant. Here and later we shall employ units for which $\hbar=c=m=1$ (m is the electron mass).

We shall use the exact relativistic one-electron Hamiltonian but we shall assume that the interaction between electrons is purely of the Coulomb type. Clearly, this can be done provided $Z^{-1} \ll 1$ and $(\alpha Z)^2 \ll 1$. If the first condition is satisfied, the relativistic corrections to the interaction are smaller than the one-electron relativistic terms, and if the second condition is satisfied, the Coulomb interaction is stronger than the magnetic and retarded interactions. Thus, we are going to ignore corrections of the order of $Z^{-1}(\alpha Z)^2$ and in its simplified form our theory is applicable to ions with $10 \leqslant Z \leqslant 50$.

In applying the Dirac theory the wave functions of a two-electron system are most naturally based on the jj coupling:

$$\psi_{JMj_1j_2}(12)=\frac{1}{\sqrt{2}}\sum_{m_1m_2} C^{j_1j_2}_{JM}(m_1m_2)\{\psi_{n_1j_1l_1m_1}(1)\psi_{n_2j_2l_2m_2}(2)-\psi_{n_2j_2l_2m_2}(1)\psi_{n_1j_1l_1m_1}(2)\}, \tag{2}$$

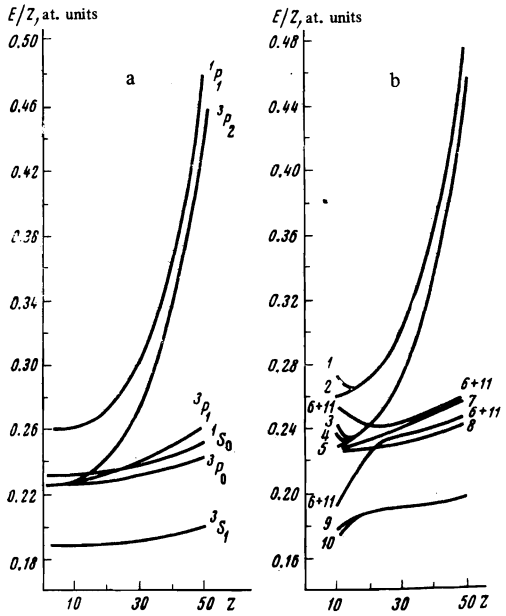

FIG. 1. Dependences of the energy levels on Z: a) in the absence of a field; b) in the presence of a field $F = 5.14\times10^9$ V/cm (the numbers alongside the curves are the indices of the levels E_i).

where ψ_{njlm} are one-electron wave functions; $C^{j_1j_2}_{JM}$ are the Clebsch–Gordan coefficients; $njlm$ are the sets of the one-electron quantum numbers (n is the principal quantum number, j and m are the total one-electron momentum and its projection, and l is the orbital momentum for the upper component of a Dirac bispinor, governing the parity of the state); J and M are the total momentum of an atom and its projection.

The Coulomb interaction of electrons mixes states with different values of j_1 and j_2, and the interaction with the external field mixes states with different values of J (in an external field the only quantum number is the projection of the total momentum M). Thus, the diagonalization of the Hamiltonian (1) based on the wave functions (2) gives a complete description of the splitting of levels in an electric field subject to the Coulomb interaction of electrons. The general expressions for the matrix elements of the Coulomb interaction operator based on the wave functions (2) are given in[2] and the corresponding matrix elements for the operator of the interaction with the electric field can be found in[3].

3. We shall now consider the specific configuration $1s2s + 1s2p$ (the configurations $1s2s$ and $1s2p$ cannot be discussed separately because of the Coulomb degeneracy). In the absence of an external field this configuration splits into six levels, which we shall describe—as in[2]—by specifying the quantum numbers J and M, and by indicating the corresponding terms in the limits of the LS and jj coupling (corresponding to small and large values of Z, respectively): $E_{JM}(^{2S+1}L, jj')$. These six levels are

$$E_{2M}(^3P,\ ^1/_2{}^3/_2),\quad E_{1M}(^3P,\ ^1/_2{}^1/_2),\quad E_{00}(^3P,\ ^1/_2{}^1/_2),$$
$$E_{1M}(^1P,\ ^1/_2{}^3/_2),\quad E_{1M}(^3S,\ ^1/_2{}^1/_2),\quad E_{00}(^1S,\ ^1/_2{}^1/_2).$$

In a homogeneous electric field these levels become split in respect of $|M|$, i.e., a total of eleven levels is formed. We shall use the following labeling system for these levels:

$$E_{11}(^1P,\ ^1/_2{}^3/_2)=E_1,\quad E_{10}(^1P,\ ^1/_2{}^3/_2)=E_2,\quad E_{20}(^3P,\ ^1/_2{}^3/_2)=E_3,$$
$$E_{21}(^3P,\ ^1/_2{}^3/_2)=E_4,\quad E_{22}(^3P,\ ^1/_2{}^3/_2)=E_5,\quad E_{10}(^3P,\ ^1/_2{}^1/_2)=E_6,$$
$$E_{11}(^3P,\ ^1/_2{}^3/_2)=E_7,\quad E_{00}(^3P,\ ^1/_2{}^1/_2)=E_8,\quad E_{10}(^3S,\ ^1/_2{}^1/_2)=E_9,$$
$$E_{11}(^3S,\ ^1/_2{}^1/_2)=E_{10},\quad E_{00}(^1S,\ ^1/_2{}^1/_2)=E_{11}.$$

The complete eleventh-order matrix, subject to the symmetry properties of the states and the rules for addition of the momenta, splits into four submatrices corresponding to the following combinations of states:

$$(E_1+E_4+E_7+E_{10})_1,\quad (E_2+E_6+E_{11})_0,\quad (E_3+E_8+E_9)_0,\quad (E_5)_2.$$

The indices after the parentheses represent the projection of the total momentum $|M|$. Diagonalization of these values gives new levels E_i', which are linear combinations of the old levels. The level E_5 is not affected by the electric field (if we ignore the interactions with other configurations).

In a relatively weak (compared with the Coulomb interaction of electrons) external field the levels E_i' are close to some of the old levels E_i. In a relatively strong field the mixing of the levels E_i is complete. This applies particularly to the levels which intersect in the absence of a field: for such levels the external field becomes strong when its intensity F is still relatively low. In spite of the mixing, the most convenient nomenclature for the levels in a strong electric field is usually the old nomenclature, i.e., it is usually most convenient to refer to a level E_i, existing in the absence of a field, from which a given level E_i' originates. This method is unsuitable only for intersecting (due to variation of Z) levels in the absence of a field. In the latter case a pseudocrossing of the levels takes place: two levels which are transformed by a change in Z into specific limiting LS and jj levels (in the absence of a field) exhibit an interchange of their limits in a field. This phenomenon differs from the usual pseudocrossing by the fact that Z is a discrete parameter and, consequently, there is a value of the field intensity F_{min} in which this effect appears: the fields should be sufficiently strong to mix the levels completely for that value of Z which corresponds to the minimum separations between the levels.

4. Figure 1a shows the dependence of the energy levels on Z in the absence of a field, whereas Fig. 1b shows the same dependence in a field $F = 5.14\times10^9$ V/cm. We can see that the levels E_6 and E_{11} intersecting in the absence of a field now repel one another. More exactly, we should speak of the "upper" $(E_6+E_{11})'$ and "lower" $(E_6+E_{11})''$ levels because the old nomenclature loses completely its meaning in the case of these two levels. We can also see that there are new crossings: the level $(E_6+E_{11})'$ intersects now the levels E_3, E_4, and E_5 when $Z = 20$. The level E_3 has the same value of the projection of the momentum $M = 0$ as the level $(E_6+E_{11})'$. Nevertheless, intersection is possible because the levels E_3 and E_6, E_{11} do not combine in an external electric field. The latter is evident from the rules govern-

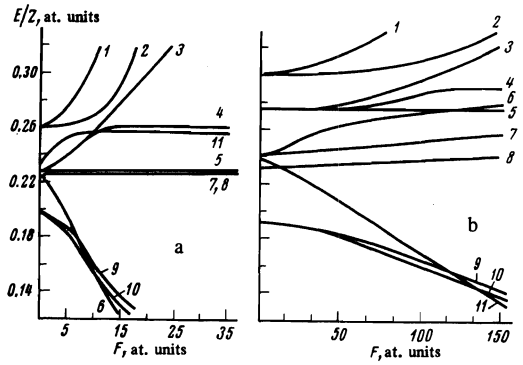

FIG. 2. Dependences of the level energies on the field intensity: a) for $Z=10$; b) for $Z=30$. The numbers alongside the curves are the indices of the levels E_i.

ing the addition of momentum and parity conservation. If the levels do not combine, i.e., if the nondiagonal matrix elements of the operator of the external field between the corresponding states vanish, the theorem on the crossing of levels with identical quantum numbers[4] is inapplicable: the levels "do not know" of the existence of one another and there can be no mutual repulsion.

Figure 2 shows dependences of a different kind: the level energies are plotted as a function of the field F for fixed values of Z. The maximum values of the field intensity in Fig. 2 are of the order of the internal atomic field for the corresponding values of Z. The curves in Fig. 2 demonstrate also repulsion of the levels and the appearance of new crossings in an electric field.

It should be noted that, in contrast to Z, the field is a continuous parameter, i.e., we are dealing here with real intersections. In all the graphs the level energies are divided, by convenience, by Z and represented in atomic units; the field intensity F is also given in atomic units (1 at. unit = 5.14×10^9 V/cm). It is clear from Figs. 1b and 2 that the influence of an external field of fixed intensity F rises when Z is reduced. This is fairly self-evident: the matrix element of the Coulomb interaction of electrons is proportional to Z and the Stark matrix element is proportional to Z^{-1}.

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Nonresonant charge exchange in dense gases

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It is shown that the increase of density of a medium can result in a pronounced change in the nonresonant charge exchange cross section, even though the pairing condition for the process is satisfied with sufficient margin. At a large bare resonance defect the final result is determined by competition between an exponentially small cross section corresponding to a nonadiabatic transition and a low probability of particle configurations in the medium such that the effective defect is negligible.

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When the density of a gas medium is increased, its influence on the inelastic collisions of atoms and molecules begins to come into play even before triple collisions become significant. Indeed, this becomes a pairing process if the criterion $n\sigma^{3/2}\ll 1$ is satisfied, where n is the density of the gas and σ is the collision cross section.[1)] However, the potential fields produced by the gas environment can lead to a shift of the terms of the colliding particles, which greatly influences the value of σ even in the region where the foregoing inequality is satisfied. The corresponding problem was considered earlier[1] with resonant charge exchange as an example, while Lisitsa[2] investigated the crossing of the atomic terms under the influence of a random field of a gas medium. The present paper is devoted to nonresonant charge exchange in gases of finite density, when the criterion for the pairing in the collisions is still satisfied.

According to Massey's adiabatic criterion the cross section for nonresonant charge exchange is exponentially small in comparison with the gas-kinetic cross section if the resonance defect Δ greatly exceeds the quantity γv, where v is the relative collision velocity and γ is of the order of the atomic momentum. The ion that takes part in the charge exchange polarizes the particles of the surrounding gas, and this leads to a shift of the terms of the quasi-molecule made up of the colliding atoms. Thus, an effective renormalization of Δ takes place and, in particular, particle configurations are possible in which the resonance defect is practically completely suppressed, that is, $|\Delta_{eff}|$ becomes less than