

¹In the course of a nonradiative annihilation of a positron and a K electron the whole system (i. e., the nucleus and the electron shell of the atom) go over to an intermediate state which is in resonance with the initial state; in this intermediate state the nucleus is excited to a level E_2 and a hole appears in the K shell of an atom. The amplitude of this intermediate state of the whole system decays as a result of subsequent nuclear (radiative, conversion, nucleon evaporation, etc.) transitions from the level E_2 and also as a result of transitions in the electron shell (radiative or Auger) resulting in the filling of the K hole. Only in the case of hydrogen- and helium-like ions can we regard the K -hole lifetime as infinitely long. The width of a resonance state of the system is thus governed by the total contribution of the nuclear and electron processes: $\Gamma = \hbar/\tau_N + \hbar/\tau_K$, where τ_N is the lifetime of the nucleus at the level E_2 and τ_K is the lifetime of a K hole. As a rule, for $Z > 40$ and $E_2 < 6$ MeV, we have $\tau_K \ll \tau_N$ but there may be exceptions (for example, the $^{208}_{82}\text{Pb}$ nucleus).

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Translated by A. Tybulewicz

Effects of nonconservation of spatial and temporal parities in spectra of diatomic molecules

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(Submitted 18 July 1978)

Zh. Eksp. Teor. Fiz. **76**, 414–421 (February 1979)

It is shown that, after allowance for the Λ doubling, the degree of nonconservation of the spatial parity in the scattering of light by homonuclear diatomic molecules can reach values of the order of 10^{-4} for the hydrogen molecule (H_2) and of unity for the iodine molecule (I_2). The effects of nonconservation of the temporal parity (T -invariance violation) in the spectra of heteronuclear diatomic molecules with the Λ doubling of the ground states are enhanced by five orders of magnitude, compared with the atomic spectra, in electric fields of a few kilovolts per centimeter.

PACS numbers: 33.80. – b, 31.90. + s

Much theoretical work has been done recently on the effects of nonconservation of the spatial parity in atoms associated with the existence of weak neutral currents (see, for example, the reviews in Refs. 1–4). The results of the first experimental investigations have been published.^{5–7} Similar effects in molecules have also been considered.^{8,9} Quite a few papers have been devoted also to the search of the effects of nonconservation of the temporal parity in atoms and molecules, namely to the discovery of the influence of the dipole moments of an electron and a proton and of the constants of the scalar and tensor interactions violating the temporal parity on the dipole moments of atoms and molecules.^{10–14}

We shall show that the effects of nonconservation of the spatial and temporal parity in diatomic molecules may be enhanced considerably in the case of the levels exhibiting the Λ doubling effect.

1. NONCONSERVATION OF THE SPATIAL PARITY

We shall consider resonance fluorescence emitted by the hydrogen molecule as a result of its transition from the ground para state $^1\Sigma_g^+(I=0, K=0; +)$ to the ground ortho state $^1\Sigma_g^+(I=1, K=1; -)$. Here, I is the total nuclear spin and K is the rotational quantum number; the sign in parentheses is the sign of the state (total spatial

parity of the whole molecule). It is assumed that the incident radiation is tuned to resonance with an electronic transition

$${}^1\Sigma_g^+(I=0, K=0; +) \rightarrow {}^1\Pi_u^-(I=1, K=1; +).$$

This transition occurs under the influence of the hyperfine interaction V_{hf} and, therefore, it is strongly forbidden. Next, the molecule in the excited state ${}^1\Pi_u^-$ undergoes an allowed $E1$ transition to the ground ortho state ${}^1\Sigma_g^+(I=1, K=1; -)$, emitting a fluorescence photon.

The amplitude of the process is described by the Feynman diagram shown in Fig. 1. Apart from the diagram in Fig. 1, the transition amplitude includes contributions from a diagram with transposed $M1$ and V_{hf} interactions, in which the intermediate states are ${}^1\Sigma_g^+(I=0, K=1; +)$ and ${}^1\Pi_u^-(I=0, K=1; +)$ with different quantum numbers n . It is quite difficult to calculate all these diagrams. We shall, therefore, confine ourselves to order-of-magnitude estimates of the transition amplitude, especially as its exact value can be determined by direct experiments.

Allowance for a weak interaction V_p which mixes states of different parities gives rise to an amplitude correction shown in Fig. 2. The Hermitian P -odd and T -even weak interaction operator V_p has the following form in the nonrelativistic approximation and momentum representation¹⁻³

$$\langle p_2 | V_p | p_1 \rangle = Z\beta_i \sigma_e \frac{p}{m} + \beta_2 \sigma_N \frac{p}{m} + \beta_3 i [\sigma_e \sigma_N] \frac{q}{m},$$

$$p = p_2 + p_1, \quad q = p_2 - p_1, \quad (1)$$

where p_i and m are the electron momenta and mass; σ_e and σ_N are the Pauli spin matrices for electrons and nucleons; β_i are independent constants. In the first term containing the Pauli electron matrix the interactions of an electron with all the nucleons in the nucleus are summed and, therefore, the factor Z appears explicitly in front of this term. The other terms, containing the nucleon spin do not include the factor Z . In universal models of the Weinberg-Salam type the constants β_i are of the order of the weak Fermi constant G .

The ortho and para states which have different signs and different total nuclear spin momenta of the molecule, and are singlets in respect of the electron spin, can be mixed only by the second term in Eq. (1). However, the states Π_u^+ and Π_u^- are not mixed at all by the T -even operator (1). In fact, we have¹⁵

$$\Pi_u^\pm = 2^{-1/2} (\Pi_u(\Lambda=1) \pm \Pi_u(\Lambda=-1)), \quad \Lambda = K_n, \quad (2)$$

where K is the operator of the total momentum of the molecule and n is the direction of the molecular axis.

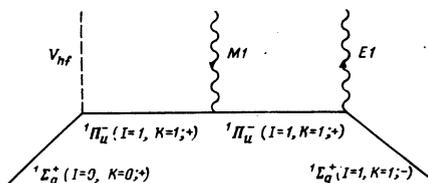


FIG. 1. Feynman diagram of resonance fluorescence emitted by a hydrogen molecule.

The matrix elements V_p diagonal in respect of Λ vanish because T is even and P is odd:

$$\langle \Lambda | V_p | \Lambda \rangle^T = \langle -\Lambda | V_p | -\Lambda \rangle^P = -\langle \Lambda | V_p | \Lambda \rangle = 0. \quad (3)$$

The equalities (3) are obtained by successive transformations of T and then P inversion. The matrix elements of V_p nondiagonal in respect of Λ vanish because the vector operator (1) cannot alter the projection of Λ by two units in one step, i.e., it cannot mix the states with $\Lambda=+1$ and $\Lambda=-1$. Therefore, the graph of Fig. 2 is supplemented by the operator V_B representing the interaction of the electron motion with rotation mixing the states $\Lambda=\pm 1$ and $\Lambda=0$ (Ref. 15):

$$V_B = -2B_e K_L, \quad B_e = \hbar^2 / 2Mr_e^2, \quad (4)$$

where L is the electron orbital moment, M is the reduced mass of the nuclei, and r_e is the equilibrium distance between the nuclei. The operator V_B transforms the states Π to Σ without a change in the other quantum numbers.

In the case of the H_2 molecule the energy denominator of the second intermediate state in Fig. 2 is governed by the nearest level ${}^1\Sigma_u^+$, which is admixed by the interaction V_B to ${}^1\Pi_u^+$, and its numerical value is $\Delta E_B \sim 0.1\omega$, where ω is the energy of the ${}^1\Sigma_g^+ - {}^1\Pi_u^-$ transition:

$$\omega = E({}^1\Pi_u^-(I=1, K=1; +)) - E({}^1\Sigma_g^+(I=0, K=0; +)) \approx 10^5 \text{ cm}^{-1}.$$

The energy denominator of the first intermediate state in Fig. 2 is equal to the Λ splitting of the ${}^1\Pi_u^+$ levels. It is governed by the shift of the ${}^1\Pi_u^+$ level in the second order of the perturbation V_B and the intermediate state ${}^1\Sigma_u^+$ is the same so that $\Delta E_\Lambda \sim K(K+1)B_e^2/\Delta E_B$. Transposition of the operators V_B and V_p in Fig. 2 results in the replacement of the nearest intermediate level ${}^1\Sigma_u^+$ with the level ${}^1\Sigma_u^-$, which is in the continuous spectrum. Therefore, such a diagram (like the shift of the level ${}^1\Pi_u^+$) is approximately an order of magnitude smaller than the diagram in Fig. 2. The diagrams without allowance for the Λ doubling (for example, without the intermediate state ${}^1\Pi_u^+$ and the operator V_B) are two orders of magnitude smaller than the diagram in Fig. 2. Thus, in the case of the H_2 molecule only the weak-interaction diagram in Fig. 2 is important.

Interference of the amplitudes in Figs. 1 and 2 results in parity nonconservation effects and the degree of nonconservation of the parity \mathcal{P} is equal to twice the ratio of the moduli of the amplitudes of Figs. 2 and 1:

$$\mathcal{P} \approx 2 \frac{\langle V_p \rangle B_e \omega}{\Delta E_\Lambda \Delta E_B \langle V_{hf} \rangle} \left(\frac{\Gamma_{E1}}{\Gamma_{M1}} \right)^{1/2} \approx 2 \frac{\langle V_p \rangle \omega}{\langle V_{hf} \rangle B_e} \left(\frac{\Gamma_{E1}}{\Gamma_{M1}} \right)^{1/2}, \quad (5)$$

where Γ_{E1} and Γ_{M1} are the widths of the corresponding

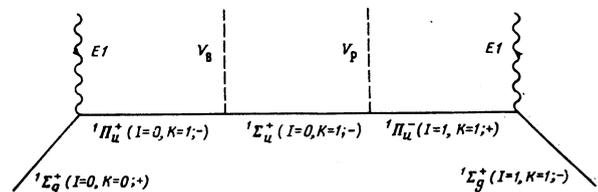


FIG. 2. Weak corrections to the resonance fluorescence process.

electromagnetic transitions. A similar formula applies also to molecules consisting of atoms with a large nuclear charge Z . Then, the part of the weak potential dependent on the nuclear spin is

$$\langle V_p \rangle \sim 10^{-10} Z^2 \text{ a.u.},$$

and the hyperfine interaction is

$$\langle V_{hf} \rangle \sim 10^{-7} Z \text{ a.u.}, \quad (\Gamma_E/\Gamma_{M1})^{1/2} \sim \alpha^{-1} \sim 10^2.$$

In this way we obtain the estimate

$$\mathcal{P} \sim 10^{-7} Z \omega / B_e. \quad (6)$$

In the case of the hydrogen molecule (resonance transition $^1\Sigma_g^+ \rightarrow ^1\Pi_u^+$, $\lambda = 100.04 \text{ nm}$, $B_e \approx 61 \text{ cm}^{-1}$ - Ref. 16), we obtain $\mathcal{P} \sim 10^{-4}$. For the iodine molecule ($Z = 53$, $i = \frac{5}{2}$, resonance transition $^1\Sigma_g^+ \rightarrow ^3\Pi_u$ with $\Omega = 1$, $\lambda = 850 \text{ nm}$, $B_e \approx 10^2 \text{ cm}^{-1}$ - Ref. 16) the estimated \mathcal{P} is of the order of unity. It should also be noted that the wavelength of this transition in the iodine molecule is within the range of the existing lasers.⁹

In the case of resonance fluorescence from the $^1\Pi_u^-$ level the parity nonconservation effect is manifested by the dependence of the transition probability on the circular polarization of the incident photons. Tuning to the resonance fluorescence from the $^1\Pi_u^+(I=0, K=1; -)$ level makes it possible to observe circular polarization of the final photon using an unpolarized initial beam. The diagram describing this process is obtained from Fig. 1 by altering the direction of motion of $E1$ and $M1$ photons, transposition of the V_{hf} and $E1$ lines, and substitution of the intermediate state $^1\Pi_u^+(I=1, K=1; +)$ with the state $^1\Pi_u^-(I=0, K=1; -)$. If we ignore the Λ splitting energy, we find that the diagram in Fig. 1 is not affected and there is no change in the diagram in Fig. 2 so that the value of \mathcal{P} remains as before. If the width of the incident radiation line is greater than the Λ splitting of the $^1\Pi_u^-$ and $^1\Pi_u^+$ levels, resonance fluorescence appears from both levels and the formula for the probability of the process becomes

$$\Gamma = \Gamma_0 \{1 + \mathcal{P} (n_i s_i - n_f s_f)\}, \quad (7)$$

where Γ_0 is the probability without allowance for the weak interaction; \mathcal{P} is the degree of parity nonconservation given by Eq. (6); n_i , s_i and n_f , s_f are the directions of motion and the spin of the initial and final photons, respectively.

We shall consider briefly the possibility of experimental detection of the above parity nonconservation effects. In view of the similarity of the Λ -doublet levels and the Doppler line broadening when the laser radiation is tuned to the resonance frequency of the $^1\Pi_u^+$ level, there is an additional background process involving the allowed transitions

$$^1\Sigma_g^+(I=0, K=0; +) \xrightarrow{E1} ^1\Pi_u^-(I=0, K=1; -) \xrightarrow{M1} ^1\Sigma_g^+(I=0, K=0; +),$$

whose probability is approximately 18 orders of magnitude higher than of the process in Fig. 1. This background process does not transfer the molecules from the para to the ortho state and does not affect the magnitude of the parity nonconservation effects. However, it is this process that governs the absorption length (free path) of laser photons. If the absorption length is $l \sim 1 \text{ cm}$, then the maximum permissible density of molecules in the target is restricted and, therefore,

there is a minimum time in which an experiment can be carried out.¹⁾ In the case of the H_2 molecule at $\sim 10^\circ \text{ K}$ the Doppler width is an order of magnitude less than the Λ splitting of the $^1\Pi_u^+$ levels. The cross section of the $E1$ transition to the $^1\Pi_u^-(I=0, K=1; -)$ space level is governed by the Breit-Wigner wing of the natural width of this level. The permissible target density is $\sim 10^{15}$ molecules/cm³ and the minimum time to detect the parity nonconservation effects is ~ 1 month when the laser photon flux is $\sim 10^{16}$ photons.cm⁻².sec⁻¹. For the I_2 molecule the Doppler width is greater than the Λ splitting at any reasonable temperature and, therefore, it governs the cross section of the $E1$ transition. The permissible target density is 10^8 molecules/cm³ and the measurement time is governed only by the sensitivity of ortho-molecule detectors.

2. VIOLATION OF THE TEMPORAL INVARIANCE

In the nonrelativistic approximation of the Hermitian T - and P -odd operator V_{PT} has the following form in the momentum space:

$$\langle p_2 | V_{PT} | p_1 \rangle = Z \gamma_i i \sigma_{i1} \frac{\mathbf{q}}{m} + \gamma_2 i \sigma_{i2} \frac{\mathbf{q}}{m} + \gamma_3 [\sigma_i \sigma_N] \frac{\mathbf{p}}{m}, \quad (8)$$

where γ_i are real constants; the rest of the notation is the same as in Eq. (1). The expression (8) represents the nonrelativistic limit of the interaction between vector currents of the type

$$i G_V [\bar{u}_2 \gamma_\mu u_1]_N \left[\bar{u}_2 \gamma_\nu \sigma_{\mu\nu} \frac{q_\nu}{m} u_1 \right]_e + (e \leftrightarrow N), \quad (9)$$

and also of the scalar and tensor variants of the interaction

$$i G_S [\bar{u}_2 u_1]_N [\bar{u}_2 \gamma_5 u_1]_e, \quad i G_T [\bar{u}_2 \sigma_{\mu\nu} u_1]_N [\bar{u}_2 \sigma_{\mu\nu} \gamma_5 u_1]_e. \quad (10)$$

The constants γ_i are linear combinations of the constants G_V , G_S , and G_T with coefficients of the order of unity. The last term in Eq. (8) appears only in the case of the tensor variant (10).

In contrast to V_P [see Eq. (3)], the matrix elements of V_{PT} diagonal in respect of Λ do not vanish:

$$\langle \Lambda | V_{PT} | \Lambda \rangle = C \mathbf{K} \mathbf{n} = C \Lambda, \quad (11)$$

where C is a real constant and $\mathbf{K} \cdot \mathbf{n} = \Lambda$ is a quantity which is odd in respect of P and T . Therefore, the operator (8) mixes the Π_u^+ and Π_u^- states of Eq. (2). In the presence of the interaction (8) the application of an external electric field $\vec{\mathcal{E}}$ to a molecule results in a linear (in respect of the field) shift of the levels, which depends on the projection of Λ . This effect is described by the diagrams in Fig. 3. For the interaction (8) the diagrams a and b in Fig. 3 make the same contribution

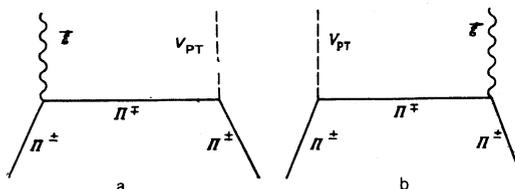


FIG. 3. Diagrams of the linear Stark effect in the case of T -invariance violation.

and have to be added. When V_{PT} is replaced with V_P of Eq. (1), the diagrams *a* and *b* of Fig. 3 cancel out in any order of the perturbation theory for the functions Π^\pm , including the case when allowance is made for the interaction V_B of Eq. (4) governing the difference between the energies of the levels Π^\pm , for the imaginary parts associated with the level instability, etc.²⁾

The correction to the energies of the states Π^\pm corresponding to the total contribution of the diagram in Fig. 3 is

$$\Delta E_\pm = \pm \frac{2\langle \pm | V_{PT} | \mp \rangle}{\Delta E_\Lambda} \langle \mp | S | \pm \rangle, \quad (12)$$

where $\Delta E_\Lambda = E_+ - E_-$ is the separation between the components of the Λ doublet; $\langle \mp | S | \pm \rangle = e \langle \mp | r_\alpha | \pm \rangle \mathcal{E}_\alpha$ is a Stark matrix element; $\langle r_\alpha \rangle$ is a matrix element of the coordinate. Clearly, ΔE_\pm increases on increase of the field \mathcal{E} until the value $\Delta E_\Lambda \sim \langle S \rangle$ is reached. In higher fields \mathcal{E} the separation between the components of the Λ doublet is governed by the Stark splitting, which exceeds ΔE_Λ , and then ΔE_\pm ceases to rise. Thus, the maximum value of ΔE_\pm is attained in a field described by the condition

$$\mathcal{E} = \frac{\Delta E_\Lambda}{e \langle z \rangle}, \quad \Delta E_\pm^{\max} = \pm 2 \langle \pm | V_{PT} | \mp \rangle. \quad (13)$$

The diagrams in Fig. 3 describe the effects associated directly with the T -invariance violation (temporal parity nonconservation) in the contact interaction of electrons with nucleons. The intrinsic dipole moment of electrons appears (because of the T -invariance violation) also in the linear Stark effect of Eq. (13). The diagrams describing this phenomenon are obtained from Fig. 3 by replacing V_{PT} with the potential representing the interaction of the Coulomb field of the nucleus with the dipole moment of the electron. The vertex of this interaction is

$$ig_V \left[\bar{u}_2 \gamma_\mu \sigma_{\nu\mu} \frac{q_\nu}{m} u_1 \right] \approx ig_V \left(\sigma_\nu \frac{q}{m}, 0 \right). \quad (14)$$

Moreover, we must add a diagram corresponding to the direct interaction of the external field \mathcal{E} with the electron dipole moment. In the lowest relativistic approximation in respect of q/m these three diagrams cancel out (Schiff theorem¹⁸⁾. The remaining relativistic corrections $\sim q^2/m^2$ cancel out the Coulomb propagator $\alpha Z/q^2$ in the diagrams of the type shown in Fig. 3. Consequently, there is a contact interaction in the form of the first term in Eq. (8) with $\gamma_1 \sim g_V \alpha/m^2$. Therefore, measurements of the level shift (13) can give the same restrictions on the constants³⁾ $Z\gamma_1$, $g_V \alpha Z/m^2$, γ_2 , γ_3 .

We shall now consider the sensitivity of the proposed experiments. The smallest energy shifts in an electric field can be discovered in magnetic resonance experiments.^{10,13} This method is acceptable for the ground-state levels which are relatively narrow. A suitable molecule with $\Lambda \neq 0$ in the ground state is, for example, PbF (ground state $^2\Pi_{1/2}$). In general, heteronuclear molecules even in the case of T -invariance conservation can have a dipole moment different from zero and directed along the molecular axis n . However, this moment does not appear in the phenomena under dis-

cussion because it is either lost as a result of averaging over the molecular rotation or it shifts by the same amount all the components of the Λ doublet.

In the case of the $^2\Pi_{1/2}$ state the splitting of the components of the Λ doublet is given by the formula¹⁶

$$\Delta E_\Lambda = A(B_e/\omega)(J+1/2), \quad (15)$$

where J is the total momentum of a molecule, including the spin ($J = \frac{1}{2}, \frac{3}{2}, \dots$); B_e is the rotational constant; A is the spin-orbit interaction constant; ω is the characteristic value of the transition frequency of a molecule. Using the values $A \sim 10^3 \text{ cm}^{-1}$, $B \sim 0.1 \text{ cm}^{-1}$, and $\omega \sim 10^4 \text{ cm}^{-1}$ typical of the heavy molecules¹⁶ and assuming that $J = \frac{1}{2}$, we find that the application of Eq. (14) to ΔE_Λ gives an estimate $\Delta E_\Lambda \sim 0.1 \text{ cm}^{-1}$. The electric field is found from the condition (13), which gives 10^3 V/cm for the example in question. The magnetic resonance method¹⁰ makes it possible to detect a value of ΔE_\pm of the order of 10^{-3} Hz . The matrix element of V_{PT} given by Eq. (8) is of the order of⁴⁾

$$\langle V_{PT} \rangle = (C_1 Z \gamma_1 + C_2 \gamma_2 + C_3 \gamma_3) (\alpha Z)^2 m^2 \text{ a.u.}, \quad C_i \sim 1. \quad (16)$$

Hence, if the linear Stark effect cannot be determined experimentally with this precision, i.e., if $\langle V_{PT} \rangle < 10^{-3} \text{ Hz}$, the following limits are obtained for the constants γ_i and g_V :

$$m^2 \gamma_1, \quad g_V \alpha, \quad m^2 \gamma_2/Z, \quad m^2 \gamma_3/Z < 10^{-20}. \quad (17)$$

The electric dipole moment d_e is related to the constant g_V by $d_e = e g_V/m$. The condition (17) imposes the following limit on the possible values of the electron dipole moment:

$$d_e/e < 10^{-28} \text{ cm}, \quad (18)$$

which is five orders of magnitude lower than the best limit obtained so far.^{10,13} This enhancement of the sensitivity is due to the fact that in the previously considered experimental variance the Stark matrix element $\langle S \rangle$ cannot be made of the same order of magnitude as the separation between the levels being mixed in electric fields attainable under laboratory conditions.

Similar effects can be also observed in molecules of the TiO and ZrO type, in which the ground state is Δ . These molecules have a separation of the order of $10^{-8} - 10^{-9} \text{ cm}^{-1}$ between Λ -doublet levels and, therefore, the maximum value of ΔE_\pm^{\max} of Eq. (13) is reached already in fields of $\mathcal{E} \sim 10^{-6} \text{ V/cm}$ and the limits applicable to the constants γ_i and g_V are still given by Eq. (17). For molecules with the ground state which is an electron-spin singlet the matrix elements of the first and third terms in Eq. (8) vanish. For these molecules we can find only the limit applicable to the constant γ_2 , which is Z times less than the limit (17) applicable to the constant γ_1 .

The authors are grateful to A. E. Barzakh, Yu. I. Neronov, and R. M. Ryndin for numerous discussions.

¹⁾The authors are grateful to A. Barzakh and Yu. Neronov for pointing out this aspect.

²⁾An incorrect calculation of the diagrams in Fig. 3 with the weak interaction (1) has led to an erroneous conclusion of the occurrence of the linear Stark effect in the case of unstable states in the T -even and P -odd interactions of neutral cur-

- rents.¹⁷
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Translated by A. Tybulewicz

Bohr-Sommerfeld quantization of n -dimensional neutral and charged pulsions

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(Submitted 2 July 1978)

Zh. Eksp. Teor. Fiz. **76**, 422-429 (February 1979)

The Klein-Gordon equation with logarithmic nonlinearity is used as an example to show that a scalar field can form n -dimensional oscillating field bunches held together by self-action forces and having apparently a Lyapunov stability. The Bohr-Sommerfeld quantization condition is used to obtain within the framework of this model the mass spectra of n -dimensional pulsions (localized oscillating extended solutions) that are either neutral or have an elementary charge $Q = 1$.

PACS numbers: 03.70. + k

Ideas of constructing a quantum-field theory of elementary particles treated as excited states of a system of fundamental fields have been advanced numerous times. An example of such a theory is quantum chromodynamics, which is actively being developed at present and is called upon to explain hadron physics. It is known that its Lagrangian determines the interaction of spinor fields and nonlinear Yang-Mills fields. Next, one of the possible methods of representing the so-called "structureless" particles of nonzero mass is to assume that they are extended field "bunches" of finite dimensions (nonlinear-field quanta) held together by self-action forces. In the classical approach such modes are described by relativistically invariant (RIN) field equations, and the particle-like solutions of these equations can be regarded as classical proto-types of elementary particles. The development of methods of quantizing

fields described by RIN equations is one of the pressing problems of the theoretical high-energy physics. At the present time, RIN models are quantized as a rule by quasiclassical methods (see, e.g., Refs. 1-3), which yield directly the energy spectrum of particle-like excitations if classically localized solutions (LS) of the RIN equations are known.

The most investigated LS of nonlinear wave equations are solitons (see the reviews^{4,5}). These will be defined here as LS of the type $R(\mathbf{x}) \exp(-i\omega t)$, having a finite energy, charge, etc; $R(\mathbf{x})$ can in general be a scalar, a vector, or a spinor. It is clear that there can exist LS of nonlinear equations, and in particular RIN equations, of more general type, e.g., periodic in time, $u(\mathbf{x}, t+T) = u(\mathbf{x}, t)$, and even more general ones, which determine time-periodic distributions of physical quan-