

Nonconservation of spatial and combined parity in molecules with inversion level doubling

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Effects of spatial and combined parity nonconservation in molecules with inversion level doubling, in particular in the ammonia molecule, are considered. Because of the closeness of the opposite-parity components of the inversion doublet, these effects become enhanced. The operator that violates only the spatial parity does not mix the doublet components, so that the degree of spatial-parity nonconservation still turns out to be small, of the order of 10^{-17} . Nonetheless, at the high accuracy of modern radio-frequency measurements, this effect can be revealed by the splitting of the ammonia-maser mode. When combined parity is violated, the doublet components are intermixed in the lower order. By observing the linear Stark effect in the molecules NH_3 and AsH_3 , it is possible to estimate the constants of the combined-parity violating interaction and the electric dipole moment of the proton.

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Nonconservation of spatial (P) and combined (CP or T) parity in atoms and molecules is a problem that is being intensively investigated in recent years both theoretically and experimentally. The results of experiments aimed at observing optical rotation as a consequence of P -parity violation in the vapor of the Bi atom¹, and the corresponding theoretical predictions,² are widely discussed. Experiments with Tl, Cs, and Xe atoms³ yielded the best upper-bound estimates for the electric dipole moment d_e of the electron. Similar effects were considered theoretically⁴⁻⁶ also for the diatomic molecules TiF , BiS , and PbF , and was shown that for BiS and PbF (Refs. 5 and 6) the upper bound of d_e can be improved by another factor 10^5 . In Refs. 5-7 were also considered possible effects of P -parity nonconservation in the spectra of diatomic molecules.

In the present paper we consider the effects of P - and T -parity nonconservation in molecules with inversion level doubling, particularly in the ammonia molecule. This analysis is of interest for several reasons. First, parity nonconservation in such molecules manifests itself somewhat differently than in diatomic molecules, and the experiment can be performed in a different manner. Second, parity nonconservation effects in ammonia can be observed directly on the maser transition, and this seems to enhance the productivity of the experiment.

The most thoroughly investigated example of a molecule with a noticeable inversion doubling of the levels is the ammonia molecule NH_3 . The configuration of the nuclei of the NH_3 molecule in the ground state constitutes a triangular pyramid, with the nitrogen nucleus at the apex and a triangle of hydrogen nuclei at the base. Since there are two equally probable configurations in which the nitrogen nucleus is on opposite sides of the hydrogen-nuclei plane, the potential curve of the corresponding normal vibration takes the form of a double well with a barrier of finite height. The wave functions that describe the real vibrational states of the molecule are linear combinations of the wave functions for each of the wells. These functions can be symmetrical or antisymmetrical with respect to operation of the reflec-

tion of the nitrogen nuclei in the plane of the hydrogen nuclei. Then the total wave function of the molecule will have a definite parity with respect to the operation of inversion of the coordinates of all the nuclei and electrons. When the tunneling probability is taken into account, the vibrational levels corresponding to the mode under consideration split into two, and to each of the split sublevels corresponds a state with definite parity.

The magnitude of this splitting, within the framework of the one-dimensional model, is given by⁸

$$\Delta E = 2\mu^{-1}\varphi(0)\varphi'(0), \quad (1)$$

where $\varphi(0)$ and $\varphi'(0)$ is the vibrational wave function and its derivative at the point corresponding to the center of the barrier, and μ is the reduced mass. Since the function φ is assumed to be centered on the (right or left) well, the value of ΔE will be smaller the higher the barrier. Despite the relative smallness of the barrier in the NH_3 molecule, the inversion splitting still remains small: $\Delta E = 0.66 \text{ cm}^{-1}$. The idea of the present paper was to use this smallness, i. e., the proximity of the levels of opposite parity, to enhance the observable parity nonconservation effects.

The general form of the effective potentials of the interaction of the electron with the nucleus, V_P and V_{CP} , which violate the space and combined parity, respectively, is according to Refs. 6 and 9

$$V_P = \frac{1}{c^2 m^3} \{ (Z_{\text{nuc}} f_1 s + f_2 I) [p\delta^{(3)}(\mathbf{r}-\mathbf{R})]_+ + i f_3 [sI] [p\delta^{(3)}(\mathbf{r}-\mathbf{R})]_- \}, \quad (2)$$

$$V_{CP} = \frac{1}{c^2 m^3} \{ i(Z_{\text{nuc}} g_1 s + g_2 I) [p\delta^{(3)}(\mathbf{r}-\mathbf{R})]_- + g_3 [sI] [p\delta^{(3)}(\mathbf{r}-\mathbf{R})]_+ \}. \quad (3)$$

We use here the atomic units $\hbar = e = 1$, with c the speed of light, m the electron mass, Z_{nuc} the nuclear charge, s and I the electron and nuclear spin operators, p the electron momentum operator, and f_i and g_i dimensionless real constants; $[...]^\mp$ denotes a commutator or an anticommutator.

We examine now how the operators V_P and V_{CP} mix states of different parity in molecules with inversion doubling of the levels. The total molecule wave function corresponding to a state with definite parity can be

written in the adiabatic approximation in the form

$$\begin{aligned} \psi_{\pm}(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}; \mathbf{R}_1, \dots, \mathbf{R}_{N_{\text{nuc}}}) &= \psi_{\text{el}}(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}; \mathbf{R}_1, \dots, \mathbf{R}_{N_{\text{nuc}}}) \\ &\times \varphi_{\pm}(\xi_1) \varphi_{\text{vib}}(\xi_2, \dots, \xi_s) \chi_{JKM_J}(\alpha\beta\gamma) \\ &\times \eta_{SM_S}(\sigma_1^e, \dots, \sigma_{N_e}^e) \eta_I N_M I^H M_I^H (\sigma_1^{\text{nuc}}, \dots, \sigma_{N_{\text{nuc}}}^{\text{nuc}}). \end{aligned} \quad (4)$$

Here $\psi_{\text{el}}(\mathbf{r}_1, \dots; \mathbf{R}_1, \dots)$ is the electronic wave function of the fully symmetrical ground state (this function depends parametrically on the coordinates of the nuclei and is written in a reference frame rotating together with the nuclei); $\varphi_{\pm}(\xi_1)$ is the wave function of the vibrational state and corresponds to the inversion vibration; $\varphi_{\text{vib}}(\xi_2, \dots)$ is the wave function of the ground state for all the remaining vibrations; ξ_2, \dots, ξ_s are the normal coordinates; $\chi_{JKM_J}(\alpha\beta\gamma)$ is the rotational function; α, β , and γ are the rotation angles; J is the total angular momentum of the molecule; K and M_J are its projections on the molecule axis and on an arbitrary external direction; $\eta_{SM_S}(\sigma_1^e, \dots)$ is the spin function of the electrons; $\eta_I N(M_I^H)$ is the spin function of the nuclei; $I^H M_I^H$ are the spin of the nitrogen nucleus and its projection; $I^H M_I^H$ is the combined spin of the hydrogen nuclei and its projection; N_e and N_{nuc} are the numbers of the electrons and nuclei in the molecule. When the hyperfine structure is taken into account, the angular momentum of the molecule J and the spin momentum of the electrons S must also be connected with the spin momenta I^N and I^H of the nuclei.

To simplify the deviations that follow, we retain only the interaction of the electrons with the heaviest nitrogen nucleus and take into account only inversion vibrations, assuming that the threefold axis coincides with the movable axis z . We locate the origin in the plane of the hydrogen nuclei. We consider now the calculation of the matrix element $\langle \psi_{\pm} | V | \psi_{\pm} \rangle$, which determines the mixing of the states ψ_{\pm} by the operators V_P and V_{CP} . Since the ground state of the ammonia is a singlet, the averaging of operators (1) and (2) with the spin functions of the electrons causes the vanishing of those terms of (1) and (2) which contain the electron spin \mathbf{s} . Thus, experiments with ammonia yield information on the constants f_2 and g_2 .

The dependence on the rotational quantum numbers J and K , as well as on the nuclear spin I^N in the matrix elements for the molecules of the symmetrical-top type is determined in exactly the same manner as for diatomic molecules.⁸ We can therefore use the results obtained in Ref. 7 for diatomic molecules, and write

$$\begin{aligned} \langle + | V | - \rangle &= (-1)^{J-K} \frac{[I^N(I^N+1)+J(J+1)-F(F+1)]K}{4J(J+1)} \\ &\times \langle \psi_{\text{el}} \varphi_{+} \varphi_{\text{vib}} | U_z | \psi_{\text{el}} \varphi_{-} \varphi_{\text{vib}} \rangle, \end{aligned} \quad (5)$$

where F is the quantum number that determines the components of the hyperfine structure, and U_z is the component of the electron vector defined by the equation

$$V = IU \quad (6)$$

in the rotating coordinate system.

Since the nitrogen nucleus is assumed by us to be located on the z axis and the normal coordinate coincides with the coordinate z of this nucleus in the c.m.s., the operators $[\mathbf{p}\delta^{(3)}(\mathbf{r}-\mathbf{R})]_{\pm}$ in (1) and (2) can be replaced by

$$-i\kappa \left[\frac{\partial}{\partial z} \delta(z-Z) \right]_{\pm},$$

where the factor $\kappa = 17/3$ results from the changeover to the c.m.s. The operator is now independent of the coordinates ξ_2, \dots, ξ_s , and since we are disregarding also the dependence of ψ_{el} on these coordinates, we can now integrate with respect to the coordinates and obtain unity by virtue of the normalization of the function φ_{vib} . In the electron wave function $\psi_{\text{el}}(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}; Z)$ we must put $x_i = y_i = 0$. The matrix element now takes the form

$$\begin{aligned} \langle + | V_{P,CP} | - \rangle &= -\frac{i\hbar_2}{c^2 m^3} (-1)^{J-K} \frac{[I^N(I^N+1)+J(J+1)-F(F+1)]K}{4J(J+1)} \\ &\times \int \psi_{\text{el}}^*(z_1, \dots, z_{N_e}; Z) \varphi_{+} \sum_i \left[\frac{\partial}{\partial z_i} \delta(z_i-Z) \right]_{\pm} \\ &\times \psi_{\text{el}}(z_1, \dots, z_{N_e}; Z) \varphi_{-}(Z) dz_1, \dots, dz_{N_e} dZ, \end{aligned} \quad (7)$$

where $\hbar_2 = f_2, ig_2$.

In the single-electron approximation, Eq. (7) is rewritten in the form

$$\begin{aligned} \langle + | V_{P,CP} | - \rangle &= -\frac{i\hbar_2}{c^2 m^3} A_{JKIN_F} \\ &\times \sum_n \int \psi_n^*(z; Z) \varphi_{+}^*(Z) \left[\frac{\partial}{\partial z} \delta(z-Z) \right]_{\pm} \psi_n(z; Z) \varphi_{-}(Z) dz dZ, \end{aligned} \quad (8)$$

where A_{JKIN_F} denotes the rotational spin factor, and the summation extends over all the occupied states. Integrating in (8) by parts, we obtain

$$\begin{aligned} \langle + | V_{P,CP} | - \rangle &= \frac{i\hbar_2}{c^2 m^3} A_{JKIN_F} \sum_n \int \left[\left(\frac{\partial}{\partial z} \psi_n^*(z; Z) \right) \right. \\ &\times \psi_n(z; Z) \mp \psi_n^*(z; Z) \frac{\partial}{\partial z} \psi(z; Z) \left. \right] \varphi_{+}^*(Z) \varphi_{-}(Z) \delta(z-Z) dz dZ. \end{aligned} \quad (9)$$

Since ψ_n can be regarded as real, it follows from (9) that the operator V_P , in contrast to V_{CP} , does not mix the states ψ_{\pm} . The reason is that the T -odd operator $[\mathbf{p}\delta^{(3)}(\mathbf{r}-\mathbf{R})]_{\pm}$, when averaged over the functions ψ_{el} , yields some nuclear T -odd vector. On the other hand, it is clear that at fixed positions of the nuclei there are simply no nuclei vectors other than the T -odd space vectors that determine the directions of the molecule axes.

Mixing of the states ψ_{\pm} with nonconservation of only spatial parity can be attained only by taking into account the other term in the interaction operator, i.e., by replacing V_P by

$$V'_P = \frac{f_2'}{c^2 m^2 M} [\mathbf{P}\delta^{(3)}(\mathbf{r}-\mathbf{R})]_{\pm} \mathbf{I}, \quad (10)$$

where \mathbf{P} is the nuclear momentum operator and M is the mass of the nucleus. In view of the Galilean invariance, the potential of the electron-nucleus interaction can depend only on the relative velocity

$$\mathbf{V} = \mathbf{p}/m - \mathbf{P}/M,$$

whence $f'_2 = -f_2$.

The operator V'_P adds to the matrix elements an additional small factor of the order $(m/M)^{1/2}$ (see below). Replacing V_P by V'_P in (8) and again integrating by parts, we obtain in place of (9) the expression

$$\begin{aligned} \langle + | V'_P | - \rangle &= -\frac{if_2\kappa}{c^2 m^2 M} A_{JKIN_F} \\ &\times \int \rho(z; Z) \left[\left(\frac{\partial}{\partial Z} \varphi_{+}^*(Z) \right) \varphi_{-}(Z) - \varphi_{+}^*(Z) \frac{\partial}{\partial Z} \varphi_{-}(Z) \right] \delta(z-Z) dz dZ, \end{aligned} \quad (11)$$

where

$$\rho(z; Z) = \sum_n |\psi_n(z; Z)|^2 \quad (12)$$

is the expression for the electron density in the molecule at fixed positions of the nuclei.

Substituting in (11) the wave functions $\varphi_{\pm}(Z)$ in the form

$$\varphi_{\pm}(Z) = \frac{1}{\sqrt{2}} (\varphi(Z-Z_0) \pm \varphi(Z+Z_0)), \quad (13)$$

where $\varphi(Z \mp Z_0)$ are centered respectively in the upper and lower wells, we obtain

$$\langle + | V_p' | - \rangle = - \frac{i f_2 \kappa}{c^2 m^2 M} A_{JKLN_F} \times \int \rho(Z; Z) \left[\varphi(Z-Z_0) \frac{\partial}{\partial Z} \varphi(Z+Z_0) - \varphi(Z+Z_0) \frac{\partial}{\partial Z} \varphi(Z-Z_0) \right] dZ. \quad (14)$$

Using the explicit expressions for the vibrational functions of the ground state in the form⁸

$$\varphi(Z \pm Z_0) = (\mu\omega/\pi)^{1/2} \exp\{-1/2\mu\omega(Z \mp Z_0)^2\}, \quad (15)$$

we transform (14) into

$$\langle + | V_p' | - \rangle = \frac{2if_2\kappa}{c^2 m^2 M} A_{JKLN_F} \times \left(\frac{\mu\omega}{\pi}\right)^{1/2} \mu\omega Z_0 \exp\{-\mu\omega Z_0^2\} \int \rho(Z; Z) \exp\{-\mu\omega Z^2\} dZ. \quad (16)$$

Recognizing that in order of magnitude the vibration frequency ω is equal to $m(m/M)^{1/2}$ at. un., and that the characteristic scale for the electron function $\psi_n(z; Z)$ is $Z \sim 1/m$ at. un., we replace $|\psi_n(z; Z)|^2$ under the integral sign by $|\psi_n(0; 0)|^2$. Then

$$\langle + | V_p' | - \rangle = \frac{2if_2\kappa}{c^2 m^2 M} A_{JKLN_F} \mu\omega Z_0 \exp\{-\mu\omega Z_0^2\} \rho^N, \quad (17)$$

where ρ^N is the electron density at the nitrogen nucleus. As seen from (16), the matrix element $\langle + | V_p' | - \rangle$ contains one more smallness given by the factor

$$\exp\{-\mu\omega Z_0^2\} \sim \exp\{-(\mu/m)^{1/2}\}$$

and connected with the poor overlap of the vibrational functions of the different wells.

We consider now the possible manifestations of space parity nonconservation in molecules with inversion doubling. Parity nonconservation leads to a difference between the emission and absorption probabilities W_{\pm} of the left- and right-polarized quanta, and consequently to a difference between the absorption coefficients k_{\pm} , the refractive indices n_{\pm} , and the dielectric constants ϵ_{\pm} . As shown in Ref. 10, the ϵ_{\pm} difference can be revealed in principle by the splitting of the optical-resonator mode. This idea can be used also in the radio-frequency band. Generally speaking, if we disregard the hyperfine structure, the effect turns out to be of zero order, since the admixtures of the state $|+\rangle$ to $|-\rangle$ and of the state $|-\rangle$ to $|+\rangle$ cancel each other. When the hyperfine structure is taken into account this is valid for transitions with $\Delta F=0$, but not for transitions with $\Delta F=\pm 1$. In the latter case the effect is proportional to the difference

$$A_{JKLN_F} - A_{JKLN_F \pm 1}.$$

According to Ref. 10, the frequency splitting is determined by the expression

$$\Delta\omega = \omega_+ - \omega_- \sim c\rho\sigma\mathcal{P} \frac{\gamma}{\omega - \omega_0}, \quad (18)$$

where ρ is the gas density, σ is the cross section for absorption on the working transition, γ is the line width, $\omega - \omega_0$ is the frequency deviation from the line center, and \mathcal{P} is the degree of parity nonconservation in the given transition. If, as in our case, the main transition is electric and the admixture is magnetic, we get

$$\mathcal{P} \approx \frac{2\langle + | V_p' | - \rangle}{\Delta E} \left(\frac{W_{M1}}{W_{E1}}\right)^{1/2}, \quad (19)$$

where $\langle + | V_p' | - \rangle$ is the matrix element of the interaction that does not conserve parity, ΔE is the interval between the mixed levels of opposite parity, and W_{E1} and W_{M1} are the probabilities of the electric and magnetic dipole transitions.

We estimate now the value of $\Delta\omega$ for the ammonia molecule. The presence in (17) of an exponential that varies rapidly with the molecular parameters makes this formula unreliable. We therefore substitute in expression (1) for ΔE the vibrational functions (15) at $Z=0$. Then

$$\Delta E = 4\omega Z_0 (\mu\omega/\pi)^{1/2} \exp\{-\mu\omega Z_0^2\}. \quad (20)$$

Now $\langle + | V_p' | - \rangle / \Delta E$ contains no exponential and we obtain

$$\frac{\langle + | V_p' | - \rangle}{\Delta E} = \frac{if_2\kappa}{2c^2 m^2} \frac{(\pi\omega\mu)^{1/2}}{M} A_{JKLN_F} \rho^N. \quad (21)$$

We shall assume that the order of magnitude of f_2 is determined by the order magnitude of the weak-interaction Fermi constant: $f_2 \sim Gm^2 \sim 10^{-5} (m/m_p)^2$, where m_p is the proton mass. The frequency of the oscillation of interest to us is $\omega = 6 \times 10^3 \text{ cm}^{-1} = 3 \times 10^{-2}$ at. un.¹¹. The reduced mass of the NH₃ molecule is $\mu = 2.5m_p$.

To determine ρ^N we use the single-electron wave functions constructed by the MO LCAO method¹¹:

$$\begin{aligned} \psi_1 &= 1.0\psi_{1s}^{(N)} - 3 \cdot 10^{-3}\psi_{2s}^{(N)} - 10^{-3}(\psi_{1s}^{(H_1)} + \psi_{1s}^{(H_2)} + \psi_{1s}^{(H_3)}) - 2 \cdot 10^{-3}\psi_{2p_z}^{(N)}, \\ \psi_2 &= 0.03\psi_{1s}^{(N)} + 0.8\psi_{2s}^{(N)} - 0.3(\psi_{1s}^{(H_1)} + \psi_{1s}^{(H_2)} + \psi_{1s}^{(H_3)}) + 0.2\psi_{2p_z}^{(N)}, \\ \psi_3 &= 0.03\psi_{1s}^{(N)} - 0.4\psi_{2s}^{(N)} - 0.3(\psi_{1s}^{(H_1)} + \psi_{1s}^{(H_2)} + \psi_{1s}^{(H_3)}) + 0.9\psi_{2p_z}^{(N)}, \\ \psi_4 &= 0.6(\psi_{2p_x}^{(N)} + \psi_{2p_y}^{(N)}) \\ &\quad + 0.5[2 \cdot 6^{-n} \psi_{1s}^{(H_1)} + 2^{-n} (1 - 3^{-n}) \psi_{1s}^{(H_2)} - 2^{-n} (1 + 3^{-n}) \psi_{1s}^{(H_3)}]. \end{aligned} \quad (22)$$

There are two electrons each in the states ψ_1 , ψ_2 , and ψ_3 , and four electrons in the state ψ_4 . The atomic functions used were of the Slater type with screened charge of the nucleus for the nitrogen atom, and hydrogen functions for the hydrogen atoms, centered on the corresponding nuclei. Calculation yields $\rho^N \approx 2 \times 10^2 \text{ m}^3$ at. un. and for the ratio $\langle + | V_p' | - \rangle / \Delta E$ we get the estimate $\approx 10^{15}$. Recognizing that $(W_{M1}/W_{E1})^{1/2} \approx 10^{-2}$, we obtain the estimate $\mathcal{P} \approx 10^{-17}$.

The absorption cross section σ for the electric dipole transition depends little on the transition frequency and is of the order of $\sigma \sim 10^{-13} \text{ cm}^2$. As seen from (18), the effect is directly proportional to the gas density ρ . In the ammonia-maser resonator itself, the density is relatively low, $\rho \leq 10^{15} \text{ cm}^{-3}$.¹² Therefore the experiment must be so performed that a cell with denser ammonia should be placed inside the resonator. This produces in (18) an additional factor L_c/L_r , where L_c and L_r are

the dimensions of the cell and resonator. The density is limited by the absorption, which is determined by the factor

$$\exp \left\{ -\rho \sigma L_c \left(\frac{\gamma}{\omega - \omega_0} \right)^2 \right\}.$$

The quadratic dependence on the frequency detuning in this exponential makes it possible to decrease the absorption by increasing the detuning and simultaneously increasing the density. Assuming, just as in Ref. 10, that the maximum permissible absorption is e^{-10} , and putting $L_c \sim L_r \sim 1$ cm, we obtain $\rho \gamma^2 / (\omega - \omega_0) \approx 10^{14} \text{ cm}^{-3}$. If we take the gas density in the cell to be 10^{18} cm^{-3} and a detuning $(\omega - \omega_0) \sim 10^2 \gamma$, then we obtain in (18) a value

$$\Delta \omega \sim 10^{-4} - 10^{-3} \text{ Hz}, \quad (23)$$

that seems to lend itself to experimental verification. In fact, an electric dipole transition with $\Delta F \neq 0$ between the inversion sublevels is suppressed in ammonia.¹² If the corresponding magnetic transition has a normal value, this can lead to an increase of $\Delta \omega$. Thus, even though \mathcal{P} is very small compared with the discussed atomic experiments,^{1, 9, 10} experimental observation of spatial parity nonconservation using the ammonia molecule is not a hopeless task, owing to the very high accuracy of the radio-frequency measurements.

We proceed now to investigate effects of nonconservation of combined parity. In this case the states ψ_{\pm} , as seen from (9), are directly mixed by the operator V_{CP} . Substituting in (9) the wave functions (13), we arrive after simple transformations at the expression

$$\langle + | V_{CP} | - \rangle = \frac{g_2}{2c^2 m^3} A_{JKI} \int \rho^N(Z; Z) [\varphi^*(Z - Z_0) - \varphi^*(Z + Z_0)] dZ \quad (24)$$

making in the second term the substitution $Z \rightarrow -Z$ and taking the symmetry properties $\varphi(-Z) = \varphi(Z)$ and $\rho^N(-Z; -Z) = \rho(Z; Z)$ into account, we obtain

$$\langle + | V_{CP} | - \rangle = \frac{g_2}{c^2 m^3} A_{JKI} \int \rho'_N(Z; Z) \varphi^*(Z - Z_0) dZ, \quad (25)$$

where $\rho'_N(Z; Z)$ means differentiation of ρ^N with respect to only the first argument. Recognizing, as we did before the difference between the characteristic scales of the functions ψ_{el} and φ , we can take the quantity $\rho'_N(Z_0; Z_0)$ outside the integral sign in (25). Then, taking into account the normalization of the functions $\varphi(Z - Z_0)$, we get

$$\langle + | V_{CP} | - \rangle = \frac{g_2}{c^2 m^3} A_{JKI} \rho'_N, \quad (26)$$

where ρ'_N is the derivative of the electron density at the nitrogen nucleus.

It is convenient to divide $\rho^N(Z)$ into two parts, symmetrical and antisymmetrical with respect to the replacement of Z by $-Z$: $\rho^N = \rho^N_+ + \rho^N_-$. Obviously, only the derivative of ρ^N_- can differ from zero. Therefore, when the wave functions (22) are multiplied, a contribution to ρ'_N is made only by terms of the type $\psi_{1s}^{(N)} \partial \psi_{2p_z}^{(N)} / \partial Z$ or $\psi_{2s}^{(N)} \partial \psi_{2p_z}^{(N)} / \partial Z$, but not of the type $\psi_{1s}^{(N)} \partial \psi_{1s}^{(N)} / \partial Z$. Calculation yields for ρ'_N a value $\rho'_N \approx 24 m^4$ at. un. and we obtain ultimately for $\langle + | V_{CP} | - \rangle$ the estimate

$$\langle + | V_{CP} | - \rangle \approx 16 g_2 \alpha^2 m \text{ a.u.}, \quad (27)$$

where α is the fine-structure constant.

We consider now the possibility of experimentally measuring the effects of combined-parity nonconservation, bearing in mind experiments of the magnetic-resonance type.⁴ Let the molecule be in an external electric field. Owing to the mixing of the components of the inversion doublet by the interaction V_{CP} , a linear Stark effect is produced, i.e., splitting of the levels in accord with the sign of the projection of the total angular momentum M_J . The magnitude of this splitting is given by⁶

$$\Delta E = \frac{4 \langle + | V_{CP} | - \rangle}{\Delta E_0} \langle - | D | + \rangle, \quad (28)$$

where ΔE_0 is the inversion splitting in a zero field, F is the intensity of the external electric field, and D is the operator of the electric dipole moment of the molecule. When an additional external magnetic field is applied, the Zeeman splitting of the levels changes also by an amount ΔE , and this change depends on the direction of the electric field F . By the magnetic-resonance method we can measure the value of ΔE with high accuracy, to within 10^{-3} Hz.

As seen from (28), it is convenient to use external-field intensities F such that $\langle - | D | + \rangle \approx \Delta E_0$. In the case of the ammonia molecule this is reached at $F \sim 10^4$ V/cm. Now

$$\Delta E = 4 \langle + | V_{CP} | - \rangle. \quad (29)$$

Putting $\Delta E = 10^{-3}$ Hz and using the estimate (27), we get from (29)

$$g_2 \leq 2 \cdot 10^{-16}. \quad (30)$$

This is the lower limit for the constant g_2 if the linear Stark effect is not observed in the corresponding experiments. We emphasize once more that the constant g_2 cannot be measured in the experiments proposed in Refs. 5 and 6, since the corresponding effect is masked there by a stronger effect connected with the constant $Z_{nuc} g_1$ in the operator (3).

The limitation on g_2 is simultaneously a limitation on the electric dipole moment d_p of the valence proton, just as the limitation on the constant g_1 is simultaneously a limitation on the electron dipole moment d_e (see the discussion in Ref. 6 concerning this subject). This yields for the isotope N¹⁵ a limitation on the dipole moment d_p of the proton. According to Ref. 6, the presence of the proton dipole moment leads to an effective interaction of the type of the second term of (3), with the substitution

$$\frac{g_2}{c^2 m^3} \rightarrow \alpha \frac{1}{m_p} \frac{d_p}{e}, \quad (31)$$

from which follows, taking (30) into account, the limitation

$$d_p/e \leq 5 \cdot 10^{-20} \text{ c.m.} \quad (32)$$

The limitations (30) and (31) are of the same order as those obtained in experiment with the molecule TlF (Ref. 13):

$$g_2 \leq 6 \cdot 10^{-16}; \quad d_p/e \leq 5 \cdot 10^{-20} \text{ c.m.}$$

To observe parity nonconservation effects it is more convenient, generally speaking, to use molecules with heavier atoms, since in that case the electron density

ρ^N at the nucleus and its derivative ρ'_N , and with them also the matrix elements V_P and V_{CP} , increase by $(Z_{\text{nuc}}/Z_N)^4$ times, respectively. So large an increase is due to the fact that in molecules with inversion doubling of the levels the effect is determined by all the electrons, including the internal ones. From this point of view it is more convenient to use the molecules PH_3 , and particularly AsH_3 or BiCl_3 . It is necessary, however, that the inversion splitting be not too small, so that the compensating field can be monitored in the experiment. Its value for PH_3 is $1.5 \times 10^{-4} \text{ cm}^{-1}$ (corresponding to a field $F \sim 1-10 \text{ V/cm}$). The increase of Z_{nuc} yields in this case for the PH_3 and AsH_3 an amplification by 10 and 400 times, respectively.

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Vacuum polarization in a strong field and the renormalization group

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Using the renormalization group, the behavior of the polarization operator for a photon in a static external electromagnetic field is found for the following two asymptotic cases: a) in the presence of a strong crossed field, and b) at low energies in the presence of a strong magnetic field. For soft photons, the polarization operator is expressed in terms of the effective Lagrangian and is calculated in the two-loop approximation for the asymptotic cases of weak and strong magnetic fields. The structure of the perturbation series in the radiation field is determined in both asymptotic regions for the three constituents of the amplitude: the one containing the vacuum part, and the two purely field constituents. It is found that the behavior of the vacuum and field constituents is similar to those of the polarization operator and of the invariant charge in quantum electrodynamics with no external field, respectively, at large squared momenta. One of the field amplitudes is exceptional: for it, the "massless hypothesis" underlying the renormalization-group analysis is not satisfied in region b).

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1. INTRODUCTION

A number of papers have recently appeared, whose results once more confirm the importance of investigating field theories in the presence of static classical fields in order to solve fundamental theoretical problems.

In the well-known paper of Coleman and Weinberg,¹ and in a series of papers that followed it, a dynamical symmetry-breaking mechanism was proposed in which scalar fields acquire nonvanishing vacuum expectation values. One of the methods of investigating this prob-

lem involves calculating the radiative corrections to the potential, i.e. calculating the effective potential for different variants of the theory.

Interesting results in another direction were obtained in Refs. 2 and 3 by Ritus, who found the next radiative correction after the Heisenberg-Euler correction to the Maxwell Lagrangian for a static field. Using the effective Lagrangian $L(F)$ as an example, he investigated the structure of the perturbation-theory (PT) series in the radiation field of quantum electrodynamics (QED) for an intense field whose field strengths E and H greatly exceed the critical value $F_{cr} \sim m^2/e$ (m and e