CONFIGURATION INTERACTION OF TERMS IN THE SYSTEM ZeZ'

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Submitted April 25, 1968; resubmitted August 8, 1968

Zh. Eksp. Teor. Fiz. 55, 1836–1844 (November, 1968)

We investigate the recently observed[1] phenomenon of pseudo-intersection of terms in the ZeZ′ system. The WKB method is used to obtain formulas for the level splitting δE at the pseudo-intersection point, the distance R_0 between the charges Z and Z′ at which the pseudo-intersection takes place, the values of the energy E_0 at this point, and also the function that determines the total number of such pseudo-intersections in the ZeZ′ system at specified values of the charges Z and Z′ and quantum numbers n and n′ of the interacting terms. The obtained formulas are compared with the numerical calculations.

1. Recently[1] there were observed in the ZeZ′ system pseudo-intersections of the terms, i.e., of the energy levels of the electron e in the field of two fixed charges Z and Z′ separated by a distance R. This unique phenomenon (configuration interaction of the terms) is an internal property of the ZeZ′ system, and is not connected with an external dynamic perturbations (there is one electron in the system, and the nuclei are fixed). Pseudo-intersections appear at large but finite distances R between the nuclei, and have the form shown schematically in Fig. 1[1].

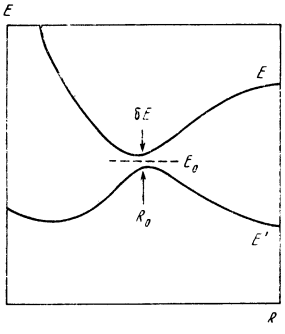

FIG. 1. Diagram of pseudo-intersections: at the point R_0 the terms E and E′ are symmetrical with respect to the value $E_0 = -(1/2)[(Z'-Z)/(n'-n)]^2$. The magnitude of the splitting δE is determined by the formula (21).

In many problems of atomic physics (for example, in the problem of asymmetrical charge exchange of the type $p\mu^- + Z \to Z\mu^- + p$[1,2]), it is just these pseudo-intersections which determine the course of the processes. To calculate the crosssections of such processes it is necessary to know the distance R_0 between the nuclei Z and Z′, at which the pseudo-intersection of the terms E and E′ takes place, and the magnitude δE of their splitting at this point. It is remarkable that the quantities R_0 and δE can be expressed analytically in terms of the quantum numbers of the levels E and E′, although the entire problem as a whole, as is well known, can be solved only numerically. We obtain these quantities in this paper with the aid of the WKB method, and therefore all subsequent calculations are also of independent interest, being a nontrivial example of the use of the quasiclassical approach[3].

2. In the WKB method, the two-center problem of quantum mechanics reduces to a problem of quantization in a double well of the type shown in Fig. 2a. The quasi-classical conditions for quantization in such a well were found in[4], and are given by ($Z' > Z$)

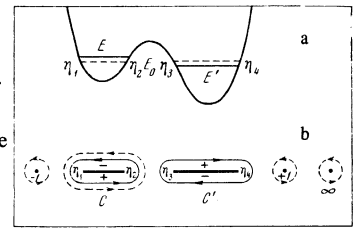

FIG. 2. Quantization scheme in a double well near the point of pseudo-intersection R_0 and diagram of the complex plane for the quasimomentum $Q(\eta)$.

$$\operatorname{ctg}\omega_2 \operatorname{ctg}\omega_2' = \operatorname{tg}^2(e^{-K}/2), \qquad \omega_1 = \pi(n_1 + 1/2), \tag{1}$$

where

$$\omega_2 = \int_{\eta_1}^{\eta_2} Q(\eta)\,d\eta, \quad \omega_2 = \int_{\eta_3}^{\eta_4} Q(\eta)\,d\eta, \quad K = \int_{\eta_2}^{\eta_3} |Q(\eta)|\,d\eta,$$

$$\omega_1 = \int_{\xi_1}^{\xi_2} R(\xi)\,d\xi,$$

$$Q(\eta) = \left[\frac{-p^2(1-\eta^2)+b\eta-\lambda}{1-\eta^2} - \frac{m^2}{(1-\eta^2)^2}\right]^{1/2},$$

$$R(\xi) = \left[\frac{-p^2(\xi^2-1)+b'\xi+\lambda}{\xi^2-1} - \frac{m^2}{(\xi^2-1)^2}\right]^{1/2},$$

$$p^2 = -1/2R^2E, \quad b = R(Z'-Z), \quad b' = R(Z'+Z),$$
$$p = 1/2R\varkappa, \quad \varkappa = \sqrt{-2E}, \tag{2}$$

E and λ are the energy and the separation constant of the two-center problem, and η_i and ξ_i are the corresponding roots of the equations $Q(\eta) = 0$ and $R(\xi) = 0$[4]. When $R \gg 1$, the following expansions[4] (all in atomic units $\hbar = m = e = 1$) hold true for the eZ terms (i.e., for the terms which go over into the levels of the isolated atom eZ as $R \to \infty$):

$$E = -\frac{1}{2}\left(\frac{Z}{n}\right)^2 - \frac{Z'}{R} + \frac{3}{2}n(n_1-n_2)\frac{Z'}{ZR^2},$$

$$\lambda + b = -4p\nu\left[1 - \frac{1}{2p}(\nu+\alpha) - \frac{1}{8p^2}(2\nu^2+2\alpha^2+3\nu\alpha)\right]. \tag{3}$$

Here n, n_1, n_2, and m are the parabolic quantum numbers of the eZ level and the following notation is introduced

$$\nu = n_2 + 1/2, \qquad \alpha = b/2p. \tag{4}$$

The formulas for the eZ′ terms are obtained from (3) following the substitutions $Z \leftrightarrow Z'$, $n_1 \to n_1'$, $n_2 \to n_2'$, and $n \to n'$ and—as a consequence—of the substitutions $\nu \to \nu'$, $b \to -b$, and $\alpha \to -\alpha$. We shall designate all the quantities in the right-hand well by primes:

$$E' = -\frac{1}{2}\left(\frac{Z'}{n'}\right)^2 - \frac{Z}{R} + \frac{3}{2}n'(n_1' - n_2')\frac{Z}{Z'R^2},$$

$$\lambda' - b = -4p\nu'\left[1 - \frac{1}{2p}(\nu' - \alpha) - \frac{1}{8p^2}(2\nu'^2 + 2\alpha^2 - 3\nu'\alpha)\right]. \quad (3')$$

3. The expansions (3) and (3′) were obtained from the equations

$$\omega_2(p, \lambda) = \pi\nu, \quad \omega_2'(p', \lambda') = \pi\nu', \quad (5)$$

i.e., under the assumption that the influence of the second well can be neglected in the quantization condition (1). When $R \to \infty$, we simultaneously have $K \to \infty$, and this neglect is perfectly legitimate so long as the levels E and E′ differ greatly from each other. However, if at a certain point R_0 (but under the barrier!) these levels come closer together, then they can no longer be quantized independently in each of the wells. In this case it is necessary to solve the transcendental equation (1), for which it is necessary to find one more condition relating the phase integrals ω_2 and ω_2'.

In order to find this condition, let us consider the complex plane of the quasimomentum $Q(\eta)$ (see Fig. 2b). Fixing the signs on the cuts, we obtain directly

$$2\omega_2 = \oint_C Q(z)\,dz, \quad 2\omega_2' = \oint_{C'} Q(z)\,dz. \quad (6)$$

Deforming the contour C′ as shown in Fig. 2b, we obtain the relation[3]

$$2\omega_2' = 2\omega_2 + 2\pi i[\mathrm{Res}(-1) + \mathrm{Res}(+1) - \mathrm{Res}(\infty)]. \quad (7)$$

The residues at the points $z = \pm$ cancel each other, and $\mathrm{Res}(\infty) = ib/2p$. We finally obtain an equation that is valid for all values of p and λ:

$$\omega_2'(p, \lambda) - \omega_2(p, \lambda) = \pi b / 2p. \quad (8)$$

We find the values of p_0 and λ_0 from the conditions

$$\omega_2(p_0, \lambda_0) = \pi\nu, \quad \omega_2'(p_0, \lambda_0) = \pi\nu', \quad (9)$$

which determine the fictitious point of intersection of the levels E and E′ (actually there is no such point, since the conditions (9) contradict Eq. (1) at all finite values of R). Substituting them in (8), we obtain

$$b / 2p_0 = \nu' - \nu = n_2' - n_2 = \alpha. \quad (10)$$

In addition, it follows from the conditions (9) that the "radial" phase integrals ω_1 and ω_1' should coincide at the point (p_0, λ_0), for in this case the potential of the "radial" equation has the form of a simple oscillator well, which is the same for both levels E and E′[4]:

$$\omega_1(p_0, \lambda_0) = \pi k = \omega_1'(p_0, \lambda_0) = \pi k', \quad k = n_1 + 1/2, \quad k' = n_1' + 1/2. \quad (11)$$

From this we conclude immediately that pseudo-intersections are possible for only those levels, in which the radial quantum numbers are equal: $n_1 = n_1'$, in agreement with the previously established empirical rule[1].

Taking this condition into account, and also the definitions (2) and the equalities $n = n_1 + n_2 + n + 1$ and $n' = n_1' + n_2' + m + 1$ from relation (10), we obtain the energy E_0 at the pseudointersection point

$$\varkappa_0 = \frac{Z' - Z}{\alpha} = \frac{Z' - Z}{n' - n}, \quad \alpha = n' - n,$$
$$E_0 = -\frac{1}{2}\left(\frac{Z' - Z}{n' - n}\right)^2. \quad (12)$$

It is curious that the set of energy values E_0 at the pseudo-intersection points forms the Coulomb series of a hydrogen-like atom with charge $Z' - Z$ and principal quantum number $n' - n$.

4. At the point of pseudo-intersection R_0, all three energies E, E′, and E_0 are close to each other and therefore the following relations are valid:

$$\omega_2(p, \lambda) = \pi\nu + \Delta\omega_2, \quad \omega_2(p', \lambda') = \pi\nu + \Delta\tilde{\omega}_2,$$
$$\omega_2'(p', \lambda') = \pi\nu' + \Delta\omega_2', \quad \omega_2'(p, \lambda) = \pi\nu' + \Delta\omega_2', \quad (13)$$

where all the increments of the phase integrals $\Delta\omega_2$, $\Delta\omega_2'$, etc. are much smaller than unity. From (1) and (8) we can easily establish that

$$-2\Delta\omega_2 = 2\Delta\tilde{\omega}_2 = \delta\omega_2 = \frac{\partial\omega_2}{\partial p}\delta p + \frac{\partial\omega_2}{\partial\lambda}\delta\lambda,$$
$$2\Delta\omega_2' = -2\Delta\tilde{\omega}_2' = \delta\omega_2' = \frac{\partial\omega_2'}{\partial p}\delta p + \frac{\partial\omega_2'}{\partial\lambda}\delta\lambda. \quad (14)$$

In relations (14), $\delta p = p' - p$, $\delta\lambda = \lambda' - \lambda$ are the total increments of the parameters on going from the term E to the term E′, and all the quantities are taken at the point (p_0, λ_0).

It is possible to show by the same method that at the point R_0 the energy $E_0 = (E + E')/2$, apart from exponentially small corrections, i.e., the splitting of the terms E and E′ is symmetrical with respect to the value E_0. When relations (10), (13) and (14) are taken into account, the conditions (1) and (8) are equivalent to the following system of equations (we shall henceforth omit the zero subscript)

$$\delta\omega_2'\,\delta\omega_2 = e^{-2K}, \quad \delta\omega_2' - \delta\omega_2 = -\frac{\pi\alpha}{p}\delta p, \quad \alpha = n' - n, \quad (15)$$

from which we can easily see that $\delta\omega_2$ and $\delta\omega_2'$ are the roots of a quadratic equation, and following the substitutions

$$\delta p = \frac{1}{\sigma}e^{-K}, \quad a = \frac{\pi\alpha}{2p} \quad (16)$$

they take the form

$$\delta\omega_2 = (a - \sqrt{a^2 + \sigma^2})\delta p, \quad (17)$$
$$\delta\omega_2' = (-a - \sqrt{a^2 + \sigma^2})\delta p. \quad (17')$$

In addition, from (11) we get

$$\delta\omega_1 = \frac{\partial\omega_1}{\partial p}\delta p + \frac{\partial\omega_1}{\partial\lambda}\delta\lambda = 0. \quad (18)$$

Using (14), (17), and (18), we obtain an equation for σ:

$$\frac{\partial(\omega_1, \omega_2)}{\partial(p, \lambda)} + (a - \sqrt{a^2 + \sigma^2})\frac{\partial\omega_1}{\partial\lambda} = 0. \quad (19)$$

The calculations given in the appendix yield for the

case of the σ terms (m = 0)[1)]

$$\delta v = \frac{p}{\pi \sqrt{n'n}} e^{-K}. \tag{20}$$

Using the relation $\delta E = -4p\delta p/R^2$ and calculating K, we obtain ultimately

$$\delta E = \frac{2\varkappa^2}{\sqrt{n'n}} \frac{(4p)^s}{n_2'!\, n_2!} e^{-2p}. \tag{21}$$

Here $s = \nu' + \nu = n_2' + n_2 + 1$, $\kappa = \sqrt{-2E}$, and all the quantities are taken at the point of the pseudo-intersection.

In the symmetrical case Z′ = Z, n′ = n, $n_2' = n_2$, and formula (21) goes over into formula (13) of[5] for the splitting of the symmetrical and antisymmetrical terms of the molecular hydrogen ion H_2^+ as $R \to \infty$.

5. Let us compare the obtained formulas with the results of numerical calculations[1] for the terms 5gσ (n = 1, $n_1 = n_2 = m = 0$) and 4fσ (n′ = 4, $n_1' = 0$, n_2' = 3, m = 0) of the system Z = 1 and Z′ = 5. Numerical calculations yield[1]

$$R_0 = 12.960; \quad E_0 = -0.888254; \quad \delta E = 4.246 \cdot 10^{-3}. \tag{22}$$

The value of R_0 is determined here at the point where the term splitting δE is minimal, this being purely arbitrary. Indeed, inasmuch as the point R_0 is fictitious, other definitions are also possible, and only the magnitude of the splitting δE has a real meaning.

So far we have determined R_0 from relations (9) under the condition that $\delta\omega_2$ and $\delta\omega_2'$ are calculated at the value $\alpha = n' - n$, and simultaneously

$$E_0 = E(R_0) = E'(R_0). \tag{23}$$

The first of these equalities leads to the result

$$R_0 = 2Z' \left[\left(\frac{Z'-Z}{n'-n} \right)^2 - \left(\frac{Z}{n} \right)^2 \right]^{-1}. \tag{24}$$

Numerically (in this case $\kappa_0 = 4/3$ and 2p = 17.16) we get

$$R_0 = 12.87; \quad E_0 = -0.8889; \quad \delta E = 14.7 \cdot 10^{-3}. \tag{25}$$

It is easy to see that the conditions (23) are contradictory; by equating (3) with (5) we get from the second equality in (23) that $R_0 = 13.26$. This circumstance is connected with the general indeterminacy of the point R_0. It is more consistent[2)] although less lucid, to determine the values of R_0 and α from the relations (23), rewritten in the form

$$-\frac{1}{2}\left(\frac{Z'-Z}{\alpha} \right)^2 = E(R_0) = E'(R_0). \tag{26}$$

In this case α = 3.020, $\kappa_0 = 1.325$, and 2p = 17.56, and in lieu of (25) we obtain

$$R_0 = 13.26; \quad E_0 = -0.8771; \quad \delta E = 10.4 \cdot 10^{-3}. \tag{27}$$

When account is taken of the corrections proportional to 1/p (A.3) we obtain in place of (25) and (27), respectively,

$$\delta E = 11.4 \cdot 10^{-3}, \quad \delta E = 8.0 \cdot 10^{-3}.$$

The values in (25) and (27) differ insignificantly from each other, but they coincide with the exact value (22) only in order of magnitude. The cause of this difference is apparently not the approximate character of the WKB method, but the asymptotic nature of formula (21): its region of applicability has not yet been reached at the given values of n, n′, Z, and Z′.

6. The pseudo-intersection phenomenon is a sui-generis form of quantum-mechanical exchange interaction[3)], which arises even in the absence of spin, and is connected with the approximate degeneracy of the levels of the ZeZ′ system at certain values of the parameters in the Hamiltonian. However, the term responsible for this degeneracy cannot be separated from the Hamiltonian, and in this lies the peculiarity of the phenomenon, unlike the well known spin degeneracy.

It is established in[1] that in the ZeZ′ system at Z = 1 the pseudo-intersections arise only at values $Z' \geq 5$. We derive a general condition under which pseudo-intersections appear in the ZeZ′ system, and also a formula for the total number of such pseudo-intersections, if they are possible.

Just as in the problem of the molecular hydrogen ion H_2^+, the degeneracy of the levels E and E′ is possible only in the case when they are separated by a potential barrier, i.e., under the condition

$$U_{max}(R) > E_0, \tag{28}$$

where $U_{max}(R) = -(\sqrt{Z} + \sqrt{Z'})^2/R$ is the height of the potential barrier separating the two wells eZ and eZ′[1]. Taking into account the equalities (24) and (12), we obtain from this a limitation on the value of α:

$$\alpha > n(x-1)\sqrt{1+2x}, \quad x = (Z'/Z)^{1/2}. \tag{29}$$

Further, the pseudo-intersection of the eZ term is possible only with those eZ′ terms which lie deeper than the chosen eZ term when $R \to \infty$, i.e., under the condition $Z'/n' > Z/n$ (n and n′ are the parabolic quantum numbers of the isolated eZ and eZ′ atoms). Putting

$$n' = nZ'/Z - r,$$
$$\alpha = n(Z'/Z - 1) - r = n(x^2 - 1) - r, \tag{30}$$

we determine from the inequality (28) the value of r, i.e., the number of eZ′ terms that pseudo-intersect with the chosen eZ term n (see Fig. 3):

$$r < n(x-1)(x+1-\sqrt{1+2x}) = ng(x),$$
$$r_0 = \mathrm{Ent}\,[ng(x)]. \tag{31}$$

Figure 4 shows a plot of the function ng(x) at different values of n. It follows from it immediately that when Z = 1 the first pseudo-intersection (r = 1) for the term n = 1 (ground state of the eZ atom) in the system ZeZ′ occurs only when Z′ = 5; this agrees with the result of[1]. With increasing values of n and Z′, the number of such pseudo-intersections increases

[1)] The derivation of (20) actually does not depend on the concrete form of the potential of the type shown in Fig. 2a. It is therefore applicable not only to the two-center problem, but to all problems of quantum mechanics in which systems consisting of two weakly coupled subsystems are investigated (for example, in the collision of complex atoms).

[2)] This circumstance was pointed out to the author by A. V. Matveenko.

[3)] This phenomenon has an exact classical analog: the interaction of two resonators coupled by a narrow channel, at definite relations between their dimensions (the so-called parametric resonance).

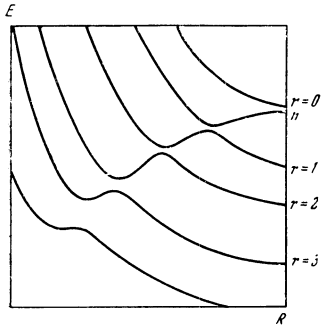

FIG. 3. Pseudo-intersection scheme of eZ term (n, n_1, n_2, m) with eZ′ terms (n′, n_1', n_2', m): $n' = nZ'/Z - r$, $n_1 = n_1'$. When r = 0 we have $n' = nZ'/Z$, and when $R \to \infty$ the eZ and eZ′ terms coincide. The number r runs through the values $r = 1, 2, \ldots, r_0$.

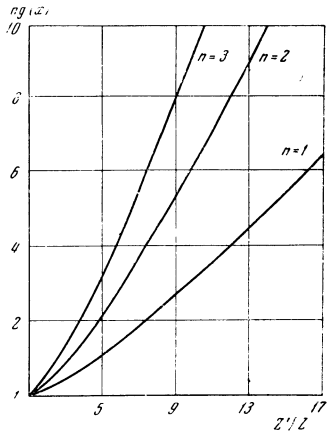

FIG. 4. Plot of the function ng(x), which determines the maximum number of pseudo-intersections r_0 at fixed values of the radial quantum number $n_1 = n_1'$ and different values of n – the principal quantum number of the eZ term. At fixed values of n_1 and m we have $r_0 = \mathrm{Ent}[ng(x)]$. The total number of pseudo-interactions of the eZ term with the eZ′ term is

$$r_{max} = \frac{n(n+1)}{2} r_0,$$

$$g(x) = (x-1)(x+1-\sqrt{1+2x}), \quad x = \sqrt{Z'/Z}$$

rapidly[4)], and therefore they must be taken into account in asymmetrical charge-exchange processes.

7. A few general remarks concerning the ZeZ′ system. Although there exists a developed algorithm for the calculation of any term of this system[1,6], it has been impossible so far to express analytically the energy $E = E(n_\xi, n_\eta, m; R)$ as a function of the elliptic quantum numbers n_ξ, n_η, m, and the intercenter distance R (and it is not clear whether such an expression exists at all). These exist, however, four characteristic values of R, at which such expressions do occur, and in each such case a Coulomb series of levels appears:

At $R \to \infty$

$$E = -\frac{1}{2}\left(\frac{Z}{n}\right)^2, \quad E' = -\frac{1}{2}\left(\frac{Z'}{n'}\right)^2;$$

At $R \gg 1$, at the pseudo-intersection points

$$E_0 = -\frac{1}{2}\left(\frac{Z'-Z}{n'-n}\right)^2;$$

At $R \sim 1$ the wave functions of the system are expressed in terms of polynomials at the points where the energy of the system obeys the condition[7] (N, L, n--integers):

$$E = -\frac{1}{2}\left(\frac{Z'+Z}{N}\right)^2 = -\frac{1}{2}\left(\frac{Z'-Z}{L}\right)^2 = \begin{cases} -1/2n^2 \\ -2/n^2 \end{cases}$$

and finally, at R = 0 the problem again becomes degenerate

$$E_N = -\frac{1}{2}\left(\frac{Z'+Z}{N}\right)^2.$$

The foregoing regularities are too simple to be accidental, and should therefore have a common and deeper cause.

This investigation was a result of stimulating discussions with I. V. Komarov and S. Yu. Slavyanov, who considered this problem by a method proposed by them earlier[8]. I consider it my pleasant duty to express my gratitude to them, and also to S. P. Alliluev, S. S. Gershteĭn, Yu. N. Demkov, and Ya. A. Smorodinskiĭ for fruitful discussions.

APPENDIX

For σ terms, the azimuthal quantum number m = 0, $\eta_1 = -1$, $\eta_4 = 1$, $\eta_2 = -q = -1 + \beta$, $\eta_3 = q' = 1 - \beta'$, $\xi_1 = 1$, and $\xi_2 = 1 + \rho$, and β, β′, ρ ≪ 1 when p ≫ 1. Using (2), (3), and the results of an earlier paper[4], get

$$\beta = \frac{2\nu}{p}\left(1 + \frac{\nu+\alpha}{2p}\right), \quad \beta' = \frac{2\nu'}{p}\left(1 + \frac{\nu'-\alpha}{2p}\right),$$
$$\rho = \frac{2k}{p}\left(1 + \frac{\alpha'-k}{2p}\right), \quad \alpha' = \frac{b'}{2p} = \frac{Z'+Z}{\varkappa},$$
$$\nu = n_2 + 1/2, \quad \nu' = n_2' + 1/2, \quad k = n_1 + 1/2, \quad \alpha = \nu' - \nu. \quad \text{(A.1)}$$

All the integrals of the problem are calculated either in terms of B (the Euler integrals) or in terms of complete elliptic integrals. For example:

$$\frac{\partial\omega_2}{\partial p} = -p\int_{-1}^{-q} d\eta \left[\frac{1-\eta^2}{-p^2(1-\eta^2)+b\eta-\lambda}\right]^{1/2}$$
$$\approx -\frac{\pi\beta}{2}\sqrt{\frac{2}{2-\beta'}}\left(1 + \frac{\beta\beta'}{16}\right).$$

Ultimately we get ($s = \nu' + \nu$)

$$\frac{\partial\omega_1}{\partial p} = -\frac{\pi k}{p}\left(1 + \frac{\alpha'-k}{p}\right), \quad \frac{\partial\omega_1}{\partial\lambda} = \frac{\pi}{4p}\left(1 + \frac{\alpha'-2k}{2p}\right),$$
$$\frac{\partial\omega_2}{\partial p} = -\frac{\pi\nu}{p}\left(1 + \frac{s+\alpha}{2p}\right), \quad \frac{\partial\omega_2}{\partial\lambda} = -\frac{\pi}{4p}\left(1 + \frac{s}{2p}\right),$$
$$\frac{\partial(\omega_1,\omega_2)}{\partial(p,\lambda)} \Big/ \frac{\partial\omega_1}{\partial\lambda} = \frac{\pi}{p}\left[\nu\left(1 + \frac{s+\alpha}{2p}\right) + k\left(1 + \frac{s+\alpha'}{2p}\right)\right]. \quad \text{(A.2)}$$

For σ we obtain from (19) the equation

$$\sqrt{a^2+\sigma^2} = \frac{\pi}{2n}\left[(n'+n) + \frac{2n'n - k(n'+n-\alpha')}{p}\right]. \quad \text{(A.3)}$$

Neglecting the terms ~1/p, we obtain from this

[4)] Actually it is even larger than follows from Fig. 4: according to condition (11), only those terms for which $n_1 = n_1'$ interact. But when m = 0 and at a specified n, the number n_1 runs through the series of values $n_1 = 0, 1, 2, \ldots, n-1$, and therefore the total number of the pseudo-interactions of the level n is equal to $r = n\,\mathrm{Int}[ng(x)]$, where Int[x] denotes the integer part of x. On the other hand, if pseudo-interactions of the terms with $m \neq 0$ are also taken into account, then their total number is $r_{max} = n(n+1)r_0/2$.

$$\sigma = \frac{\pi}{p}\sqrt{n'n}. \tag{A.4}$$

In the symmetrical case Z′ = Z, n′ = n, α' = 2n, and for σ we obtain the more exact expression:

$$\sigma = \frac{\pi n}{p}\left(1+\frac{n}{p}\right). \tag{A.5}$$

The integral K can be easily calculated, after breaking down the integration region (−q, q′) into two regions (−q, 0) and (0, q′), in terms of complete elliptic B-integrals[9]:

$$K \approx p[q^2B(q)+(q')^2B(q')]+O\left(\frac{1}{p}\right), \quad B(q)=\int_0^{\pi/2}\frac{\cos^2\varphi}{\sqrt{1-q^2\sin^2\varphi}}d\varphi. \tag{A.6}$$

When q → 0, the following asymptotic formula is valid[9]

$$q^2B(q) \approx q^2\left[1-\frac{1}{2}\left(\ln\frac{4}{\sqrt{1-q^2}}-\frac{3}{2}\right)(1-q^2)\right] \approx 1-\frac{\nu}{p}\ln\frac{4pe}{\nu}. \tag{A.7}$$

Using the Stirling formula

$$n! = \sqrt{2\pi}\left(\frac{n+1/2}{e}\right)^{n+1/2},$$

we obtain the relation

$$e^{-K} = 2\pi\frac{(4p)^s}{n_2!\,n_2'!}e^{-2p}, \tag{A.8}$$

which, with allowance for (16) and (A.4) leads to the final formula (21). In the symmetrical case, the WKB method leads to the result:

$$\delta E = \frac{2\varkappa^2}{n}\frac{(4p)^{2n_r+1}}{n_2!\,n_2!}e^{-2p}\left(1+\frac{n}{p}\right)^{-1}. \tag{A.9}$$

This example can be used to trace the usual singularity of the quasiclassical approach: formula (A.8) has been derived under the assumption $n_2 \gg 1$ and $n_2' \gg 1$ but it remains valid down to values $n_2 = 0$.

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Translated by J. G. Adashko
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