Asymptotic electron terms of colliding identical heavy nuclei

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The change in the energy levels of the inner shells of heavy nuclei upon bombardment by identical nuclei (e.g. in uranium-uranium collisions) is investigated in the adiabatic approximation. The problem is considered in the asymptotic limit when the distance between the nuclei is large compared to the electron Compton wavelength. A formula is derived for the dependence of the electron-term energy on the charges of and the distance between the nuclei. A corresponding quasiclassical formula for excited states with a large number of nodes is obtained which gives the splitting of the levels of two identical three-dimensional wells separated by a high barrier. The preexponential factor in the quasiclassical problem of the splitting of the levels of two identical one-dimensional wells separated by a high barrier is discussed.

When heavy nuclei are bombarded by heavy nuclei (e.g., uranium nuclei by uranium nuclei), the electron terms of the inner shells can drop down drastically and even cross the lower boundary of the Dirac continuum. In fact, if an uranium nucleus ($Z = 92$) comes close to another uranium nucleus, then the combined system has a charge $Z = 184$; this is higher than the critical charge $Z = 170$ corresponding to the attainment of the ground state of the lower limit of the Dirac continuum[1]. In this connection it is of interest to compute the motion of the electron levels as the nuclei approach each other.

Of special interest are the inner shells. The motion of the nuclei takes place adiabatically slowly; therefore we can consider the electron terms of the inner shells for a fixed distance R between the centers of the nuclei[2].

The problem is essentially relativistic. In contrast to the Schrödinger equation, the Dirac equation for an electron in the field of two nuclei does not admit of separation of the variables in elliptic coordinates, and this makes its solution difficult. In the present paper we investigate the limiting case $R \gg 1$ (further, we use the system of coordinates with $\hbar = m = c = 1$; a unit length in these units is an electron Compton wavelength equal to 386 F).

It is of interest to consider the collision of identical nuclei, since in this case the solution has a simple analytical form. Furthermore, it is well known that in this case the cross section of the secondary effect connected with direct pair production by the strong Coulomb field decreases by many orders of magnitude. The method of solving the problem is similar to the method in the nonrelativistic case[3].

The Dirac equation for the bispinor

$$\psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

has the form

$$\sigma \mathbf{p} \xi = (\varepsilon + 1 - V)\eta, \quad \sigma \mathbf{p} \eta = (\varepsilon - 1 - V)\xi.$$

Here V is the total Coulomb potential of both nuclei. Eliminating from this the spinor η and making the functional substitution[2] $\xi = (\epsilon + 1 - V)^{1/2}\varphi$, we obtain the following equation for φ found by Popov[1]:

$$\Delta\varphi + k^2\varphi = 0. \tag{1}$$

Outwardly it looks like the Schrödinger equation, but in the case under consideration the quantity k^2 has the form

$$k^2 = (\varepsilon - V)^2 - 1 - \frac{\Delta V}{2W} - \frac{3}{4}\frac{(\nabla V)^2}{W^2} - \frac{1}{W}[\nabla V \times \mathbf{p}]\sigma, \tag{2}$$

where $W \equiv \epsilon + 1 - V$. Because of the spin-orbit term, it is not Hermitian; however, we shall see later that this is not important.

For $R \gg 1$, we represent the solution φ in the form of a superposition of the solutions $\varphi_0(x, y, z)$ and $\varphi_0(-x, y, z)$ respectively localized near the right ($x = R/2$) and left ($x = -R/2$) charges:

$$\varphi = \varphi_0(x, y, z) \pm \varphi_0(-x, y, z).$$

The equation for φ_0 has the form

$$\Delta\varphi_0 + k_0^2\varphi_0 = 0. \tag{3}$$

On the face of it, it seems that φ_0 is the solution in the right well, and that this solution needs not be corrected for the presence of the left nucleus. But we shall see that, as in the nonrelativistic case, this is incorrect. Therefore, under the potential V in k_0^2 we shall also understand the total potential of both charges, while under the energy ϵ in k_0^2 we shall understand the energy of an electron in the right well, which energy has been corrected in the first approximation for the presence of the left well, i.e., the quantity $\epsilon_0 - Z/R$ (allowance for the next correction, which corresponds to dipole interaction, is discussed at the end of the article); here and below under Z we shall understand $Z/137$.

Let us multiply Eq. (1) from the left by $\varphi_0(x, y, z)$ and Eq. (3) from the left by φ; then let us take the difference between the resulting equations and integrate it over the region $0 < x < \infty$, $-\infty < y, z < \infty$. Let us consider the individual terms arising from the integration:

$$\pm \int_{x>0} (\varphi_0\Delta\varphi - \varphi\Delta\varphi_0)\,d\mathbf{r} = \pm 2\int \left(\varphi_0 \frac{\partial\varphi_0}{\partial x}\right)_{x=0} dS. \tag{4}$$

Here the integration is over the area $dS = dydz$ passing through the middle ($x = 0$) of the distance between the nuclei.

Let us describe the individual terms obtained in the integration of the expression

$$\int (\varphi_0 k^2\varphi - \varphi k_0^2\varphi_0)\,d\mathbf{r}.$$

We have

$$\int_{x>0} \left\{ \left[(\varepsilon - V)^2 - 1 - \frac{3}{4}\left(\frac{\nabla V}{W}\right)^2 \right] \right.$$

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$$-\left[(\varepsilon_0-V)^2-1-\frac{3}{4}\left(\frac{\nabla V}{W_0}\right)^2\right]\Big\}\varphi\varphi_0\,d\mathbf{r}. \tag{5}$$

Let us replace φ by φ_0 in the integrand, since the integration virtually takes place in the vicinity of the right charge where the function $\varphi_0(-x, y, z)$ is exponentially small. We also retain from the total potential V only the potential $V_0 = -Z/r$ of the right nucleus, since the contribution of the potential of the left nucleus to the integral is smaller by a factor of R. Then the expression (5) is approximately equal to

$$(\varepsilon-\varepsilon_0)\int\left[2(\varepsilon_0-V_0)+\frac{3}{2}\frac{(V_0')^2}{W_0^3}\right]\varphi_0^2\,d\mathbf{r}. \tag{6}$$

The term containing $-\nabla V/2W$ in the expression (2) for k^2 does not contribute to the integral. Indeed, the quantity ΔV is proportional to δ-functions at the points where the nuclei are located. In the present case the dominant contribution is made by the δ-function $\delta(r)$ at the location of the right nucleus. We shall first of all be interested in the change in the ground term $1s_{1/2}$. Then the solution φ_0 has the form (nor normalized)[4]

$$\varphi_0 = r^{\varepsilon_0-1}e^{-Zr}/W_0^{1/2}, \tag{7}$$

where $\epsilon_0 = (1 - Z^2)^{1/2}$. The bottom component of the spinor φ_0 can be neglected, since we shall see that in the problem under consideration the spin-orbit potential, which couples the spinor components, is unimportant. The quantity

$$\int\Delta V\left(\frac{1}{W}-\frac{1}{W_0}\right)\varphi_0^2\,d\mathbf{r}$$

is proportional to the integral

$$\int\frac{1}{W_0^2}\varphi_0^2\delta(\mathbf{r})\,d\mathbf{r}.$$

Since $\varphi_0^2/W_0^2 \propto r^{2\epsilon_0+1}$ as $r \to 0$, this integral vanishes.

Let us finally consider the spin-orbit term in the expression (2). Because of its non-Hermiticity, there are two types of contributions. Let us first set $\epsilon = \epsilon_0$. We then obtain the contribution

$$\int\limits_{x>0}\frac{1}{W_0}\{\varphi_0[\nabla V\times\mathbf{p}]\sigma\bar{\varphi}_0-\bar{\varphi}_0[\nabla V\mathbf{p}]\sigma\varphi_0\}\,d\mathbf{r}.$$

Here we have set $\bar{\varphi}_0 \equiv \varphi_0(-x, y, z)$. We shall further see that because of the exponential decrease of the functions φ_0 and $\bar{\varphi}_0$, such type of integrands are substantially different from zero only in the region of the thin tube joining the charges. Its length is equal to R and the diameter is of the order of $\sqrt{R}$. Consequently, the volume $\int d\mathbf{r}$ is of the order of R^2. Since $\nabla V \propto 1/R^2$, the integral in question is of the order of $R^{2\epsilon_0-2}e^{-ZR}$. As we shall see below, this is R times smaller than the integral (4). Thus, the contribution due to the non-Hermiticity of the spin-orbit operator can be neglected.

Let us now estimate the contribution made by this same operator, a contribution which is proportional to the energy shift $\epsilon - \epsilon_0$:

$$(\varepsilon-\varepsilon_0)\int\frac{1}{W_0^2}\varphi_0[\nabla V,\mathbf{p}]\sigma\varphi_0\,d\mathbf{r}.$$

Here we have already made the substitution $\varphi \to \varphi_0$ for the same reasons as was done earlier. The potential V consists of two parts. Let us first consider the potential V_0 of the right nucleus. The expression $[\nabla V\cdot\mathbf{p}]\sigma$ is proportional to the spin-orbit operator $l\sigma$. When it acts on φ_0 it yields the factor $(\kappa + 1)$, where the quantum number κ is, for the states with the angular momenta $j = l \pm 1/2$, equal to $\pm(j + 1/2)$[4]. For the state $1s_{1/2}$ under consideration the quantity $\kappa = -1$ and the contribution vanishes. The contribution of the potential of the left nucleus can be neglected, since it is proportional to $1/R^2$.

Collecting the expressions (4) and (6) together, we find

$$\varepsilon-\varepsilon_0=\mp\left[\int(\varphi_0\partial\varphi_0/\partial x)_{x=0}\,dS\right]\Big/\int\left[\varepsilon_0-V_0+\frac{3}{4}\frac{(V_0')^2}{W_0^3}\right]\varphi_0^2\,d\mathbf{r}. \tag{8}$$

Let us first compute this expression, assuming that φ_0 is the regular solution (7) to the Dirac equation in the right well. In computing the numerator of the expression (8), we go over to polar coordinates. Then it has the form

$$\mp\frac{1}{2}\frac{ZR}{1+\varepsilon_0}\int\limits_0^\infty 2\pi\rho d\rho\, r^{2\varepsilon_0-3}e^{-2Zr}.$$

It can be seen from this that typical values of the coordinates y, z, and $\rho = (r^2 - R^2/4)^{1/2}$ at which the integrand is different from zero are of the order of $\sqrt{R}$. Computing the integral, we obtain

$$\mp\frac{\pi}{1+\varepsilon_0}\left(\frac{1}{2}R\right)^{2\varepsilon_0-1}e^{-ZR}.$$

The computation of the denominator of the expression (8) leads to incomplete gamma functions and their derivatives[5]. However, as a result of tedious calculations, the incomplete gamma functions cancel each other out in the answer, and the right-hand side of the expression (8) can be written in the comparatively simple form

$$\mp Z^2(ZR)^{2\varepsilon_0-1}e^{-ZR}/\Gamma(2\varepsilon_0+1). \tag{9}$$

This is still not the final answer. In fact the pre-exponential factor of the wave function $\varphi_0(0, y, z)$ changes substantially if the influence of the potential of the left nucleus is taken into account. Let us compute this change. Let us represent the wave function φ_0 in the form of a product of the solution (7) in the right well and a factor α which varies smoothly with distance. The characteristic distance over which the the quantity a varies is of the order of R. Let us substitute this solution into Eq. (3) and retain in it only the terms that are inversely proportional to R. Consequently, we neglect the terms containing Δa, the spin-orbit potential, and the term $-\frac{3}{4}(\nabla V/W)^2$: they contain higher inverse powers of R. Furthermore, the quantity a essentially depends only on the coordinate x, since the derivatives in the y and z directions contain the small parameter $1/\sqrt{R}$. It is important to retain in the energy ϵ_0 the term $-Z/R$, which is inversely proportional to the first power of R; it corresponds to the interaction between the left nucleus and an electron located near the right nucleus.

The differential equation for a assumes, after all these operations, the form

$$\frac{da}{dx}+\varepsilon_0\left[-\frac{1}{R}+\frac{1}{1/2R+x}\right]a=0.$$

Its solution, which becomes unity in the vicinity of the right charge, has the form

$$a(x)=\left(\frac{2R}{R+2x}\right)^{\varepsilon_0}\exp\left\{\varepsilon_0\left(\frac{x}{R}-\frac{1}{2}\right)\right\}.$$

Consequently, the wave function $\varphi_0(0, y, z)$ differs from the solution (7) of the Dirac equation by the factor

$$a(0) = (4/e)^{\varepsilon_0/2}. \quad (10)$$

Let us make a slight digression at this point. In considering the splitting of the terms in the case of two identical symmetric potential wells separated by a high barrier (see[3], p. 213), one uses quasiclassical wave functions in the right well, neglecting the left well. Because of the left well the preexponential factor in the quasiclassical wave function at x = 0, which is equal to

$$\left(\frac{\omega}{2\pi|p_0|}\right)^{1/2}\exp\left\{-\int_0^a |p|dx\right\}$$

(a is the distance of closest approach, $|p_0|$ is the momentum at x = 0, and ω is the frequency of the classical motion in the well), substantially changes; this change is easily taken into account in the general form. Let us seek the solution of the one-dimensional Schrödinger equation

$$\varphi'' + 2(\varepsilon - V_0 - v)\varphi = 0,$$

which is concentrated in the neighborhood of the right well in the form of the product $\varphi = a(x)\varphi_0$, where φ_0 is the solution of the equation

$$\varphi_0'' + 2(\varepsilon_0 - V_0)\varphi_0 = 0,$$

and a(x) is a slowly varying (over the distance ~R) function. The quantity a(x) satisfies the approximate equation

$$\frac{da(x)}{dx} + (\Delta\varepsilon - v)a(x)\frac{\varphi_0}{\varphi_0'} = 0, \quad (11)$$

where $\Delta\epsilon = \epsilon - \epsilon_0$. The ratio φ_0/φ_0' is equal to $1/|p|$ in the quasiclassical approximation. The solution of Eq. (11) satisfying the condition that $a(x) \to 1$ in the right well has the form

$$a(x) = \exp\left\{-\int_a^x \frac{\Delta\varepsilon - v}{|p|}dx\right\}.$$

Consequently, the correction factor to the wave function φ_0 at x = 0 is equal to

$$a(0) = \exp\left\{\int_0^a \frac{\Delta\varepsilon - v}{|p|}dx\right\}.$$

When this factor is taken into account the exponential factor in φ_0 assumes the form

$$\exp\left\{-\int_0^a\left[|p| + \frac{-\Delta\varepsilon + v}{|p|}\right]dx\right\},$$

where $|p| = [2(V_0 - \epsilon_0)]^{1/2}$. The same expression can, to the same degree of accuracy, be written in the form

$$\exp\left\{-\int_0 [2(V_0 + v - \varepsilon)]^{1/2}dx\right\} = \exp\left\{-\int_0 [2(V - \varepsilon)]^{1/2}dx\right\}.$$

Thus, the well-known answer[3] for the splitting of the terms

$$\varepsilon - \varepsilon_0 = \mp\frac{\omega}{2\pi}\exp\left\{-2\int_0 |p|dx\right\}$$

is correct, but only under |p| we should understand here the momentum $[2(V - \epsilon)]^{1/2}$, where ϵ is not simply the energy of a particle in the right well, but the energy which has been corrected for the influence of the left well. This fact can be reflected in an essential manner in the preexponential function if the correction $\Delta\epsilon$ is proportional to 1/R (as in the Coulomb case being considered), or if it decreases even more slowly. On this note we conclude the digression.

Multiplying (9) by $a^2(0)$, where a(0) is given by the expression (10), we finally obtain for the energy splitting of the term $1s_{1/2}$ for $R \gg 1$ the following expression:

$$\mp 2Z^2(2ZR)^{2\varepsilon_0 - 1}e^{-ZR - \varepsilon_0}/\Gamma(2\varepsilon_0 + 1).$$

In this case of the hydrogen atom this expression goes over, as it should be, to the well-known answer $\mp(2/e)Re^{-R}$.

To find the change in the term energy, we must add to the obtained expression the energy of interaction between the left nucleus and an electron concentrated near the right nucleus, i.e., -Z/R. Furthermore, the right nucleus and an electron concentrated near it can interact as one dipole with the left nucleus. Let us estimate this small term. The dipole-interaction potential is equal to $(Z/R^2)r\cos\theta$. It contributes to the energy in second-order perturbation theory. Let us denote it by $-c(Z)/R^4$. The largest contribution to the sum over the excited states is made by the states $2p_{3/2,1/2}$ (their contribution in the case of the hydrogen atom constitutes about 50% of the sum). Using the well-known bispinor expressions for the relativistic wave functions of the states $1s_{1/2}$ and $2p_{3/2,1/2}$, we found that when we go over from hydrogen to uranium the contribution of the $2p_{3/2,1/2}$ terms to the coefficient c(Z) changes by only 10%. This indicates that c(Z) weakly depends on Z. Consequently, we can simply use the case of the hydrogen atom to make a rough estimate of it: $c(Z) \approx c(1) = -9/4$[3]. Thus, for $R \gg 1$ the change for the ground term is determined by the formula

$$\varepsilon - \varepsilon_0 \approx -\frac{Z}{R} \mp 2Z^2(2ZR)^{2\varepsilon_0 - 1}\frac{e^{-ZR - \varepsilon_0}}{\Gamma(2\varepsilon_0 + 1)} - \frac{9}{4R^4}. \quad (12)$$

Figure 1 shows the individual contributions of the terms on the right hand side of (12) as functions of R, while Fig. 2 shows the total dependence $\epsilon(R)$ for uranium. Notice that at very large distances the dipole term, which decreases according to a power law, certainly becomes larger than the exponentially damped term (for R > 16). However, even for R = 12 the exponential term is still greater than the dipole term by a factor of three, to say nothing of small distances where the dipole term is negligibly small. This situation is analogous to the nonrelativistic case.

For excited terms with a large number of nodes we can use the quasiclassical formula for term splitting. In this case the effective nuclear charge is small, because of screening, and the well-known nonrelativistic formula[3] will do. However, the formula has to be modified, since it is obtained for the one-dimensional case, while the case of two three-dimensional wells separated by a high barrier is being considered here. The energy splitting in the three-dimensional case is equal to

$$\varepsilon - \varepsilon_0 = \mp\int\left(\varphi_0\frac{\partial\varphi_0}{\partial x}\right)_{x=0}dS. \quad (13)$$

The quasiclassical wave function φ_0 in the classically forbidden region has the form

$$\varphi_0 = \frac{1}{(4\pi)^{1/2}}\frac{1}{r}\left(\frac{\omega}{2\pi|p_r|}\right)^{1/2}\exp\left\{-\int_0^r |p_r|dr\right\}. \quad (14)$$

Substituting (14) into (13), we find

$$\varepsilon - \varepsilon_0 = \mp\frac{1}{2}\int_{R/2}^{\infty} r\,dr\frac{1}{r^2}\frac{\omega}{2\pi}\exp\left\{-2\int_0^r |p_r|dr\right\}.$$

Integrating by parts, we approximately obtain

$$\varepsilon - \varepsilon_0 = \mp\frac{1}{2|p_r(0)|R}\frac{\omega}{2\pi}\exp\left\{-\int_{-R/2}^{R/2}|p_r|dr\right\}. \quad (15)$$

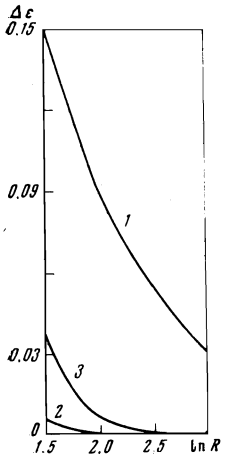

FIG. 1

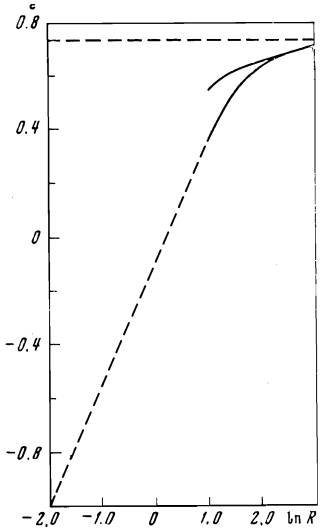

FIG. 2

FIG. 1. Absolute values of the contributions of the monopole (1), dipole (2), and exchange (3) terms to the energy of the ground state. The values were computed from the formula (12) as functions of the distance between the nuclei. The case of collisions between uranium nuclei is considered. The internuclear distance R is measured in units of $\hbar/mc$ = 386 F. The energy is measured in units of mc^2.

FIG. 2. Splitting of the electron term $1s_{1/2}$ in uranium-uranium collisions. The units are the same as in Fig. 1. The dashed horizontal straight line is the energy of the $1s_{1/2}$ term for the isolated uranium nucleus. The inclined dashed line is a hypothetical interpolated behavior of the ground term in the region R ~ 1. This line ends, for R = 50 F, at the point $\epsilon = -1$ found in [6].

Here $|p_r(0)|$ is the radial momentum at the point midway between the nuclei. Comparing with the one-dimensional case, we see that in the three-dimensional case, in the preexponential factor appears the additional factor $1/2|p_r(0)|R \ll 1$. The formula (15) can, in the problem being considered, be used to determine the term splitting in the case of highly excited states with a large number of nodes, to which case the quasiclassical approximation is applicable.

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