WKB method at $Z > 137$ and its applications to the theory of supercritical atoms

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Formulas are obtained in the WKB approximation for the Dirac equation in a strong external field (defined as a field in which the electron binding energy exceeds $2m_ec^2$ and the discrete-spectrum level can drop to the lower continuum). The forms of the wave functions in the classically allowed and forbidden regions are obtained, and conditions for their joining at the turning point are obtained. The following applications of the WKB method are considered: 1) Generalization of the Bohr-Sommerfeld quantization condition with allowance for relativistic effects and spin. 2) Calculation of the pre-exponential factor in the probability of spontaneous positron production. 3) The level energy and width in the relativistic two-center problems. 4) The effect of screening on the critical distance R_{cr} between colliding nuclei. 5) Tunneling through a nonspherical barrier and the angular distribution of positrons. 6) Allowance for the finite velocity of nuclei. Some problems outside the scope of the WKB method are also considered, viz., the electron spectrum at $Ze^2 = 1$ and deep level in the lower continuum [$Ze^2 \gg 1, j \lesssim (Ze^2)^{1/2}$].

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INTRODUCTION

The WKB method is one of the most important approximate methods of quantum mechanics. It is known[1-3] that in the case of a Coulomb field it is highly accurate even for small quantum numbers. Its application to a strong ($Ze^2 > 1$) Coulomb field is a timely problem, expecially in connection with experimental observation[4,5] of the production of positrons in slow ($v < 0.1c$, $E/A = 3 - 5$MeV/nucleon) collisions of heavy nuclei. A calculation of the spontaneous[6-8] and induced[9] emission of the positrons, and of their energy and angular spectra, as well as a comparison of the theoretical calculations with experiment, provide a check on quantum electrodynamics in the region of strong external fields (outside the framework of perturbation theory), a problem of fundamental interest.[10-13]

For such calculations we need the solution of the two-center problem for the Dirac equation. Since the variables do not separate in this case, this problem has no analytic solution, and the numerical calculations are quite cumbersome and were carried out[14,15] only in the region below critical $R > R_{cr}, \varepsilon \geq -1$ (i.e., where spontaneous positron production is still impossible). The purpose of the present paper is to develop a consistent scheme for obtaining the WKB expansions for the Dirac equation in a strong field.[1)] This makes it possible to obtain an approximate analytic solution of the two-center problem, and also to consider a large group of problems in the theory of supercritical atoms. It must be emphasized that the WKB method usually yields the answer in a convenient analytic form, thus avoiding cumbersome numerical calculations. In those cases when the results of the WKB method can be compared with the exact calculation, the difference between them is small even for the ground level $1s_{1/2}$, and decreases rapidly with increasing Ze^2. This indicates good accuracy of the WKB approximation for a strong Coulomb field.

In Sec. 1 we obtain the quasiclassical formulas for the solutions of the Dirac equation and the conditions for their continuity in the transition through the turning point. These formulas are valid for an arbitrary potential $V(r)$ of spherical symmetry. The generalization to noncentral potentials is discussed in Sec. 2. The succeeding sections consider the applications of these formulas to particular problems of the theory of supercritical atoms. A brief discussion of the results and a comparison with other studies is contained in the concluding Sec. 11.

We use the system of units with $\hbar = c = m_e = 1$ and the following notation: ε is the level energy in units of m_ec^2, R is the distance between the nuclei, Z_1 and Z_2 are their charges, $Z = Z_1 + Z_2$ is the total charge (or the charge of a spherical superheavy nucleus), $\zeta = Ze^2 \approx Z/137$, $g = (\zeta^2 - \varkappa^2)^{1/2}$, r_N is the radius of the nucleus, and R_{cr} is the critical distance at which the level of the discrete spectrum drops to the boundary of the lower continuum.

1. THE WKB METHOD FOR THE DIRAC EQUATION IN A STRONG EXTERNAL FIELD

The first to consider the limiting transition from the Dirac equation in an external field to the Hamilton-Jacobi equation for a classical relativistic particle was Pauli,[17] followed by a number of more detailed studies by others.[18,19] The case of deep levels (with binding energy $> 2mc^2$), however, was not considered, so that this question must be examined anew.

We assume that the external potential $V = -eA_0(r)$ is electrostatic and has spherical symmetry (the generalization to noncentral potentials will be considered in the next section). After separating the angle variables in the Dirac equation, we obtain a system of first-order equations for the radial functions G and F, which we express in matrix form:

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$$\psi' = \frac{1}{\hbar} D\psi; \quad \psi = \begin{pmatrix} G \\ F \end{pmatrix}, \quad D = \begin{pmatrix} -\tilde{\varkappa}/r & m+\varepsilon-V(r) \\ m-\varepsilon+V(r) & \tilde{\varkappa}/r \end{pmatrix}. \tag{1.1}$$

Here $\varkappa = \hbar\tilde{\varkappa}$, $\tilde{\varkappa} = \mp(j+1/2)$ is the integral of motion for a Dirac particle in a central field; $j\hbar$ is the total angular momentum; the definitions and normalizations of the functions $G(r)$ and $F(r)$ are the same as in Refs. 6 and 10. Representing the solution by formal power series in $\hbar$:

$$\psi = \varphi \exp\left(\int^r y\, dr \right), \tag{1.2}$$

$$y(r) = \frac{1}{\hbar} y_{-1}(r) + y_0(r) + \hbar y_1(r) + \ldots, \quad \varphi = \sum_{n=0}^{\infty} \hbar^n \varphi^{(n)}, \tag{1.3}$$

we arrive at the chain of equations

$$(D - y_{-1})\varphi^{(0)} = 0, \tag{1.4}$$

$$(D - y_{-1})\varphi^{(1)} = \varphi^{(0)\prime} + y_0\varphi^{(0)}, \ldots, \quad (D - y_{-1})\varphi^{(n+1)} = \varphi^{(n)\prime} + \sum_{k=0}^{n} y_{n-k}\varphi^{(k)}, \tag{1.5}$$

from which the quantities y_n and $\varphi^{(n)}$ are determined consecutively.

In order for the homogeneous system (1.4) to have a nontrivial solution, $y_{-1}(r)$ must be an eigenvalue, and $\varphi^{(0)} \equiv \varphi_i$ must be one of the (two-component) eigenvectors of the matrix $D(r)$:

$$y_{-1} = \lambda_i = \pm q, \quad q = \left[1 + \frac{\varkappa^2}{r^2} - (\varepsilon - V(r))^2 \right]^{1/2}; \tag{1.6}$$

$$\varphi_i = A \begin{pmatrix} 1+\varepsilon-V \\ \lambda_i + \varkappa r^{-1} \end{pmatrix} = A' \begin{pmatrix} \lambda_i - \varkappa r^{-1} \\ 1-\varepsilon+V \end{pmatrix}. \tag{1.7}$$

Here and below $\hbar = m = c = 1$; the subscript i takes on two values, plus and minus; A and A' are normalization constants which will be fixed later on. Since the matrix $D(r)$ is not symmetrical, we must introduce besides the right-hand eigenvectors φ_i also the left-hand eigenvectors $\check{\varphi}_i$:

$$(D - \lambda_i)\varphi_i = \check{\varphi}_i(D - \lambda_i) = 0, \tag{1.8}$$

$$\check{\varphi}_i = A_i(1-\varepsilon+V, \lambda_i + \varkappa r^{-1}) = A_i'(\lambda_i - \varkappa r^{-1}, 1+\varepsilon-V). \tag{1.9}$$

We note that $\check{\varphi}_i$ does not coincide with $(\varphi_i)^T$, and the left- and right-hand vectors are mutally orthogonal:

$$(\check{\varphi}_i, \varphi_j) = \sum_{\alpha=1}^{2} (\check{\varphi}_i)_\alpha (\varphi_j)_\alpha \propto \delta_{ij}.$$

To determine y_0 we put $\varphi^{(0)} = \varphi_i$ in (1.5) and multiply both sides from the left by $\check{\varphi}_i$. By virtue of (1.8) the term with $\varphi^{(1)}$ vanishes, and we obtain for y_0 an equation from which it follows that

$$y_0(r) = -(\check{\varphi}_i, \varphi_i') / (\check{\varphi}_i, \varphi_i) \tag{1.10}$$

(the prime denotes a derivative with respect to r). We determine similarly also the next terms $y_1, \varphi^{(1)}, \ldots$ in the expansion (1.3). We confine ourselves, however, to the obtained terms y_{-1} and y_0 (which correspond to the known expression $\psi \propto p^{-1/2}\exp(i\int^r p\, dr)$ in the nonrelativisitic quasiclassical approach), since corrections of order $\hbar, \hbar^2$, etc. usually does not improve the agreement between the WKB method and the exact solution. The reason, as is well known,[1-3] is that formally the series in powers of $\hbar$ does not converge and is only asymptotic.

The remaining calculations entail no difficulty. We present the final formulas for the wave function of the quasistationary state with energy $\varepsilon < -1$ (details of the calculations can be found in Ref. 20). Expression (1.6) corresponds to an effective potential

$$U(r, \varepsilon) = \varepsilon V - {}^1\!/_2 V^2 + \varkappa^2/2r^2, \tag{1.11}$$

which represents attraction at short distances from the nucleus (where the term $-(1/2)V^2$ predominates) and repulsion at $r > r_-$. Thus, $U(r, \varepsilon)$ at $V(r) < 0$ and $\varepsilon < 0$ takes the form of a potential with a barrier.[6,10] We denote by r_0, r_-, and r_+ the turning points (see Fig. 1 in Ref. 16). The wave functions G and F have different forms in three regions: I) $r_0 < r < r_-$, II) the subbarrier region $r_- < r < r_+$, III) $r > r_+$.

I. The region $r_0 < r < r_-$ is classically allowed; the wave function in it oscillates:

$$G = C_1 \left[\frac{\varepsilon+1-V}{p(r)} \right]^{1/2} \sin\theta_1, \quad F = C_1 \operatorname{sgn}\varkappa \left[\frac{\varepsilon-1-V}{p(r)} \right]^{1/2} \sin\theta_2. \tag{1.12}$$

Here

$$p(r) = [(\varepsilon - V(r))^2 - 1 - \varkappa^2 r^{-2}]^{1/2} \tag{1.13}$$

is the quasiclassical momentum for the radial motion,

$$\theta_1(r) = \int_{r_0}^{r} \left(p + \frac{\varkappa w}{pr} \right) dr + \frac{\pi}{4}, \quad \theta_2(r) = \int_{r_0}^{r} \left(p + \frac{\varkappa \tilde{w}}{pr} \right) dr + \frac{\pi}{4},$$
$$w = \frac{1}{2}\left(\frac{V'}{1+\varepsilon-V} - \frac{1}{r} \right), \quad \tilde{w} = \frac{1}{2}\left(\frac{V'}{1-\varepsilon+V} + \frac{1}{r} \right), \tag{1.14}$$

with

$$\theta_2 - \theta_1 = \operatorname{sgn}\varkappa \cdot \arcsin\{p[(\varepsilon - V)^2 - 1]^{-1/2}\}.$$

If the level width γ is small (as confirmed by the result), then the wave function of the quasistationary state must be normalized to a single particle localized in region I, neglecting its penetration into the classically forbidden regions $r > r_-$ and $r < r_0$ (see Furry's article[21] as well as Ch. V of Ref. 3 on this subject). Hence

$$C_1 = \left[\int_{r_0}^{r_-} \frac{\varepsilon - V(r)}{p(r)} dr \right]^{-1/2} = \left(\frac{2}{T} \right)^{1/2}, \tag{1.15}$$

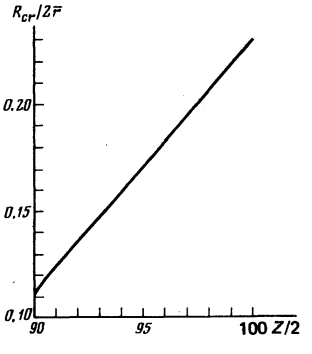

FIG. 1. The parameter $R_{cr}/2\bar{r}$, which characterizes the nonsphericity of the potential (4.1) in the subbarrier region. The values of R_{cr} were taken from Ref. 14, and the average radius $\bar{r}$ of the K shell was calculated from formula (5.3) with $\varkappa = -1$.

where T is the period of oscillations of a classical particle in an internal well:

$$T=2\int_{r_0}^{r_-}\frac{dr}{v},\quad v_r=p\left(1+p^2+\frac{\varkappa^2}{r^2}\right)^{-1/2}=\frac{p}{\varepsilon-V}.$$

We note that at the turning point $r=r_-$ we have $\varepsilon-V(r_-)=(1+\varkappa^2/r_-^2)^{1/2}$, so that the quantity $\varepsilon-V(r)$ is positive in the region I.

II. The subbarrier region $r_-<r<r_+$. Here $p^2(r)<0$, $p=iq$, and the quantities q, y_{-1}, and y_0 are real. Expressions (1.12) then go over into functions that attenuate exponentially with increasing r. For states with $\varkappa<0$ we have[2)]

$$\psi\equiv\begin{pmatrix}G\\F\end{pmatrix}=C_2(Qq)^{-1/2}\exp\left\{-\int_{r_-}^{r}\left(q-\frac{V'}{2Qq}\right)dr\right\}\begin{pmatrix}1+\varepsilon-V\\-Q\end{pmatrix},\quad(1.16)$$

where $Q=q-\varkappa r^{-1}$ and $q(r)$ is given by formula (1.6). At $\varkappa>0$ we have

$$\psi=C_2'(Qq)^{-1/2}\exp\left\{-\int_{r_-}^{r}\left(q+\frac{V'}{2Qq}\right)dr\right\}\begin{pmatrix}-Q\\1-\varepsilon+V\end{pmatrix}\quad(1.17)$$

(an example of a state with $\varkappa>0$ is the first excited level, for which $\varkappa=1$); here $Q=q+\varkappa r^{-1}$.

III. In the region $r>r_+$ the quasistationary state corresponds to a diverging wave (outgoing positron):

$$\psi=C_3(Pp)^{-1/2}\exp\left\{\int_{r_+}^{r}\left(ip-\frac{V'}{2Pp}\right)dr\right\}\begin{pmatrix}1+\varepsilon-V\\iP\end{pmatrix}.\quad(1.18)$$

Here $\varkappa<0$, $P=p-i\varkappa r^{-1}$, so that the radial momentum $p(r)$ is again positive. The flux of particles that go off to infinity is then $\gamma=2\lim\mathrm{Im}(F^*G)$ as $\gamma\to\infty$.

The obtained formulas determine the quasiclassical asymptotic form of the solutions of the Dirac equation as $\hbar\to0$ and are valid for all r with the exception of small vicinities ($\Delta r\sim\zeta^{-2/3}$) of the turning points. To get around these points and to match the solutions together, the usual procedure is employed. Thus, near $r=r_-$ the Dirac system (1.1) reduces to a Schrödinger equation whose potential depends linearly on $r-r_-$ and whose solution is expressed in terms of an Airy function; it is also possible to use Zwaan's more elegant method.[1,3] As a result we get a prescription for matching together the quasiclassical solutions, viz., the usual[1-3] formulas for joining the solutions on the left and on the right of the turning point are valid if we consider in solutions similar to (1.16) and (1.18) in the vicinity of the turning point only the behavior of the prinicpal factors of type

$$p^{-1/2}\exp\left(\pm i\int^{r}p\,dr\right),$$

which are singular as $r\to r_-$ (or $r\to r_+$).

In particular, the connection between the normalization constants in formulas (1.12)–(1.18) is of the form

$$C_2=-iC_3=\frac{\sigma}{2}C_1\left[\frac{|\varkappa|}{r_-+(\varkappa^2+r_-^2)^{1/2}}\right]^{\sigma/2}\exp\left\{-\int_{r_-}^{r_+}\left(q-\sigma\frac{V'}{2Qq}\right)dr\right\},\quad(1.19)$$

where $\sigma=-\mathrm{sgn}\,\varkappa=\pm1$.

Although formulas (1.12)–(1.18) differ substantially from the quasiclassical nonrelativistic formulas[3)] and are more complicated than the latter, their application to concrete problems encounters no difficulty, since all the quantities contained in G and F are defined in terms of quadratures.

In conclusion, we indicate the positions of the turning points in the case of a Coulomb field

$$V(r)=\begin{cases}-\zeta/r, & r>r_N\\-(\zeta/r_N)f(r/r_N), & 0<r<r_N\end{cases}.\quad(1.20)$$

Here $f(x)$ is a cutoff function that takes into account the finite dimensions of the nucleus (we consider henceforth two cases: $f(x)=1$ and $f(x)=(3-x^2)/2$, $0<x=r/r_N<1$; this corresponds to cutoff models I and II in the terminology of Refs. 6 and 10). At $\varepsilon>-\zeta/r_N$ the points $r_\pm$ lie outside the nucleus and do not depend on the cutoff model:

$$r_-=\frac{\zeta(1-\rho^2)}{(1+k^2)^{1/2}+(1+\rho^2k^2)^{1/2}},\quad r_+=\frac{\zeta}{k^2}((1+k^2)^{1/2}+(1+\rho^2k^2)^{1/2}),\quad(1.21)$$

where $k=(\varepsilon^2-1)^{1/2}$ and $\rho=|\varkappa|/\zeta$ (for levels in the lower continuum $0<\rho<1$). As $k\to0$ we have

$$r_-=\frac{\zeta^2-\varkappa^2}{2\zeta}\left[1-\frac{1-\rho^2}{2}k^2+\ldots\right],\quad r_+=\frac{2\zeta}{k^2}+\frac{1}{2}\zeta(1+\rho^2)+\ldots,\quad(1.22)$$

and for levels that drop deeply into the lower continuum

$$r_\pm=\zeta(1\pm\rho)/k,\quad k\gg1.\quad(1.23)$$

As to r_0, this turning point is determined from the equation $f(x)-\rho/x=kr_N/\zeta$, whose root is $x=r_0/r_N$. At $k\ll\zeta/r_N$ we get $xf(x)=\rho$, where $f(x)$ is the cutoff function from (1.20). We thus have $x_0=\rho$ for the cutoff model I, and in the case of model II

$$x_0=2\sin\left(\frac{1}{3}\arcsin\rho\right)=\begin{cases}{}^2/_3\rho+O(\rho^3), & \rho\to0\\1-[{}^2/_3(1-\rho)]^{1/2}, & \rho\to1\end{cases}.$$

Thus, the turning point r_0 always lies inside the nucleus, i.e., $r_0\ll r_-$. We shall hereafter set r_0 equal to zero wherever possible.

For the potential (1.20) at $r>r_N$ we have

$$p(r)=\frac{g}{r}\left[\left(1-\frac{r}{r_-}\right)\left(1-\frac{r}{r_+}\right)\right]^{1/2},\quad g=(\zeta^2-\varkappa^2)^{1/2}.\quad(1.24)$$

Therefore the condition for the applicability of the quasiclassical approach takes the form

$$\frac{d}{dr}\left(\frac{1}{p}\right)=g^{-1}\left(1-\frac{r}{r_m}\right)\left[\left(1-\frac{r}{r_-}\right)\left(1-\frac{r}{r_+}\right)\right]^{-3/2}\ll1\quad(1.25)$$

and is satisfied at $g\gg1$. Here r_m is the point at which the effective potential (1.11) reaches its maximum:

$$r_m=\zeta(1-\rho^2)/(1+k^2)^{1/2},\quad r_m^{-1}={}^1/_2(r_+^{-1}+r_-^{-1}).$$

The WKB method is actually applicable all the way to $g\sim1$, as can be verified by comparing the quasiclassical formulas with the exact calculations. Such a comparison was made in Refs. 22 and 23 for Z_{cr} and N, where $N=N(\zeta)$ is the number of discrete-spectrum levels that have dropped to the lower continuum.

2. WKB METHOD FOR NONCENTRAL POTENTIALS

The results can be generalized to the case when the potential $V(\mathbf{r})$ does not have spherical symmetry (a concrete example is the potential (4.1) of the two-center problem). We write down the Dirac equation in a form similar to (1.1):

$$-i(\alpha\nabla)\psi=\hbar^{-1}D\psi, \tag{2.1}$$

where now $D=\varepsilon-m\beta-V(\mathbf{r})$, $\psi=\varphi e^{i\sigma}$ (ψ and φ are four-component bispinors), and we expand σ and φ in powers of $\hbar$:

$$\sigma=\hbar^{-1}\sigma_{-1}+\sigma_0+\hbar\sigma_1+\ldots, \quad \varphi=\varphi^{(0)}+\hbar\varphi^{(1)}+\ldots . \tag{2.2}$$

Substitution of these series in (2.1) gives rise to a system of coupled equations

$$\begin{aligned}&\{D-(\alpha\nabla\sigma_{-1})\}\varphi^{(0)}=0,\\ &\{D-(\alpha\nabla\sigma_{-1})\}\varphi^{(1)}=\alpha\nabla\varphi^{(0)}+(\alpha\nabla\sigma_0)\varphi^{(0)},\ldots .\end{aligned} \tag{2.3}$$

The condition for the existence of a nontrivial solution $\varphi^{(0)}$ is of the form $\det(D-\alpha\nabla\sigma_{-1})=0$ and yields an equation for σ_{-1}:

$$(\nabla\sigma_{-1})^2=[\varepsilon-V(r)]^2-m^2, \tag{2.4}$$

which agrees with the Hamilton-Jacobi equation for a relativistic zero-spin particle. Thus, as expected,[17] σ_{-1} coincides with the classical action S. In contrast to the preceding case, the matrix $D-\alpha\nabla\sigma_{-1}=\varepsilon-V(\mathbf{r})-m\beta-\alpha\nabla S$ is Hermitian, therefore its left-hand and right-hand eigenvectors are Hermitian conjugates: $\tilde{\varphi}_i=\varphi_i^+$, with

$$(D-\alpha\nabla S)\varphi_i=\varphi_i^+(D-\alpha\nabla S)=0 \tag{2.5}$$

(here $i=1,2,3,4$). Using (2.5), we get from (2.3) a system of equations for the correction σ_0:

$$\varphi_i^+(\alpha\nabla\sigma_0)\varphi_j=-\varphi_i^+\alpha\nabla\varphi_j. \tag{2.6}$$

The bispinors $\varphi_i=\varphi_i(\mathbf{r})$ can be obtained in explicit form by diagonalizing the matrix $D-\alpha\nabla S$, so that the right-hand side of (2.6) contains known quantities. Determining σ_0 from this equation, we obtain the quasiclassical approximation of the solutions of the Dirac equation

$$\psi\approx\varphi_i\exp(\hbar^{-1}\sigma_{-1}+\sigma_0). \tag{2.7}$$

In practice the calculation of the functions σ_{-1} and σ_0 for noncentral potentials that do not admit of separation of the variables in (2.4) and (2.6) is a complicated mathematical problem and calls for the solution of partial differential equations (of first order). In contrast to the case when $V(r)$ is spherically symmetrical, the answer is not expressed in quadratures. This, however, is a general difficulty when the WKB method is applied to multidimensional systems without separation of the variables (see, e.g., Refs. 24–26).

We proceed now to concrete applications of the WKB method in the theory of supercritical atoms.

3. QUASISTATIONARY LEVELS IN THE LOWER CONTINUUM

Let us find the energy of the quasistationary states that are continuations of the levels of the discrete spectrum into the transcritical region $Z>Z_{cr}$, $\varepsilon<-1$. Neglecting the penetrability of the barrier in the region $r_-<r<r_+$, we obtain from (1.12) and (1.14) the quantization condition:

$$\int_{r_0}^{r_-}\left(p+\frac{\varkappa w}{pr}\right)dr=(n+\gamma')\pi. \tag{3.1}$$

Here $n=0,1,2,\ldots$ is the radial quantum number; the constant γ' is equal to 3/4 at $\varkappa=-1$ (s levels) and 1/2 at $\varkappa\neq-1$. The equation (3.1) determines the real part of the level energy $\varepsilon_{n\varkappa}$. It differs from the usual Bohr-Sommerfeld quantization rule[1] in that the momentum $p(r)$ is given by a relativistic expression and that a correction proportional to w must be introduced for the spin-orbit interaction.

This correction does not exceed the error in the WKB method. We shall demonstrate this with the Coulomb field as an example, where

$$V(r)=-\frac{\zeta}{r}, \quad w(r)=-\frac{1+\varepsilon}{2[\zeta+(1+\varepsilon)r]}, \tag{3.2}$$

and $p(r)$ is given by formula (1.24). At $r<r_-$ the momentum is $p(r)\sim g/r$, and therefore the ratio of the two terms under the integral sign in (3.1) is $\sim\varkappa g^{-2}rw\sim\zeta^{-1}$. Since the quasiclassical approximation for the wave function has at $\zeta\gg1$ an accuracy of the order of ζ^{-2} (see Ref. 27), it follows that only terms of order ζ^{-1} need be retained. On the edge of the lower continuum the function $w(r)$ vanishes identically, and (3.1) reduces to the usual Bohr-Sommerfeld condition. This justifies the calculations performed in Refs. 22 and 23 (we note however that the vanishing of w is a specific feature of the Coulomb field: if $V(r)\propto r^{-n}$, then $w=(n-1)/2r$ at $\varepsilon=-1$.

At $V(r)=-\zeta/r$ the integrals in (3.1) can be calculated exactly. The energy spectrum in the case of a spherical superheavy nucleus is described by the formula

$$\varepsilon_{n\varkappa}=-\frac{\zeta}{r_N}c(\rho)\exp\left\{-\frac{\pi}{g}\left[n+\frac{1}{2}\left(1-\operatorname{sgn}\varkappa\frac{\arccos\rho}{\pi}\right)\right]\right\}, \tag{3.3}$$

where $\rho=|\varkappa|/\zeta$, $g=(\zeta^2-\varkappa^2)^{1/2}=\zeta(1-\rho^2)^{1/2}$. The pre-exponential factor depends on the model of the cutoff:

$$\begin{aligned}c(\rho)=\exp\Big\{&(1-\rho^2)^{-1/2}\int_{x_0}^{1}[f^2(x)-\rho^2x^{-2}]^{1/2}dx\\ &+\ln(\rho^{-1}-\rho)-\frac{\operatorname{Arth}(1-\rho^2)^{1/2}}{(1-\rho^2)^{1/2}}-(1-\ln2)\Big\}.\end{aligned} \tag{3.4}$$

Here $f(x)$ is the cutoff function from (1.20), and $x_0=x_0(\rho)$ is the root of the equation $xf(x)=\rho$. We note the following concerning these results.

1. Formula (3.3) describes the "Coulomb" part of the spectrum, in the energy region $1\ll|\varepsilon|\ll\zeta/r_N$. The main contribution to the integral (3.1) is made here by the region of r outside the nucleus. The cause of the exponential dependence of $\varepsilon_{n\varkappa}$ on the level number n is that at $r_N<r\ll r_-$ the effective potential is $U\sim-g^2/2r^2$. In this case "falling to the center" takes place, and the spectrum E_n for the squared Dirac equation takes the form $E_n\sim\exp(-2\pi n/g)$. From this we get at $|\varepsilon|\gg1$

$$|\varepsilon_n|\approx(2E_n)^{1/2}\propto\exp(-\pi n/g).$$

2. The pre-exponential function (3.4) decreases monotonically with increasing parameter ρ. At $\rho\ll1$ we have

$$c(\rho)=c_0-{}^1/_2\pi\rho+{}^1/_2\rho^2\ln\rho+O(\rho^2), \tag{3.5}$$

where

$$c_0=\exp\left(-1+\int_0^1 f(x)\,dx\right),$$

$c_0=1$ for model I and $c_0=1.40$ for model II; for the maximal angular momenta ($\rho\to1$) we have $c(\rho)=c_1(1$

$-\rho(+\ldots, c_1 = 4e^{-2} = 0.541$. This means that when the angular momentum of the level increases the energy $\varepsilon_{n\varkappa}$ increases (at one and the same value of n).

3. The spin-orbit interaction causes the energy of the level to depend on the sign of the quantum number $\varkappa$. At $\zeta \gg 1$ the relative magnitude of the splitting is small:

$$\left|\frac{\varepsilon_{n\varkappa}-\varepsilon_{n,-\varkappa}}{\varepsilon_{n\varkappa}}\right| = \frac{\arccos\rho}{\zeta(1-\rho^2)^{1/2}}. \tag{3.6}$$

4. Formula (3.3) is valid under the condition $g/\pi < n < (g/\pi)\ln(\zeta/r_N)$. Because of the large logarithm $\ln(\zeta/r_N) \gg 1$, it describes the greater part of quasistationary levels that lie in the lower continuum.

We proceed now to calculate the level width $\gamma = 2\,\mathrm{Im}\,\varepsilon_{n\varkappa}$ (which coincides with the probability of spontaneous positron production[6,7]). To this end we find the flux of the particles that go off to infinity, normalized to one particle in the region $r_0 < r < r_-$. With the aid of the formulas of Sec. 1 we get

$$\gamma = \gamma_0 \exp\left\{-2\int_{r_-}^{r_+} q(r)\,dr\right\}, \tag{3.7}$$

where

$$\gamma_0 = \frac{1}{T}\exp\left\{2\varkappa\int_{r_-}^{r_+}\frac{w}{qr}\,dr\right\}, \tag{3.8}$$

and T is the period of the oscillations determined in (1.15) (the last integral is singular at the point $r = r_1$ where $V(r) = 1+\varepsilon$, and must be understood in the sense of the principal value).

In the nonrelativistic case $\gamma_0 = 1/T$ and the meaning of formula (3.7) is obvious: $1/T$ is the number of impacts, per unit time, of the particle (localized inside region 1) against the wall of the potential barrier at $r = r_-$, and the exponential corresponds to the probability of penetrating through the barrier in each impact. Allowance for the relativistic effects and for the spin $s = 1/2$ changes the expression for the period of the oscillations and adds to (3.8) a factor that depends generally speaking on the sign of $\varkappa$. In the case of a Coulomb field all the integrals can be calculated exactly, and we get

$$T = \frac{1}{\gamma_0} = \frac{2\zeta}{k^2}\left\{[(1-\rho^2)(1+k^2)]^{1/2} - \frac{1}{k}\,\mathrm{Arth}\left(k\left[\frac{1-\rho^2}{1+k^2}\right]^{1/2}\right)\right\}, \tag{3.9}$$

$$\gamma = \gamma_0 \exp\left\{-2\pi\zeta\left[\frac{(1+k^2)^{1/2}}{k} - (1-\rho^2)^{1/2}\right]\right\}, \tag{3.10}$$

where $k = (\varepsilon^2-1)^{1/2}$ is the momentum of the positron. If $k \ll \zeta^{1/2}$, then the width γ is exponentially small at any value of the angular momentum. At $|\varkappa| \gg (\zeta/\pi)^{1/2}$ the exponential smallness of γ is preserved even for very deep levels:

$$\gamma \approx \frac{k}{2\zeta(1-\rho^2)^{1/2}}\exp\{-2\pi\zeta[1-(1-\rho^2)^{1/2}]\} \tag{3.11}$$

(with the exclusion of the physically unreal values $k \gtrsim \exp(2\pi\zeta)$). Finally, at $|\varkappa| \lesssim (\zeta/\ )^{1/2}$ and $k \gg 1$ the exponential factor becomes of the order of unity, and the quasiclassical approximation ceases to be valid. We shall return to this case in Sec. 10.

The obtained formulas describe the spectrum of the quasistationary levels in the lower continuum (their position and width) for a spherical superheavy nucleus with charge $Z > Z_{cr}$. A realistic method of obtaining such states is by collision between two heavy nuclei. We now proceed to consider this problem.

4. RELATIVISTIC TWO-CENTER PROBLEM

Simple estimates show that the motion of the nuclei is nonrelativistic,[4] whereas the electron on the lower levels of the quasimolecule (Z_1, Z_2, e) has a velocity $v \sim c$. Therefore the level spectrum of an electron in the field of colliding nuclei can be calculated in the adiabatic approximation: $\varepsilon = \varepsilon(R(t))$, where $\varepsilon(r)$ is the position of the level in the two-center problem (i.e., for immobile nuclei located at a distance R). This problem could be solved previously[7] only in the limiting case $\zeta = (Z_1+Z_2)\times e^2 \to 1$. The WKB method yields a formula for $\varepsilon(R)$ for arbitrary values of the parameters ζ and R/R_{cr}.

For nuclei in the uranium region, the average radius $\bar{r}$ of the K shell exceeds by several times the critical distances R_{cr} (see Fig. 1), so that to calculate $\varepsilon(R)$ we need not know the wave function in the region $r \lesssim R/2$, where the specific features of the two-center problems are important. At distances $r \sim \bar{r}$, the potential is close to spherically-symmetrical:

$$V(\mathbf{r}) = -\frac{\zeta}{2}\left(\frac{1}{r_1}+\frac{1}{r_2}\right) = -\frac{\zeta}{r}\left[1+\left(\frac{R}{2r}\right)^2 P_2(\cos\theta)+\ldots\right], \tag{4.1}$$

where $r_{1/2} = |\mathbf{r} \pm R/2|$. We consider therefore a spherical nucleus with total charge $Z = Z_1 + Z_2$ and with a variable radius equal to $R/2$ (the monopole approximation[8,9]).

In a Coulomb field $V(r) = -\zeta/r$ the quasiclassical momentum is

$$p(r) = r^{-1}F(r,\varepsilon) \approx r^{-1}(a-2br+cr^2)^{1/2}. \tag{4.2}$$

The parameters a, b, and c can be easily obtained from (3.1). In this case, however, it is possible to obtain for them also more accurate[5)] expressions, by starting from the squared Dirac equation (see the Appendix). The equation for the level energy $\varepsilon = \varepsilon(R)$ follows from the quantization condition:

$$\int_{R/2}^{r_-} F(r,\varepsilon)\frac{dr}{r} = \int_{R_{cr}/2}^{r_-^{(0)}} F(r,-1)\frac{dr}{r}, \tag{4.3}$$

where $r_-^{(0)} = (\zeta^2-\varkappa^2)/2\zeta$ is the position of the turning point r_- at $\varepsilon = -1, k = 0$. Allowance is made here also for the fact that the dependence on ε is negligible, in the integral $\int p\,dr$ over the region $r < R/2 \ll 1$ since $|V(\mathbf{r})| \gg |\varepsilon|$. The integrals (4.3) diverge logarithmically at the lower limit (as $R \to 0$), and once they are regularized the dependences on R and R_{cr} can be separated in explicit form:

$$\ln\frac{R}{R_{cr}} = \Phi(\varepsilon, \zeta, \varkappa), \tag{4.4}$$

where

$$\Phi = \frac{1}{g}\left\{\int_0^{r_-^{(0)}}[F(r,\varepsilon)-F(r,-1)]\frac{dr}{r} + \int_{r_-^{(0)}}^{r_-} F(r,-1)\frac{dr}{r}\right\}.$$

The function Φ is obtained from this numerically. It

is also possible to obtain for it approximate expressions (see the Appendix) that allow us to rewrite Eq. (4.4) in simpler form:

$$\left[1-\left(1+\frac{1-2\varkappa}{4\zeta^2}\right)(\varepsilon+1)\right]\psi(x)=\frac{R_{cr}}{R}, \tag{4.5}$$

where

$$\varkappa=\left[1-\left(\frac{\varkappa}{\zeta}\right)^2\right]^{1/2}\left[\varepsilon^2-1+\left(\varkappa-\frac{5}{4}\right)\frac{(\varepsilon+1)^2}{\zeta^2}\right]^{1/2}$$
$$\times\left[1-\left(1+\frac{1-2\varkappa}{4\zeta^2}\right)(\varepsilon+1)\right]^{-1},$$

$0<|\varkappa|/\zeta<1$, and $\psi(x)$ is defined by formula (A.10). Figure 2 shows a plot of $\varepsilon(R)$ for the ground term $1s\sigma(\varkappa=-1)$ as calculated from these equations. It turned out that the results of calculation by (4.4) and (4.5) practically coincide: at all $\varepsilon-1$ the difference is $\lesssim 0.1\%$.

As $\varepsilon\to-1$ we get from (4.5)

$$\varepsilon=-1+\beta\left(\frac{R}{R_{cr}}-1\right)+\ldots,\quad \beta=\frac{3}{2}\left(1+\frac{4\varkappa^2-6\varkappa+3}{8\zeta^2}\right)^{-1}. \tag{4.6}$$

The slope of the level β at the boundary of the lower continuum determines the threshold behavior of the cross section for spontaneous positron production.[7] In the other limiting case, when $|\varepsilon|\gg 1$, we have

$$\varepsilon(R)\approx-\left[\left(1+\frac{1-2\varkappa}{4\zeta^2}\right)\psi(x_\infty)\right]^{-1}\frac{R_{cr}}{R} \tag{4.7}$$

(x_∞ is defined in (A.12)).

It is seen from Fig. 2 that at $\zeta=1$ the results of the WKB method (curve 1) and of the small subcriticality approximation[7] (dashed curve 4) practically coincide. This attests to the good accuracy of the WKB approximation for the ground level $1s\sigma$. For the first excited level, the difference between these approximations is ~10%.

The probability of spontaneous positron production at $R<R_{cr}$ is determined by formulas (3.7) and (3.10), where the energy ε must be taken from Eq. (4.5). The exponential factor in γ was obtained previously,[6] but the pre-exponential γ_0 could not be calculated without using the formulas of Sec. 1. We note that γ_0 depends substantially on the positron momentum k and on the total charge of the nuclei:

$$\gamma_0=\frac{k^2}{2\zeta}\left\{[(1-\rho^2)(1+k^2)]^{1/2}-\frac{1}{k}\operatorname{Arth}\left(k\left[\frac{1-\rho^2}{1+k^2}\right]^{1/2}\right)\right\}^{-1}$$
$$=\begin{cases}c_0, & k\to 0\\ c_1 k, & k\gg 1\end{cases}; \tag{4.8}$$

here

$$c_0=3[2\zeta(2+\rho^2)(1-\rho^2)^{1/2}]^{-1},\quad c_1=[2\zeta(1-\rho^2)^{1/2}]^{-1}$$

(see Fig. 3). The pre-exponential factor γ_0 increases with increasing ρ and grows sharply as $\rho\to 1$. In this region, however, $g=(\zeta^2-\varkappa^2)^{1/2}\to 0$ and the condition for the validity of the quasiclassical approach is violated-[see (1.25)]. The value of γ_0 at $\zeta=\rho=1$ can be obtained from the small-supercriticality approximation,[7] and is shown by the dashed curve of Fig. 3. It is interesting to note the fact that although the analytic form of $\gamma_0(k)$ is quite complicated, the dependence of γ_0 on ε is nearly linear.

It follows from Figs. 2 and 3 that the level energy ε and the width γ depend not only on the ratio R/R_{cr}, but also on the total charge Z of the nuclei. This points to the approximate character of the self-similarity (i.e., to a universal dependence of ε and γ on the ratio R/R_{cr}

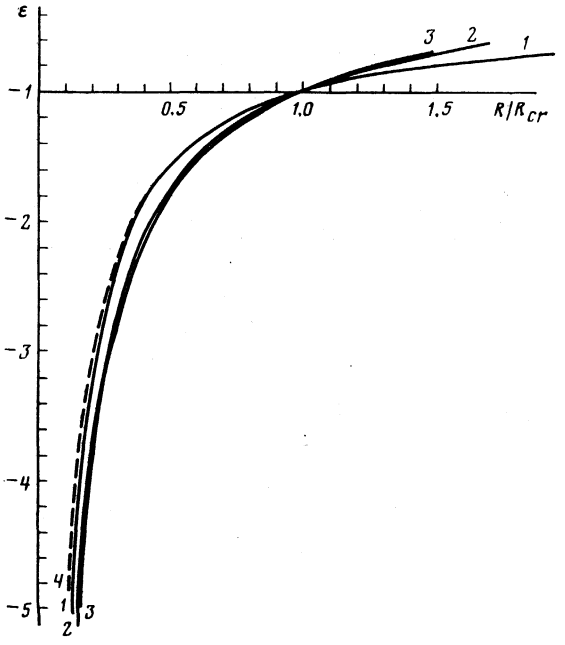

FIG. 2. Energy of the ground level $1s\sigma$ as a function of the distance R between the colliding nuclei. The values of the total charge $Z=Z_1+Z_2$ are the following: curve 1—$Z=137$, curve 2—$Z=184$, curve 3—$Z=200$; curve 4—result of calculation of $\varepsilon(R/R_{cr})$ in the small-supercriticality approximation[7] at $Z=137$.

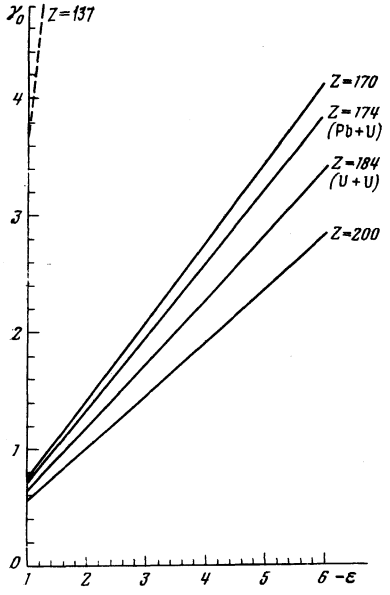

FIG. 3. Pre-exponential factor $\gamma_0(\varepsilon,\zeta)$ in formula (3.9); $Z=Z_1+Z_2$ is the total charge of the nuclei. The curves with $Z=174$ and 184 correspond to Pb+ U and U +U collisions. The dashed curve was constructed in accordance with the "small supercriticality" approximation.[7]

at arbitrary ζ) obtained in the small-supercriticality approximation. In the calculation of the cross section and of the energy spectrum of the positrons for the $U+U$ collision, they used in Ref. 7 curves corresponding to $Z=137$, whereas the curve with $Z=184$ should be taken. This correction is significant (especially the change in the position of the level on Fig. 2, since the probability w depends exponentially on the momentum k), and must be taken into account in the comparison of theory with experiment.

5. THRESHOLD BEHAVIOR OF THE LEVEL WIDTH γ

As $\varepsilon \to -1$, i.e., at the threshold of the spontaneous positron production, the Dirac equation with Coulomb potential has a simple analytic solution.[6] Since $r_N \sim 0,03 \ll 1$ (in units of $\hbar/m_e c$), we can expect the probability of finding the electron inside the nucleus to be of the order of several percent. This is confirmed by numerical calculation (see Fig. 5 of Ref. 28). Using the smallness of r_N, we can develop a calculation method that is valid in the energy region $\varepsilon \approx -1$ and is more accurate than the WKB approximation.

Let us examine, following Ref. 7, the determination of the width γ. At $r \ll r_+ \approx 2\zeta/k^2$ the wave function of the quasistationary state is practically independent of the energy ε and coincides with the wave function of the level in the critical point, which is known in analytic form [see formulas (2.22)–(2.28) in Ref. 10]. On the other hand, at $r > \zeta/2$ the substitution $\chi_2 = [1-\varepsilon V(r)]^{-1/2} F(r)$ no longer has any singularities, so that we can write for $\chi_2(r)$ the usual quasiclassical formulas.[1] If $k \ll 1$, then we can choose the matching point r such that $r_- \ll r \ll r_+$. In this region of r, the quasiclassical asymptotic form of $\chi_2(r)$ goes into the "tail" of the wave function at the critical point, and this determines the normalization constant in χ_2. Calculating next with the aid of χ_2 the flux of particles as $r \to \infty$, we obtain for the probability of the spontaneous production of positrons formula (3.10) with the pre-exponential factor

$$\gamma_0 = \frac{3\zeta^2[1-\exp(-4\pi g)]}{[4\zeta^2+(\varkappa-1)(2\varkappa-1)]g} \tag{5.1}$$

(see Fig. 4). This formula is exact at $k \to 0$. Under the condition $\zeta \gg |\varkappa| \gg 1$ it goes over into the quasiclassical formula (4.8); the dependence of γ_0 on the sign of $\varkappa$ then drops out.

We can similarly determine also other physical quantities at $\varepsilon = -1$. Thus for the moments

$$\langle r^\nu \rangle = \int_0^\infty (G^2+F^2) r^\nu dr,$$

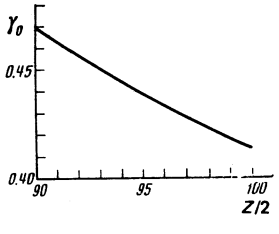

FIG. 4. Pre-exponential factor γ_0 at the positron-production threshold ($k \to 0$).

which characterize the dimensions of the electron cloud we obtain

$$\langle r^\nu \rangle = \frac{3\pi^{1/2}(\nu+2)}{2^{3(\nu+1)}\zeta^\nu} \frac{\Gamma(\nu+1)}{\Gamma(\nu+{}^5/_2)} \left| \frac{\Gamma(\nu+1+2ig)}{\Gamma(1+2ig)} \right|^2 \times \frac{(\nu+2)\zeta^2+(\nu+1)[\varkappa^2-(\nu+{}^3/_2)\varkappa+{}^1/_4(\nu^2+3\nu+2)]}{2\zeta^2+\varkappa^2-{}^3/_2\varkappa+{}^1/_2}, \tag{5.2}$$

where $\zeta = \zeta_{cr}(r_N, \varkappa)$. In particular, the average radius is

$$\langle r \rangle = \frac{3}{10\zeta}\left(\zeta^2-\varkappa^2+\frac{1}{4}\right)\frac{\zeta^2+({}^2/_3\varkappa^2-{}^5/_3\varkappa+1)}{\zeta^2+{}^1/_2(\varkappa^2-{}^3/_2\varkappa+{}^1/_2)}. \tag{5.3}$$

For the first three levels $1s_{1/2}, 2p_{1/2}$ and $2s_{1/2}$ we therefore get $\langle r \rangle \approx 0.301$, 0.227 and 0.532, while exact calculation (numerical solution of the Dirac equation) yields respectively 0.303, 0.229, and 0.534. This approximation is thus quite accurate.

Unfortunately, the region of its applicability is limited to energies near the boundary of the lower continuum: at $k \gtrsim 1$ the solutions of the Dirac equation are no longer expressed in terms of MacDonald functions (see Ref. 6), and furthermore the region where the solutions are matched together vanishes. The WKB method is cruder, but its applicability is not limited to the case $\varepsilon \approx -1$. It is important to note that where regions of applicability of these two methods overlap, their results coincide. Thus, calculation of the moments $\langle r^\nu \rangle$ with the aid of (1.12) yields

$$\langle r^\nu \rangle_{cl} = \frac{3\pi^{1/2}}{8} \frac{(\nu+2)\Gamma(\nu+1)}{\Gamma(\nu+{}^5/_2)} \left(1+\frac{\nu+1}{\nu+2}\rho^2\right) \frac{[{}^1/_2\zeta(1-\rho^2)]^\nu}{1+{}^1/_2\rho^2}, \tag{5.4}$$

which agrees with (5.2) if $|\varkappa| \gg 1$. As already noted, the situation is similar for γ.

6. INFLUENCE OF SCREENING ON THE CRITICAL DISTANCE BETWEEN NUCLEI

When two heavy nuclei come close together, a quasimolecule is produced for a short time ($\tau_{coll} \sim 10\hbar/m_e c^2 \approx 10^{-20}$ sec). The electric field exceeds in this case the critical value if $R_{min} < R_{cr}$. If the colliding nuclei are not fully stripped (as under the experimental conditions[4,5]), the quasimolecule is surrounded by an electron cloud whose screening action weakens the attraction of the K electron to the nuclei. As a result, the critical charge Z_{cr} increases (in the case of a spherical superheavy nucleus) and R_{cr} decreases. A numerical calculation of the screening effect in the spherical-nucleus model was carried out in Ref. 29.

We present a sample calculation of this effect, which is valid not only for a spherical nucleus but also for a system of two nuclei. We use the fact that nuclei in the uranium region satisfy the conditions

$$R_{cr} \ll \bar{r} \ll a, \tag{6.1}$$

where $a \sim (Ze^6)^{-1/2} \approx 30\zeta^{-1/3}$ is the average radius of the atom in accordance with the Thomas-Fermi model. This makes it possible to use the nonrelativistic Thomas-Fermi model for the description of the outer electron shells. The level shift $\Delta\varepsilon$ is determined by the perturbation $\delta V = V(\mathbf{r}) - V_0(\mathbf{r})$, where V_0 is the potential (4.1) for bare nuclei, and V is the potential corrected for the electron shell. The characteristic radius for δV is $r \sim a$, so that accurate to $\sim (R_{cr}/a)^2$

~10^{-3} the perturbation δV should be regarded as spherically symmetrical:

$$\delta V=\frac{\zeta}{a}\cdot\begin{cases}[1-\varphi(x)]/x-q/x_0, & 0<x\leqslant x_0\\ (1-q)/x, & x\geqslant x_0\end{cases}. \tag{6.2}$$

Here

$$a^{-1}=\left[\frac{128}{9\pi^2}(Z_1+Z_2)e^6\right]^{1/3}=0.0425\zeta^{1/3},$$

$x=r/a$, $q=(Z_1+Z_2-N)/(Z_1+Z_2)$ is the degree of ionization, N is the total number of electrons in the quasimolecule shell, $\varphi(x)$ is the solution of the Thomas-Fermi equation with suitable boundary conditions,[1] $r_0=ax_0$ is the radius of the positive ion, and $x_0=x_0(q)$. Using the expansion of $\varphi(x)$ at small x, we find the correction for the screening in the two-center problem:

$$\Delta R_{cr}=-\frac{\zeta R_{cr}}{\beta a}\sum_{n=0}c_n\langle r^{n/2}\rangle a^{-n/2}. \tag{6.3}$$

Here β is the slope of the level on the boundary of the lower continuum [see formula (4.6)],

$$\langle r^\nu\rangle=\int\psi_0^2(\mathbf{r})r^\nu d^3r, \tag{6.4}$$

where $\psi_0(\mathbf{r})$ is the wave function in the critical point ($\varepsilon=-1, R=R_{cr}$) and is normalized by the condition $\int\psi_0^2(\mathbf{r})d^3r=1$; the coefficients c_n depend on the degree of ionization q:

$$c_0=\gamma-q/x_0,\quad c_1=-1/2,\quad c_2=0,\ c_3=2/5\gamma,$$
$$c_4=-1/2,\ c_5=-3/70\gamma^2,\ \ldots; \tag{6.5}$$

$\gamma=\gamma(q)=-\varphi'(0)$ is the slope of the $\varphi(x)$ curve at zero. For a neutral atom we have $q=0, x_0=\infty, c_0=\gamma=1.588$ (see Ref. 1). The quasimolecule produced when a bare nucleus collides with a neutral atom corresponds (at $Z_1=Z_2$) to the parameters $q=1/2, x_0=2.952, \gamma=1.607$.

The series (6.3) converges rapidly. The quantities β and $\langle r^{n/2}\rangle$ can be obtained by numerically solving the two-center problem for the Dirac equation. A rough estimate (with the moments $\langle r^{n/2}\rangle$ replaced by their values for a spherical nucleus) shows that the correction for the screening is appreciable: $\Delta R_{cr}/R_{cr}\approx 12\%$ at $q=0$ and $\Delta R_{cr}/R_{cr}\approx 10\%$ at $q=0.5$.

7. ANGULAR DISTRIBUTION OF THE POSITRONS

In the quasiclassical approximation the probability of passage of the particle through the barrier, accurate to the pre-exponential factor, is equal to

$$w\approx\exp(-2\operatorname{Im}S), \tag{7.1}$$

where $S=\int L dt$; the integral is taken along the extremal trajectory that minimizes ImS.

As seen from (4.1), the potential of the system of two nuclei contains at $r\gg R$ a quadrupole correction. For uranium nuclei this correction in the subbarrier region $r_-<r<r_+$ does not exceed $(R_{cr}/2r_-)^2\sim 10^{-2}$. Therefore the problem reduces to a calculation of the penetrability of a three-dimensional barrier that differs little from a spherically symmetrical one, and can be solved with the aid of an expansion in powers of R^2. Substituting

$$V=V_0+R^2V_1+\ldots,\quad S=S_0+R^2S_1+\ldots \tag{7.2}$$

in the Hamilton-Jacobi equation (2.4), we get

$$(\nabla S_0)^2=2(E-U_0),\ \nabla S_0\cdot\nabla S_1=-U_1,\ \ldots, \tag{7.3}$$

where

$$E=\frac{\varepsilon^2-1}{2},\quad U_0=-\left(\frac{\zeta^2}{2r^2}+\frac{\varepsilon\zeta}{r}\right),\quad U_1=-\frac{\zeta}{4r^2}\left(\varepsilon+\frac{\zeta}{r}\right)P_2(\cos\theta).$$

Since $U_0=U_0(r)$, it follows that θ is a cyclic variable. Therefore the first equation is directly integrated:

$$S_0(r,\theta)=\int^r p dr+\varkappa\theta,$$

where $p(r)$ is the radial momentum (1.13). The imaginary part of the action is acquired when the particle moves in the subbarrier region, where $p=iq$. The equation for S_1 in the region $r_-<r<r_+$ is of the form

$$iq(r)\frac{\partial S_1}{\partial r}+\frac{\varkappa}{r^2}\frac{\partial S_1}{\partial\theta}=-U_1(r,\theta) \tag{7.4}$$

and is solved by the method of separation of the variables. Putting $r^2U_1(r,\theta)=u(r)(3/4\cos 2\theta+1/4)$ and taking into account the boundary condition $\operatorname{Im}S_1(r_-)=0$ we obtain at $r=r_+$, i.e., at the emergence from under the barrier:

$$\operatorname{Im}S_1(r_+,\theta)=aP_2(\cos\theta)+a',$$

where

$$a=\int_{r_-}^{r_+}dr\frac{u(r)}{q(r)}\operatorname{ch}\left(2\varkappa\int_r^{r_+}\frac{dr'}{q(r')r'^2}\right),$$
$$a'=-\frac{1}{2}\int_{r_-}^{r_+}dr\frac{u(r)}{q(r)}\operatorname{sh}^2\left(\varkappa\int_r^{r_+}\frac{dr'}{q(r')r'^2}\right) \tag{7.5}$$

(the constant a' is immaterial for the angular asymmetry of positron emission).

A most remarkable fact is that the expression for a acquires a hyperbolic cosine that enhances of the angular anisotropy of the emitted particles compared with the anisotropy of the potential. The cause of this effect is that the subbarrier trajectory of a tunneling particle with nonzero angular momentum is not a straight line. One-dimensional motion corresponds to $\varkappa=0$; in this case

$$\operatorname{Im}S_1(r_+,\theta)=\int_{r_-}^{r_+}\frac{U_1(r,\theta)}{q(r)}dr \tag{7.6}$$

and there is no enhancement. Formula (7.6) can also be obtained by varying the expression

$$\operatorname{Im}S=\int_{r_-}^{r_+}[2(U-E)]^{1/2}dr$$

with respect to the potential U (it is assumed here that θ is constant, i.e., the "twisting" of the subbarrier trajectory is not taken into account). Since $|\varkappa|=j+1/2\geq 1$ for a Dirac particle, the anisotropy of the potential is always enhanced. This constitutes the substantial difference between the three-dimensional and one-dimensional problems.

We note that in the case of a Coulomb field we have

$$u(r)=-\frac{\zeta(\zeta+\varepsilon r)}{4r^3},\quad q(r)=\frac{k}{r}[(r_+-r)(r-r_-)]^{1/2} \tag{7.7}$$

and the integral (7.5) can be calculated exactly. This calculation, however, is hardly meaningful, since applicability of the WKB method now calls not only for quasiclassical radial motion (which is well satisfied in

a Coulomb field at $g \gtrsim 1$), but also quasiclassical values of the angle θ. The latter are obtained only at $|\varkappa| \gg 1$, a condition which does not hold for the first levels $1s\sigma$ and $2p\sigma(\varkappa = \mp 1)$. Formula (7.5) cannot claim to be quantitatively accurate for these states.

Taking (7.7) into account, we get

$$\int_{r_-}^{r_+} \frac{dr}{qr^2} = \frac{\pi}{g}.$$

An estimate of the integral (7.5) shows that the parameter α in the angular distribution of the positrons

$$w(\theta) \approx \exp(-2\operatorname{Im} S) = \text{const} \cdot \exp(\alpha P_2(\cos\theta)) \qquad (7.8)$$

is of the order of $\alpha \sim (R^2 \sinh\eta)/\eta \gg R^2$, where $\eta = 2\pi\varkappa(\zeta^2 - \varkappa^2)^{-1/2}$. For uranium nuclei, $\alpha \sim 1/3$, and we can expect therefore a noticeable angular anisotropy (the positrons are emitted predominantly along the axis that joins the nuclei at the instant of their closest approach). This question is worthy of experimental study.

8. ADIABATIC CORRECTION TO THE LEVEL WIDTH γ

In the derivation of formula (3.10) it is assumed that the positron tunneling time τ_t is too short for either the barrier itself or for the level energy ε to change noticeably. This, however, is certainly not the case in the region of R close to R_{cr}, since τ_t increases without limit as $k \to 0$.

Using the imaginary-time method,[6] we now estimate the correction due to the change of the penetrability of the Coulomb barrier as the result of the finite velocity of the nuclei. The probability of particle tunneling from a bound state (with energy ε_0) into states of the continuous spectrum is determined by the imaginary part of the action function[7]

$$\bar{S} = \int_{t_0}^{t} (L + \varepsilon_0)\, dt = \int_{t_0}^{t} \{-m(1-\dot{x}^2)^{1/2} - V(x,t) + \varepsilon_0\}\, dt. \qquad (8.1)$$

Varying this expression, we get

$$\delta\bar{S} = \int_{t_0}^{t} \left[p\delta\dot{x} - \frac{\partial V}{\partial x}\delta x - \delta V + \delta\varepsilon_0 \right] dt$$

$$= p\delta x\Big|_{t_0}^{t} + \int_{t_0}^{t} (\delta\varepsilon_0 - \delta V)\, dt, \qquad (8.2)$$

where $p = m\dot{x}(1-\dot{x}^2)^{-1/2}$ and account is taken of the equation of motion $\dot{p} = -\partial V/\partial x$. We note that $p\delta x\big|_{t_0}^{t}$ makes no contribution to $\operatorname{Im}\delta\bar{S}$, and the term $\int \delta\varepsilon_0 dt$ is fully accounted for by the fact that in the calculation of γ the level energy is taken in the form $\varepsilon_0 = \varepsilon_0(R(t))$ corresponding to the adiabatic approximation in the velocity of the nuclei. The term that remains in

$$\bar{S}_1 = -\int_{t_0}^{t} \delta V(x(t))\, dt \qquad (8.3)$$

yields the correction to the penetrability of the static barrier necessitated by the effect of interest to us—the change of $R(t)$ during the tunneling time. The integral (8.3) is then calculated along a subbarrier trajectory that satisfies formally the classical equations of motion, but with "imaginary time" $t = i\tau$, where

$$\tau = \int_{r}^{r_+} \frac{V-\varepsilon}{q(r)}\, dr = \frac{\zeta}{k^3}\{\varphi + [(1+k^2)(1+\rho^2k^2)]^{1/2}\sin\varphi\}. \qquad (8.4)$$

We have introduced here the variable $\varphi = 2\arcsin[(r_+ - r_-)/(r_+ - r_-)]^{1/2}$, which is convenient in the case of the Coulomb field. In this case $0 \leq \varphi \leq \pi$, $r = r_+\cos^2(\varphi/2) + r_-\sin^2(\varphi/2)$, while $\tau = 0$ and $\varphi = 0$ correspond to the instant of emergence from under the barrier. The total tunneling time is therefore $\tau_t = \pi\zeta/k^3$, i.e., $\tau_t \to \infty$ as $\varepsilon \to -1$, and for deep levels τ_t becomes rapidly shorter.

The kinematics of the motion of the nuclei was considered in detail in Refs. 7 and 8. Near the closest-approach point we have $R(t) = R_0 + v^2t^2/4R_0$; Taking (4.1) into account, we obtain the time-varying part of the potential:

$$\delta V = -\frac{\zeta v^2}{8r^3}t^2.$$

Substitution in (8.3) yields

$$\operatorname{Im}\bar{S}_1 = -\frac{2Z}{A}\frac{m_e}{m_N}\frac{\zeta^2}{R_0 v_p^3} I(\varepsilon_p, \eta), \qquad (8.5)$$

where $\varepsilon_p = -\varepsilon$, $v_p = (1-\varepsilon^{-2})^{1/2}$ is the positron velocity,

$$I(\varepsilon_p, \eta) = -\frac{1}{8}\int_0^{\pi} d\varphi \left[\frac{\sin\varphi + (1-v_p^2)\eta}{\cos\varphi + \eta}\right]^2 \frac{\cos\varphi + (1-v_p^2)\eta}{\cos\varphi + \eta}, \qquad (8.6)$$

$\eta = [1 - (1-\rho^2)v_p^2]^{1/2}$, and $\rho^2 = \varkappa^2/\zeta^2$. The integral (8.6) was calculated numerically (see the table for $\zeta = 1.343$, which corresponds to collision of two uranium nuclei). The ratio

$$\delta = \operatorname{Im}\bar{S}_1/\operatorname{Im}\bar{S}_0, \quad \operatorname{Im}\bar{S}_0 = \pi\zeta[v_p^{-1} - (1-\rho^2)^{1/2}] \qquad (8.7)$$

for $\zeta = 1.343$ is shown in Fig. 5, from which it is seen that $\delta < 10\%$ at $|\varepsilon| > 1.65$. Thus, the adiabatic approximation in the problem of spontaneous production of positrons is not valid only in a relatively narrow energy region near $\varepsilon = -1$, where the positron production cross section itself is quite small.

Numerical calculations have shown[14,15] that R_{cr} increases rapidly with increasing total charge $Z_1 + Z_2$ for nuclei in the uranium region. The cross section for spontaneous production of positrons increases in this case in proportion to $R_{cr}^{7/2}$ (see Ref. 7), while the correction for the nonadiabaticity of the tunneling process decreases in proportion to $1/R_{cr}$ [at a fixed energy of the emitted positron–see formula (8.5)]. To check on the theory developed in the adiabatic approximation, it is convenient therefore to perform the experiments on heavier nuclei.

When heavy nuclei collide, induced positron pro-

TABLE I.

ε_p	$I(\varepsilon_p, \eta)$	ε_p	$I(\varepsilon_p, \eta)$	ε_p	$I(\varepsilon_p, \eta)$	ε_p	$I(\varepsilon_p, \eta)$
1.05	880	1.55	12.0	2.05	3.11	2.9	0.960
1.10	284	1.60	10.0	2.10	2.82	3.0	0.876
1.15	142	1.65	8.50	2.15	2.57	3.25	0.716
1.20	84.9	1.70	7.28	2.20	2.36	3.5	0.605
1.25	56.4	1.75	6.30	2.3	2.00	3.75	0.525
1.30	40.0	1.80	5.50	2.4	1.72	4.0	0.465
1.35	29.7	1.85	4.84	2.5	1.50	4.25	0.419
1.40	22.8	1.90	4.29	2.6	1.32	4.5	0.384
1.45	18.1	1.95	3.83	2.7	1.18	4.75	0.355
1.50	14.6	2.00	3.44	2.8	1.06	5.0	0.332

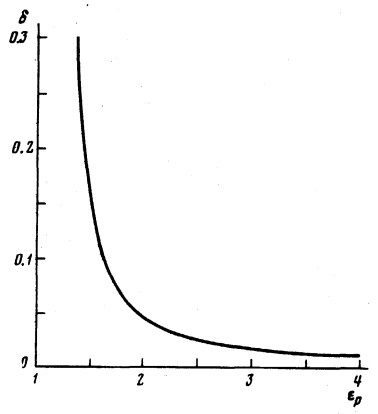

FIG. 5. Relative value of the adiabatic correction δ as a function of the positron energy $\varepsilon_p = (1+k^2)^{1/2}$. The calculation was made for uranium nuclei ($\zeta = 1.343$).

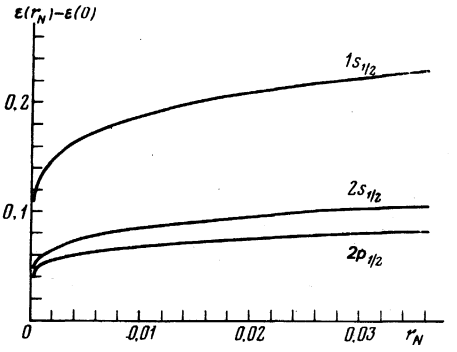

FIG. 6. The correction $\varepsilon(r_N) - \varepsilon(0)$ for the finite dimensions of the nucleus at $Ze^2 = 1$; r_N is the radius of the nucleus in units of $\hbar/m_e c = 386$ F, $\varepsilon(0)$ is the level energy in the field of a point charge ($r_N \to 0$).

duction is possible in addition to the spontaneous production. A calculation of the probability of this process is given in Ref. 9.

9. ELECTRON SPECTRUM AT $Z = 137$

The exact equation for the level energies in a potential (1.20) is quite unwieldy.[6] It can be simplified in two cases: 1) at $\varepsilon = -1$, a fact already used[6] in the calculation of the critical charge of the nucleus; 2) at $\zeta = |\varkappa| = j + 1/2$, corresponding to the start of the "falling to the center" in the field of the point charge Ze for states with angular momentum j.

We consider the second case. Since we have here $g = (\zeta^2 - \varkappa^2)^{1/2} = 0$, the condition (1.25) is violated and the WKB method cannot be used. To calculate the level spectrum it is necessary to turn to the exact solutions of the Dirac equation.

We confine ourselves to the case $\zeta = |\varkappa| = 1$ (the levels $ns_{1/2}$ and $np_{1/2}$). Introducing the function

$$\varphi_\nu(x) = \frac{1}{\Gamma(1-\nu)} \int_1^\infty e^{-xt}(t-1)^{-\nu}(t+1)^{\nu-1}dt,$$

we can transform Eq. (16) of Ref. 6 into

$$x\frac{\varphi_\nu'(x)}{\varphi_\nu(x)} = \left[\frac{1}{\varkappa + (\nu^2+1)^{1/2} - \nu} - \frac{1}{\xi_\varkappa}\right]^{-1}. \qquad (9.1)$$

Here $\nu = \varepsilon(1-\varepsilon^2)^{-1/2}$, $x = (\nu^2+1)^{-1/2} r_N$, $\varkappa = \pm 1$, ξ is the logarithmic derivative of the internal solution on the edge of the nucleus; the values of $\xi_\varkappa$ at $\zeta = 1$ are the following:

	$\varkappa=-1$	$\varkappa=1$
Cutoff model I:	0.642	1.794
Cutoff model II:	0.550	1.220

After determining the roots $\nu = \nu_{n\varkappa}$ of (9.1), we can calculate the energy spectrum from the formula $\varepsilon_{n\varkappa} = \nu(1+\nu^2)^{-1/2}$. The results of the calculation are shown in Figs. 6 and 7. Allowance for the finite dimensions of the nucleus at $\zeta = 1$ lifts the known "accidental" degeneracy of the levels with respect to the sign of $\varkappa$, which is characteristic of the Dirac equation in a Coulomb field.[8)] It follows from (9.1) that as $r_N \to 0$ the expansion parameter for ε is not the nuclear radius r_N of itself, but $\Lambda = -\ln r_N$

$$\varepsilon(r_N) = \sum_{k=0}^{\infty} \varepsilon_k \Lambda^{-k}, \quad \varepsilon_0 = (n-1)(n^2-2n+2)^{-1/2}, \ldots, \qquad (9.2)$$

with the first term of the series ε_0 corresponding to the Sommerfeld formula for a pointlike nucleus. The values of the coefficients ε_1 and ε_2 are given in Ref. 35. The splitting of the levels $ns_{1/2}$ and $np_{1/2}$ begins with Λ^{-2}.

The non-analytic character of the dependence of $\varepsilon_{n\varkappa}$ on the radius of the nucleus at the point $r_N = 0$ is connected with the behavior of the effective potential at short distances: $U = -1/8r^2 + O(r^{-1})$. This behavior is on the borderline between the cases of regular and singular potentials.[1] Therefore the influence of the finite dimensions of the nucleus at $\zeta = 1$ for states with $j = 1/2$ and $\varkappa = \pm 1$ cannot be taken into account by perturbation theory, and the correction $\varepsilon(r_N) - \varepsilon(0)$ itself turns out to be quite appreciable (see Fig. 6), although $\zeta = 1$ these states are still far from the boundary of the lower continuum.

10. DEEP LEVELS IN THE LOWER CONTINUUM

Special consideration should be given to the case

$$\zeta,\ k \gg 1; \quad |\varkappa| \leqslant (\zeta/\pi)^{1/2}, \qquad (10.1)$$

i.e., levels with relatively small ($\varkappa,\ \varkappa_{max} \sim \zeta^{-1/2} \ll 1$) angular momenta, which have dropped deeply into the

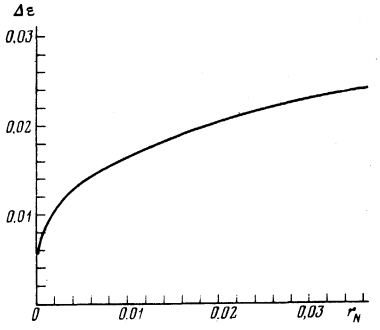

FIG. 7. Lifting of the "accidental" Coulomb degeneracy at $Ze^2 = 1$. We designate by $\Delta\varepsilon$ the difference between the energies of the levels $2s_{1/2}$ and $2p_{1/2}$, with opposite signs of the quantum number.

lower continuum. Most appropriate for such states is the term "superbound electrons," proposed in Ref. 11. At the present time the properties of such states are of purely theoretical interest, since their existence calls for nuclei with charge $\zeta = Ze^2 \gg 1$. This question, however, would become timely should supercharged nuclei, the existence of which is suggested by Migdal's theory,[36,37] be observed.

When the conditions (10.1) are satisfied, the turning points r_+ and r_- come closer together

$$\frac{r_+ - r_-}{r_+ + r_-} = \left(\frac{1+\rho^2 k^2}{1+k^2}\right)^{1/2} \sim \rho \ll (\pi\zeta)^{-1/2}$$

and the penetrability of the barrier tends to unity. Therefore the quasiclassical approximation ceases to be valid, and it becomes necessary to resort to the exact solutions of the Dirac equation.

Owing to the analytic difficulties, we confine ourselves to cutoff model I, assuming in this case that $k^2 \gg \zeta \gg 1$. Changing over in the region $r > r_N$ from the functions G and F to their linear combinations χ_+ and χ_-, which are equal to

$$\chi_\pm(r) = r^{1/2}\{(1-\varepsilon)^{1/2} G \pm i(-1-\varepsilon)^{1/2} F\}, \tag{10.2}$$

we have

$$\chi_\pm'' + p_\pm^2(r)\chi_\pm = 0,$$

$$p_\pm^2(r) = k^2 - 2\zeta\left[(k^2+1)^{1/2} \pm \frac{ik}{2\zeta}\right]\frac{1}{r} + \left(\zeta^2 - \varkappa^2 + \frac{1}{4}\right)\frac{1}{r^2}. \tag{10.3}$$

We separate from $\chi_\pm$ the factor corresponding to the quasiclassical asymptotic value $\exp(i\int^r p_\pm dr)$ as $r \to \infty$:

$$\chi_\pm(r) = \exp\{i[kr - (\zeta \pm i/2)\ln kr]\} y_\pm(r), \tag{10.4}$$

$$y_\pm'' + 2(ik + \alpha_\pm r^{-1}) y_\pm' + \beta_\pm r^{-2} y_\pm = 0, \tag{10.5}$$

where $\alpha_\pm = -i\zeta \pm 1/2$, $\beta_+ = -\varkappa^2$, $\beta_- = 2i\zeta + 1 - \varkappa^2$. Assuming $r = (\xi + t)/k$ and confining ourselves in the region $|t| \ll \zeta$ to the principal terms of the expansion in ζ^{-1}, we arrive at the equation

$$\frac{d^2 y_\pm}{dt^2} + \frac{2i}{\zeta} t \frac{dy_\pm}{dt} + \frac{k^2}{\zeta^2}\beta_\pm y_\pm = 0,$$

which can be reduced by the substitution

$$t = (i\zeta/2)^{1/2} x, \quad y_\pm(t) = \varphi_\pm(x)\exp(-x^2/4)$$

to the standard form of the equation for the parabolic-cylinder functions. The quasistationary level corresponds to the solution

$$\chi_\pm(r) = \text{const} \cdot \exp\{\pm(i/8\zeta)^{1/2} x\} D_{\nu_\pm}(x), \tag{10.6}$$

where $x = (i\zeta/2)^{-1/2}(kr - \zeta)$, $\nu_+ = 1 + \nu_- = -i\varkappa^2/2\zeta$. Inside the nucleus, the Dirac equation for the cutoff model I can be solved analytically in terms of Bessel functions. The matching of the external and internal solutions on the edge of the nucleus yields the equation

$$\frac{\Lambda_j(z) - i}{\Lambda_j(z) + i} = (i\eta)^{1/2} \frac{D_{-(1+i\eta)}(u)}{D_{-i\eta}(u)}, \tag{10.7}$$

which determines the spectrum of the quasistationary states. Here

$$z = \zeta - kr_N, \quad u = e^{3\pi i/4}(\zeta/2)^{-1/2} z, \quad \eta = \varkappa^2/2\zeta, \quad \Lambda_j(z) = J_{j+1}(z)/J_j(z).$$

The appearance of the functions D_ν in (10.6) and (10.7) is due to the fact that at $|\varkappa| \ll \zeta^{1/2} \ll k$ the effective potential becomes parabolic.

Although (10.7) is much simpler than the exact equation for the energy levels, its solution still calls for numerical calculations. We consider limiting cases, in which the answer can be obtained in analytic form:

a) $z \ll \zeta^{1/2}$. This includes the deepest levels with energy close to the bottom of the well. Since $|u| \ll 1$, we can neglect the right-hand side of (10.7). As a result

$$\varepsilon_{nj} = (-\zeta + z_{nj})/r_N, \tag{10.8}$$

where z_{nj} are the roots of the equation $\Lambda_j(z) = i$, $n = 1, 2, 3, \ldots$. Near the bottom of the well the level spectrum is approximately equidistant, as can be seen from the asymptotic ($n \gg 1$, $j \ll n \ll \zeta^{1/2}$) formula

$$\varepsilon_{nj} = \left[-\zeta + \left(n + \frac{j}{2}\right)\pi + \frac{i}{2}\ln\frac{4\pi n}{2j+1}\right] r_N^{-1}. \tag{10.9}$$

The decrease of γ_{nj} with increasing j is due to the centrifugal barrier. At fixed j, the width γ_{nj} increases with increasing n, but more slowly than the distance of the level from the bottom of the well (for details see Ref. 35).

b) $z \gg \zeta^{1/2}, j$. Substituting in (10.7) the quasiclassical asymptotic forms for the Bessel and Weber functions we obtain

$$\gamma_{nj} = -\frac{1}{2r_N}\ln(1 - e^{-2\pi\eta}). \tag{10.10}$$

The region of applicability of this formula is $\zeta^{1/2} \ll n \ll \zeta$, $n \gg j$. The width γ is determined here by the value of the angular momentum. At $j \gg \zeta^{1/2}$ we have $\eta \gg 1$ and a transition takes place to the quasiclassical exponential function (3.11):

$$\gamma \approx \frac{1}{2r_N}\exp\left(-\frac{\pi\varkappa^2}{\zeta}\right).$$

This establishes the connection between the WKB approximation and the exact solutions of the Dirac equation.

c) At $j \ll n \sim \zeta^{1/2}$ formulas (10.9) and (10.10) are joined together and yield

$$\gamma_{nj} = \frac{1}{2r_N}\left[\ln\frac{\zeta}{\varkappa^2} + O(1)\right].$$

In this energy region (still close to the bottom of the well, since the exponential factor in (3.3) is close to unity), γ reaches a maximum, with

$$\frac{\gamma_{nj}}{|\varepsilon_{nj}|} \sim \frac{\ln\zeta}{2\zeta} \ll 1, \quad \frac{\gamma_{nj}}{\varepsilon_{n+1,j} - \varepsilon_{nj}} \sim \frac{1}{2\pi}\ln\frac{\zeta}{(2j+1)^2}.$$

Thus, in this case, too, the quasistationary levels in the lower continuum overlap weakly. On the other hand, if the angular momentum is large enough, $|\varkappa| \gtrsim (\zeta/\pi)^{1/2}$, then the exponential (3.10) comes into play and decreases γ sharply.

Thus, levels with energy $\varepsilon < -1$ (even deep ones) are not "smeared out" over the lower continuum, but remain practically isolated. In addition, because of the Pauli principle, no considerable growth of the vacuum polarization takes place as $Z \to Z_{cr}$,[10] in contrast to the boson case.[37] This explains why the single-particle approximation has such good accuracy in the case of fermions in the region $Z > Z_{cr}$. The two indicated facts (the small width of γ and the allowance

for the Pauli principle) were used in the derivation[27] of the relativistic Thomas-Fermi equation that describes the electron shell of a supercritical atom.

11. CONCLUDING REMARKS

1. The application of the WKB method to a Coulomb field with charge $Z>137$ was previously based[6, 22, 23, 38] on squaring the Dirac equation. This method is good at $\varepsilon \geq -1$, but a difficulty arises for states with energy $\varepsilon<-1$: the substitutions (8.1) have singularities at the points r_1 and r_2, such that $V(r)=\varepsilon \pm 1$ (we are considering an attraction potential: $V(r)<0$, $0<r<\infty$). Consequently as $r \to r_i$ the effective potential $U_i(r) \approx 3/8(r-r_i)^{-2}+\ldots \to \infty$ and the ordinary quasiclassical formulas[1] become meaningless near the points $r=r_i$ because of the divergence of the integral $\int^r [2(E-U_i)]^{1/2} dr$. The points r_1 and r_2 are always in the region below the barrier. For example, at $V(r)=-\zeta/r$ we have

$$r_1=\frac{\zeta}{k^2}[1+(1+k^2)^{1/2}], \quad r_2=\frac{\zeta}{1+(1+k^2)^{1/2}},$$

and a comparison with (1.21) shows that $r_-<r_2<r_1<r_+$.

2. At $Z=Z_{cr}$ this difficulty still does not manifest itself. In fact, as $\varepsilon \to -1$ we have $r_-=\zeta(1-\rho^2)/2$, $r_2=\zeta/2$, and the points r_1 and r_+ go off to infinity. As a result, the potential $U_1(r, \varepsilon=-1)$ remains regular for all $0<r<\infty$, so that the usual variant of the WKB method can be used. This is how the quasiclassical formulas were obtained[22, 23] for the critical charge Z_{cr} of the nucleus, for the level energy near $\varepsilon=-1$, and for the total number of levels that go off to the lower continuum. Comparison with the numerical calculations shows that these formulas have good accuracy[9)] even for the ground state $1s_{1/2}$.

3. It was shown in the present paper that the difficulty indicated above is formal in character. Direct application of the WKB method to the Dirac system (1.1) yields for the functions G and F quasiclassical formulas that are free of singularities at the points $r=r_1$ and $r=r_2$. These formulas have numerous applications in the theory of supercritical atoms. For nuclei in the uranium region, the parameter $g=(\zeta^2-1)^{1/2} \sim 1$, so that one can count on good accuracy of the quasiclassical approach.

4. From the form of formulas (1.12)–(1.18) it is not quite obvious how the limiting transition is made to the nonrelativistic approximation. Referring the reader to Ref. 35 for details, we consider here the case when $\varkappa<0$ and $r_-<r<r_+$. Introducing the nonrelativistic energy $\mathcal{E}=\varepsilon-m=p^2/2m+V(r)$ and assuming $\tilde{q}=(q^2+\varkappa r^{-2})^{1/2} \approx q+\varkappa/2qr^2$, we transform the argument of the exponential in (1.16):

$$\int_{r_-}^{r} dr\left(q-\frac{V'}{2Qq}\right)=\int_{r_-}^{r} dr\left[\tilde{q}-\frac{1}{2q}\left(\frac{V'}{Q}+\frac{\varkappa}{r^2}\right)\right] = \int_{r_-}^{r} dr\left[\tilde{q}-\frac{1}{2}(\ln Q)'\right], \tag{11.1}$$

where $Q=q-\varkappa/r$. The last term in the integral cancels out exactly with the pre-exponential factor $Q^{-1/2}$. We now recognize that $\varkappa^2+\varkappa=l(l+1)$, and add to $\tilde{q}(r)$ the Langer correction,[10)] which improves the accuracy of the WKB approximation at small r. We obtain ultimately

$$\tilde{q}(r)=\{2m[-\varepsilon+V(r)-(l+1/2)^2/2mr^2]\}^{1/2},$$
$$G(r) \approx \text{const} \cdot \frac{1}{\tilde{q}^{1/2}(r)} \exp\left(-\int_{r_-}^{r} \tilde{q}(r)\,dr\right), \tag{11.2}$$

which coincides with the quasiclassical approximation for the Schrödinger equation. We note that $q(r)$ contains not $\varkappa=\mp(j+1/2)$ but the orbital angular momentum l, as should be the case in the nonrelativistic theory if the potential $V(r)$ does not contain the spin-orbit interaction.

5. Application of the WKB method to the quantum-mechanical many-body problem leads to the Thomas-Fermi equation (see Ref. 2), which is the basis of the theory of complex atoms. In Refs. 39 and 27 the WKB method was used to derive and solve a relativistic Thomas-Fermi equation for the vacuum shell of a supercritical atom. We note that the electrons of the vacuum shell are in the main localized in the region $r<r_-$. In this region, formulas (1.12) for $G(r)$ and $F(r)$ differ from those obtained in Ref. 27 only in that the phases $\theta_i(r)$ are of different form. The electron density averaged over the rapid oscillations ($\overline{\sin^2\theta_i}=1/2$) retains its previous form. Therefore the use of the more exact expressions of Sec. 1 does not change the relativistic Thomas-Fermi equation.

The results of Secs. 3–5 make it possible to calculate quantities that are directly measured in experiment: the cross sections (total and differential, i.e., at a definite scattering angle of the nuclei) for spontaneous production of positrons, the energy spectrum of e^+, etc. For example, in the adiabatic (with respect to the velocity v of the nuclei) approximation the total cross section σ_+ is[7]

$$\sigma_+=\frac{4\pi}{v}\int_{R_0}^{R_{cr}} \gamma(R,\zeta)R^{3/2}(R-R_0)^{1/2}dR. \tag{11.3}$$

Such calculations are presently underway, and will result in substantial refinement of the small-supercriticality approximation.

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APPENDIX

We derive here formulas (4.5)–(4.7) of Sec. 4, and determine the functions that enter in the equation for the level energy $\varepsilon=\varepsilon(R;\zeta,\varkappa)$.

In the effective-potential method[6, 10] the Dirac system (1.1) reduces with the aid of the substitutions

$$\chi_1=(\varepsilon+1-V)^{-1/2}G, \quad \chi_2=(\varepsilon-1-V)^{-1/2}F \tag{A.1}$$

to the second-order equation

$$\chi_i''+2(E-U_i)\chi_i=0. \tag{A.2}$$

Here $i=1,2$; $E=(\varepsilon^2-1)/2$, so that the states of the lower

continuum correspond to an "energy" $E>0$. The effective potential $U_i(r,\varepsilon)$ is of the form

$$U_i=\varepsilon V-\frac{1}{2}V^2+\frac{\varkappa(\varkappa\pm1)}{2r^2}\pm\frac{V''}{4W_i}+\frac{3}{8}\left(\frac{V'}{W_i}\right)^2-\frac{\varkappa V'}{2rW_i}, \qquad (A.3)$$

where $W_i=1\pm(\varepsilon-V)$; the upper and lower signs correspond to $i=1$ and $i=2$, respectively. Near the boundary of the lower continuum $D_1=-W(r)$ and the expression for U_1 simplifies considerably:

$$U_1(r;\varepsilon=-1)=-\frac{1}{2}V^2+\frac{\varkappa(\varkappa+1)}{2r^2}-V-\frac{V''}{4V}+\frac{3}{8}\left(\frac{V'}{V}\right)^2+\frac{\varkappa V'}{2rV}. \qquad (A.4)$$

We shall therefore work with the function $\chi_1(r)$. The quasiclassical momentum is equal to $p(r)=[2(E-U(r,\varepsilon))]^{1/2}$, where at $V=-\zeta/r$ we have

$$U=U_1+\frac{1}{8r^2}=-\frac{\varepsilon\zeta}{r}-\frac{1}{2r^2}\left[\zeta^2-\left(\varkappa+\frac{1}{2}\right)^2+\frac{\varkappa+1}{1-y}-\frac{3}{4(1-y)^2}\right]; \qquad (A.5)$$

$y=-(\varepsilon+1)r/\zeta$. We have added here to the potential U_1 the Langer correction,[3] which improves the accuracy of the WKB approximation in the region of small r. Hence $p(r)=r^{-1}F(r,\varepsilon)$, where

$$F=\left[\zeta^2-\varkappa^2+2\varepsilon\zeta r+(\varepsilon^2-1)r^2+\left(\varkappa-\frac{1}{2}\right)\frac{y}{1-y}-\frac{3y^2}{4(1-y)^2}\right]^{1/2}$$
$$=[a-2br+cr^2+O(y^3)]^{1/2}, \qquad (A.6)$$

$$a=\zeta^2-\varkappa^2,\quad b=\zeta\left[1-\left(1+\frac{1-2\varkappa}{4\zeta^2}\right)(1+\varepsilon)\right],$$
$$c=\varepsilon^2-1+(\varkappa-{}^3/_4)(\varepsilon+1)^2\zeta^{-2}. \qquad (A.7)$$

We have expanded here the radicand in powers of the parameter y and discarded terms of order y^2 and higher; this makes it possible to calculate the integrals in (4.3) in analytic form. To justify this approximation, we note that the quantization condition (4.3) contains only $r<r_-$. Therefore the error δ which arises when the terms $\propto y^2$ are discarded has an upper bound

$$\delta<\frac{1}{a}\left|\frac{(1+\varepsilon)r_-}{\zeta}\right|^3=\begin{cases}(1-\rho^2)^2k^2/64\zeta^2, & k\to0\\ (1-\rho)^2/(1+\rho)\zeta^2, & k\to\infty\end{cases}.$$

This leads to smallness of δ (at $k\gg1$ we have also $\zeta\ll1$).

Using the formula

$$\int_r^{r_0}(a-2br+cr^2)^{1/2}\frac{dr}{r}=a^{1/2}\left[\ln\frac{1}{r}+\ln\frac{2a}{b(1-x^2)^{1/2}}\right.$$
$$\left.-\frac{1}{2x}\ln\frac{1+x}{1-x}-1\right]+O(r),\quad r\ll r_0, \qquad (A.8)$$

where $a>0$, $b>0$, $x^2=ac/b^2$, and $r_0=a[b+(b^2-ac)^{1/2}]^{-1}$ is the zero of the radicand, we obtain for the function Φ in (4.4) the expression

$$\Phi=\ln\frac{\zeta}{b}+1-\frac{1}{2x}[(1+x)\ln(1+x)-(1-x)\ln(1-x)]. \qquad (A.9)$$

This leads to formula (4.5), in which $x=\sqrt{ac}/b$,

$$\psi(x)=\begin{cases}\exp\{[(1+x)\ln(1+x)-(1-x)\ln(1-x)]/2x-1\}, & x>0,\\ (1-x^2)^{1/2}\exp\{(-x^2)^{-1/2}\operatorname{arctg}(-x^2)^{1/2}-1\}, & x^2<0\end{cases}. \qquad (A.10)$$

Although the analytic expressions for $\psi(x)$ are different at $x^2>0$ and $x^2<0$, the point $x=0$ is not singular for this function:

$$\psi(x)=1-{}^1/_6x^2-{}^{13}/_{360}x^4+\ldots,\quad x\to0.$$

We note now that the parameter x in (4.5) varies in a restricted region:

$$x=(1-\rho^2)^{1/2}k+\ldots,\quad k\to0, \qquad (A.11)$$

$$x\to x_\infty=\frac{[(1-\rho^2)(1+(\varkappa-{}^3/_4)\zeta^{-2})]^{1/2}}{1+(1-2\varkappa)/4\zeta^2},\quad k\to\infty. \qquad (A.12)$$

For the ground level we have $x_\infty^2<0$ if $\zeta<3/2$, i.e., $x^2(\varepsilon)$ reverses sign. On the other hand if $\varkappa\neq-1$, then x^2 remains positive at all $\varepsilon<-1$. Recognizing that $\psi(x)$ is a weakly varying function of x, and putting in (4.5) $\psi(x)\approx\psi(0)=1$, we get

$$\varepsilon(R)=-\left(\frac{R_{cr}}{R}+\frac{1-2\varkappa}{4\zeta^2}\right)\Big/\left(1+\frac{1-2\varkappa}{4\zeta^2}\right). \qquad (A.13)$$

The difference between this simple formula and (4.5) is of the order of 1%; this accuracy is sufficient for many purposes.

Note added in proof (20 December 1978). 1. The quasiclassical formulas of Sec. 1 are not valid when $|r-r_-|\lesssim g^{2/3}r_-$; the same holds for r close to the turning point r_+. We have presently obtained approximate expressions for G and F, free of singularities at the turning points in terms of Airy functions. Comparison with the numerical solutions of the Dirac equation shows that the error of these formulas does not exceed 10% (for the $7s_{1/2}$ level).

2. In a number of problems of solid-state theory one encounters a Dirac system (1.1) with $\varkappa=0$. This case is special because $r_1=r_+$ and $r_2=r_-$. WKB-approximation formulas were obtained for $\varkappa=0$.

[1)] A brief exposition of the results is published in Ref. 16.
[2)] One such state is the ground level $1s_{1/2}$, for which $\varkappa=-1$.
[3)] For example, in the subbarrier region the expressions for $G(r)$ and $F(r)$ contain, besides the usual[1] pre-exponential factor $q^{-1/2}=|p(r)|^{-1/2}$, also $Q^{-1/2}$.
[4)] Thus, for uranium nuclei at $R=R_{cr}$ the relative velocity of the nuclei is $v_N\sim0.07\,c$.
[5)] Which takes into account not only the spin-orbit but also the spin-spin interaction. We note that to take such terms into account in (3.1) it would be necessary to calculate corrections $\sim\hbar$ in the expansion (1.3).
[6)] This method is quite convenient in the calculation of the probability of tunneling of the particles through an oscillating potential barrier. It was taken into account previously in a calculation of the probability of multiphoton ionization of atoms and ions by the field of a strong light wave, in a calculation of the probability of production of electron–positron pairs out of vacuum in an alternating electric field, as well as in a number of similar problems (see Refs. 30).
[7)] We confine ourselves again to calculation of the adiabatic correction to the principal (exponential) factor in γ, discarding the pre-exponential factor and the spin–orbit terms. In addition, we assume frontal collision of the nuclei, and that the positrons are emitted along the line joining the nuclei at the instant of closest approach. These assumptions, without changing the qualitative picture of the phenomenon, greatly simplify the calculation, since the problem then becomes one-dimensional.
[8)] It is caused by the existence of an additional integral of motion[31] and by the fact that the Dirac Hamiltonian $H=a\cdot p+\beta m-\zeta/r$, has a hidden symmetry group broader than the $O(3)$ group of the geometrical symmetry of the Coulomb potential.

In particular, the Sommerfeld formula for the ε_{nx} spectrum obtained by purely algebraic means—from consideration of the Lie algebra made up of the generators of the group of hidden symmetry.[32,33] A detailed discussion of the questions connected with hidden symmetry of the Coulomb field is contained in a review.[34]

[9)]This pertains in particular to the formula for Z_{cr}, obtained in Ref. 22. Krainov's results[38] are not quite correct because of the number of additional approximations that do not hold very well in the region $\zeta \gtrsim 1.25$ (this question is discussed in Ref. 22).

[10)]See Refs. 1–3. A consistent derivation of this correction within the framework of our approach should call for the calculation of the functions y_1 and $\varphi^{(1)}$ in (1.3), i.e., of terms of order $\hbar$ in the quasiclassical expansion.

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