WKB method at $Z > 137$

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WKB-approximation formulas are obtained for the Dirac equation for a strong external field ($\epsilon_0 > 2m_e c^2$, where ϵ_0 is the electron binding energy). These formulas are used to calculate the energy and width of the quasistationary states in the lower continuum and to determine the pre-exponential factor in the probability of the spontaneous positron creation. Other applications of the WKB method are briefly discussed.

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In connection with the experimental observation[1] of the positrons created in slow ($v \lesssim 0.1c$) collisions of heavy nuclei, such as Pb+Pb, Pb+U, and U+U, it becomes urgent to calculate this process in detail, and this calls for solving the Dirac equation for the two-center problem. Since the variables do not separate in this case,

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this problem has no analytic solution, and the numerical calculations are quite unwieldy and have been performed only in the sub critical region where $R \geqslant R_{cr}, \epsilon \geqslant -1$ (see[2,3]; we put hereafter $\hbar = c = m_e = 1$, ϵ is the energy of the level in $m_e c^2$ units, R is the distance between the nuclei, $\chi = \mp(j+\frac{1}{2})$; in particular $\kappa = -1$ for the ground level). It is therefore necessary to resort to approximate methods. It is natural to consider the WKB method, which has high accuracy in the case of a Coulomb field even for small quantum numbers.

The application of the WKB method to a strong ($Z > 137$) Coulomb field was based earlier[4,5] on a squaring of the Dirac equation (the effective-potential method[6,7]). At $\epsilon < -1$, however, the substitution $\chi(r) = (1+\epsilon - V)^{-1/2} G(r)$ used in that method becomes singular at the point $r = r_g$, where $V(r_g) = \epsilon + 1$. Consequently the usual quasiclassical formulas become meaningless at $r \sim r_g$ because of the divergence of the integral $\int^r p dr$. We have succeeded in overcoming this difficulty by expanding in powers of $\hbar$ in the initial Dirac system for the radial wave functions G and F. The expansion in powers of $\hbar$ leads to a chain of matrix differential equations that are solved in succession with the aid of the left and right eigenvectors of the homogeneous system, calculated in explicit form. We present the final formulas for the wave function of the quasistationary state with energy $\epsilon < -1$. These formulas have different forms in three regions: I) $r_0 < r < r_-$; II) the sub-barrier region $r_- < r < r_+$; III) $r > r_+$. Here r_- and r_+ are turning points in which the quasiclassical momentum

$$p(r) = [(\epsilon - V(r))^2 - 1 - \kappa^2 r^{-2}]^{1/2} \tag{1}$$

vanishes (see Fig. 1). At $r_0 < r < r_-$ we have:

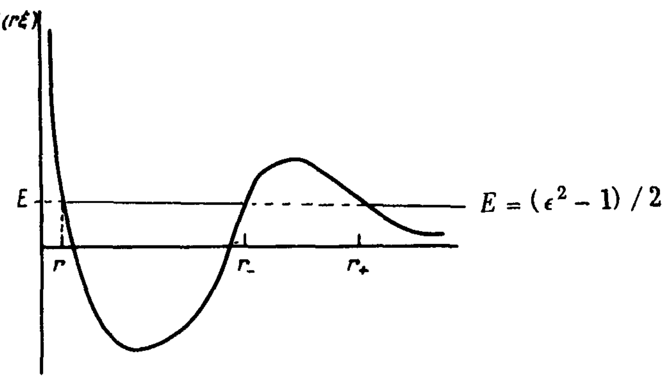

FIG. 1. Effective potential $U(r,\epsilon)$ for states with $\epsilon \leqslant -1$.

$$G = A\left[\frac{\epsilon - V + 1}{p}\right]^{1/2} \sin\theta_1, \quad F = A \operatorname{sgn}\kappa \left[\frac{\epsilon - V - 1}{p}\right]^{1/2} \sin\theta_2 \quad , \tag{2}$$

where

$$\theta_i(r) = \int_{r_0}^{r}\left(p + \frac{\kappa w_i}{pr}\right)dr + \frac{\pi}{4} ,$$

$$w_1 = \frac{1}{2}\left(\frac{V'}{1+\epsilon - V} - \frac{1}{r}\right), \quad w_2 = \frac{1}{2}\left(\frac{V'}{1-\epsilon+V} + \frac{1}{r}\right).$$

If the level width $\gamma \ll 1$ (this is verified by the results), we must put

$$\int_{r_0}^{r_-} (G^2 + F^2)dr = 1, \qquad A = \left\{\int_{r_0}^{r_-} \frac{\epsilon - V(r)}{p(r)}\, dr\right\}^{-1/2} = \left(\frac{T}{2}\right)^{-1/2}, \tag{3}$$

where T is the period of the oscillations of a classical particle localized in region I. In the sub-barrier region, the solution corresponding to a damped exponential takes at $\kappa < 0$ the form

$$G = \frac{V - \epsilon - 1}{Q} F, \qquad F = B\left(\frac{Q}{q}\right)^{1/2} \exp\left\{- \int_{r_-}^{r}\left(q - \frac{V'}{2qQ}\right)dr\right\}, \tag{4}$$

and for states with $\kappa > 0$

$$G = B\left(\frac{Q}{q}\right)^{1/2}\exp\left\{- \int_{r_-}^{r} \left(q + \frac{V'}{2qQ}\right)dr\right\}, \qquad F = \frac{\epsilon - V - 1}{Q} G . \tag{4'}$$

Here $q=|p(r)|$ and $Q=q+|\kappa| r^{-1}$. At $r > r_+$ the quasistationary state corresponds to a diverging wave; the formulas for G and F are similar to (4) and (4′). To go around the turning points we can use the Zwaan method, which joins together the solution and establishes the connection between the normalized constants. Expression (2) and (4) differ substantially from the usual quasiclassical formulas. As expected, the point $r = r_g$ is not singular for correct quasiclassical formulas, since $q(r)$ and $Q(r)$ are positive at $r_- < r < r_+$.

The obtained formulas allow us to solve a large number of problems in the theory of supercritical atoms. Thus, (2) leads to the quantization rule

$$\int_{r_0}^{r_-}\left(p + \frac{\kappa w_1}{pr}\right)dr = \left(n + \frac{1}{2}\right)\pi , \qquad n = 0, 1, 2 \ldots \tag{5}$$

which determines the real part of the level energy. It differs from the usual Bohr-Sommerfeld quantization condition by the relativistic expression for the momentum $p(r)$ and by inclusion of a correction, proportional to $w_1(r)$, which takes the spin-orbit interaction into account and leads to splitting of levels with unequal signs of κ. By calculating the particle flux as $r \to \infty$, we obtain the level width γ (i.e., the spontaneous-positron-production probability):

$$\gamma(\epsilon, \kappa) = \gamma_0 \exp \{ -2 \int_{r_-}^{r_+} q(r)\, dr \}, \tag{6}$$

where

$$\gamma_0 = \frac{1}{T} \exp\left\{ 2\kappa \fint_{r_-}^{r_+} \frac{w_1}{qr}\, dr \right\} \tag{6'}$$

(the last integral is taken in the sense of the principal value). In the case of a Coulomb field $V(r) = -\zeta/r$ we obtain

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

$$\gamma_0 = \frac{k^2}{2\zeta} \left[\sqrt{(1-\rho^2)(1+k^2)} - \frac{1}{k} \operatorname{Ar\,th}\left(k \sqrt{\frac{1-\rho^2}{1+k^2}} \right) \right]^{-1} = \begin{cases} c_0, & k \to 0 \\ c_1 k, & k >> 1 \end{cases} \tag{7}$$

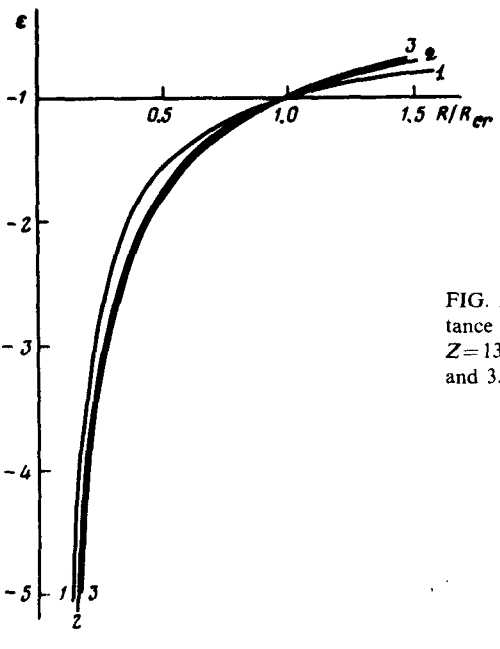

FIG. 2. Energy of the ground level $1s\sigma$ vs. the distance R between the colliding nuclei ($Z = Z_1 + Z_2$). $Z = 137$ for curve 1 and $Z/2 = 92$ and 100 for curves 2 and 3.

where $\zeta = Ze^2$, $\rho = |\kappa|\zeta^{-1}(0 < \rho < 1)$, and $k = \sqrt{\epsilon^2 - 1}$ is the positron momentum,

$$c_0 = \frac{3}{2\zeta(2+\rho^2)\sqrt{1-\rho^2}}, \quad c_1 = \frac{1}{2\zeta\sqrt{1-\rho^2}}.$$

The exponential factor in (7) was obtained earlier.[6] We note that the pre-exponential factor γ_0 depends substantially on the momentum k, a fact that must be taken into account when the theory is compared with experiment.

The application of the WKB method to the problem of two centers with charges Z_1 and Z_2 yields a simple approximate equation of the level energy $\epsilon = \epsilon(R, \zeta, \kappa)$:

$$\frac{R}{R_{cr}} = \left[1 - \left(1 + \frac{1-2\kappa}{4\zeta^2}\right)(1+\epsilon)\right]^{-1} \phi(x), \tag{8}$$

which is plotted in Fig. 2. Here $\zeta = (Z_1 + Z_2)/137$,

$$\phi(x) = \exp\left\{\frac{1}{2x}[(1+x)\ln(1+x) - (1-x)\ln(1-x)] - 1\right\},$$

$$x = \left\{(1-\rho^2)\left[\epsilon^2 - 1 + \left(\kappa - \frac{5}{4}\right)\left(\frac{(\epsilon+1)^2}{\zeta^2}\right)\right\}^{1/2}\left[1 - \left(1 + \frac{1-2\kappa}{4\zeta^2}(\epsilon+1)\right)\right].$$

In particular, the slope of the level at the boundary of the lower continuum is described by the formula

$$\epsilon = -1 + \beta\left(\frac{R}{R_{cr}} - 1\right) + \dots, \quad \beta = \frac{3}{2}\left(1 + \frac{4\kappa^2 - 6\kappa + 3}{8\zeta^2}\right)^{-1} \tag{9}$$

(the critical distance R_{cr} was calculated in[2,3]).

By way of further applications of the WKB method to the theory of supercritical atoms we point out the following problems: 1) calculation of the screening effect, i.e., the calculation of R_{cr} for a quasimolecule (Z_1, Z_2, e) surrounded by outer electron shells; 2) allowance for the finite velocity of the nuclei; 3) the angular distribution of the emitted positrons (which reduces to the problem of tunneling of a particle with nonzero angular momentum through a potential barrier with low nonsphericity). The use of the WKB method yields solutions in closed form and obeviates the need for cumbersome numerical computations.

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