The phase method for the Dirac equation and the calculation of the critical nuclear charge

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A simple method for solving the Dirac and Schrödinger equations in an arbitrary potential $V(r)$ is developed, which is convenient for qualitative analysis of the problem and for numerical calculations. The basic idea consists in replacing the equation under consideration by a first-order nonlinear equation for the phase function $\theta(r)$. Applications of the method to the problem of the appearance of a bound level and for the calculation of the critical charge Z_c are considered. An estimate is given of the effect on Z_c due to screening of the Coulomb field of the nucleus by the electron shell, and also variational calculations of Z_c are carried out for a system of colliding nuclei (the relativistic two-center problem). Other applications of the phase equation are briefly discussed, namely, the problem of determining the coefficient for reflection from a potential barrier and the problem of pair production in a variable electric field.

1. INTRODUCTION

Considerable interest has arisen recently in the electrodynamics of the strong Coulomb fields which are created by a nucleus with charge $Z \sim Z_c = 170$.[1-9] The necessity of solving the relativistic two-center problem arose in connection with a discussion of an experiment involving the spontaneous creation of positrons in heavy ion collisions.[4-6] This problem is just as important for the physics of the phenomena associated with $Z \sim Z_c$ as the calculation of the terms of the molecular hydrogen ion H_2^+ is for the quantum theory of molecules. In contrast to the case of a spherical nucleus,[8,9] the variables in the Dirac equation with the potential $V(\mathbf{r}) = -\alpha(Z_1/r_1 + Z_2/r_2)$ are not separable in any orthogonal coordinate system, which gives rise to certain mathematical difficulties. A variational principle was proposed[10,11] in order to solve the two-center problem, and preliminary calculations[12] were carried out in the case of scalar particles; however, the accuracy of these calculations turned out to be inadequate due to a not completely successful choice of the trial function. The necessary physical requirements, which the trial functions must satisfy in the variational method, are formulated in[10,13].

The results of variational calculations of the critical charge Z_c for the two-center problem are presented in the present article. In the process of carrying out these calculations we developed a method of solving the Dirac equation with an arbitrary potential $V(r)$; the new method turned out to be extremely convenient for numerical calculations and, in so far as we know, has not previously been discussed in the literature. It somewhat resembles the method of phase functions in quantum mechanics;[14-16] however, it is not identical with the latter and leads to simpler equations (see Sec. 2). In Sec. 3 this method is applied to the problem of the appearance of a bound level. This problem is frequently encountered in atomic and nuclear physics, and it is of special interest to us since by using an effective potential[1,10] the solution of the Dirac equation at the boundary of the lower continuum reduces to it. In secs. 4 and 5 the phase equation is applied to calculations of the critical charge Z_c: the influence on Z_c due to the screening of the nucleus' Coulomb field by the electron shell is investigated, and the curve $Z_c = Z_c(R)$ is determined in the two-center problem for scalar ($s = 0$) and spinor ($s = 1/2$) particles. We note that due to the sharp dependence of the cross section for the creation of positrons on the critical distance R_c between the nuclei ($\sigma \sim R_c^{7/2}$, see[5]), these calculations must be performed with a high degree of accuracy. Applications of the phase method to calculation of the coefficient for the reflection of particles from a barrier are briefly discussed in Sec. 6.

In investigations of the Dirac equation below we shall always use the relativistic system of units: $\hbar = c = m = 1$, and in the Schrödinger equation we use $\hbar = m = e = 1$ (atomic units).

2. THE PHASE METHOD

In a spherically symmetric field the Dirac equation has the form

$$G' = -\frac{\varkappa}{r}G + (1+\varepsilon-V)F, \quad F' = (1-\varepsilon+V)G + \frac{\varkappa}{r}F, \tag{2.1}$$

$$\varkappa = \begin{cases} -(l+1), & j = l+1/2 \\ l, & j = l-1/2 \end{cases}. \tag{2.2}$$

Let $\kappa < 0$ (for example, $\kappa = -1$ for the 1s level). Assuming

$$G = a\cos\theta, \quad F = a\sin\theta \tag{2.3}$$

in Eq. (2.1) (we shall call $a(r)$ and $\theta(r)$ the amplitude and the phase), we arrive at the phase equation

$$\theta' = \cos 2\theta + \varkappa r^{-1}\sin 2\theta - \varepsilon + V(r) \tag{2.4}$$

with the initial condition[1)]

$$\theta(0) = 0. \tag{2.5}$$

After this the equation for the amplitude is solved in quadratures:

$$a(r) = Ar^{-\varkappa}\exp\left[\int_0^r dr\left(\sin 2\theta + \frac{2\varkappa}{r}\sin^2\theta\right)\right]; \tag{2.6}$$

here A is a constant which is determined from the normalization condition

$$\int_0^\infty a^2(r)\,dr = 1.$$

The phase $\theta(r)$ becomes constant as $r \to \infty$. Let us denote its constant value by η:

$$\eta = \lim\theta(r) \ \text{ as } \ r\to\infty; \quad \cos 2\eta = \varepsilon. \tag{2.7}$$

Since $a(r) \propto \exp(r\sin 2\eta)$ (in the limit $r \to \infty$), the levels of the discrete spectrum are determined by the boundary condition at infinity:

$$\sin 2\eta = -\sqrt{1-\varepsilon^2} = -\lambda. \qquad (2.8)$$

The phase equation (2.4) with the boundary conditions (2.5) and (2.8) completely determines the discrete spectrum of the Dirac equation. Let us make a few remarks in connection with these equations.

1. In connection with a numerical calculation it is convenient to choose a certain point r_0 and solve Eq. (2.4) separately in the interval $(0, r_0)$ using boundary condition (2.5) and in the interval (∞, r_0) using the boundary condition (2.8), and then match these solutions at the point r_0. Such a procedure enables us to immediately extract the solution which is regular at zero and at infinity. The merit of Eq. (2.4) lies in the fact that $\theta(r)$ appears in the argument of the bounded functions $\cos 2\theta$ and $\sin 2\theta$.

2. The angular momenta $j = |\kappa| - 1/2$ and $l = |\kappa| + (\operatorname{sgn}\kappa - 1)/2$ enter into Eq. (2.4) in a very simple way, which favorably distinguishes this equation from the corresponding equation in the method of phase functions (see Chapter 17 in[14]).

3. The requisite singularity $a(r) \propto r^{-\kappa}$ for the solution, which is regular at zero, is automatically selected in Eq. (2.6). If $\kappa > 0$ then $G/F \propto r$ as $r \to 0$. Therefore, it is necessary to interchange G and F in Eq. (2.3) which gives

$$\theta' = \cos 2\theta - \varkappa r^{-1}\sin 2\theta + \varepsilon - V, \quad \theta(0) = 0. \qquad (2.9)$$

4. For the continuous spectrum, the substitution analogous to (2.3) has the form

$$G = (\varepsilon+1)^{1/2} a\cos\theta, \quad F = -(\varepsilon-1)^{1/2} a\sin\theta \qquad (2.10)$$

(for $\kappa < 0$ and $\epsilon > 1$), and hence it follows that

$$\theta' = k - \frac{1}{k}(\varepsilon+\cos 2\theta)V(r) + \frac{\varkappa}{r}\sin 2\theta, \quad k = \sqrt{\varepsilon^2-1}. \qquad (2.11)$$

As $r \to \infty$ we have $\theta(r) \approx kr + (1/2)\pi\kappa + \delta$, where δ is the scattering phase shift.

One can also treat the nonrelativistic Schrödinger equation in an analogous manner. Instead of (2.3) we assume

$$\chi(r) = a\sin\theta, \quad \chi'(r) = a\cos\theta, \qquad (2.12)$$

$$\theta' = \cos^2\theta + \{2[E-V(r)] - l(l+1)r^{-2}\}\sin^2\theta, \quad \theta(0) = 0. \qquad (2.13)$$

The amplitude a(r) is again expressed in terms of the phase with the aid of quadratures. For $E = -\lambda^2/2 < 0$ it follows from Eq. (2.13) that $\cot\eta = \pm\lambda$, which corresponds to $a(r) \propto \exp(\pm\lambda r)$. The discrete spectrum is determined by the condition $\cot\eta = -\lambda$, from which it follows that $(n_r + 1/2)\pi < \eta < (n_r + 1)\pi$ (the integer n_r is equal to the number of nodes in the radial function χ).

We note the following interesting property. In contrast to the energy E, the asymptotic phase η does not "experience an accidental degeneracy" since η contains not only information about the energy levels $E = -(1/2)\cot^2\eta$ but also about the number of nodes, $n_r = n - l - 1$, in the radial wave function. For example, for the hydrogen atom we have

$$E_{nl} = -1/2n, \quad \eta_{nl} = (n-l)\pi - \operatorname{arc\,tg} n, \qquad (2.14)$$

i.e., the levels with angular momenta $l = 0, 1, \ldots, n-1$ (which are degenerate with respect to energy) have different values of η.

3. THE FORMATION OF A BOUND LEVEL

The case E = 0 requires a separate investigation since the asymptotic form of $\psi(r)$ as $r \to \infty$ does not have the usual form $\psi \propto e^{-\lambda r}$. In addition, this case is important in connection with the fact that the determination of the critical nuclear charge (see[1,2,8]) reduces to precisely this case.

For the Dirac equation the energy $E = (\epsilon^2 - 1)/2 = 0$ on the boundaries of both continua. Here $\epsilon = 1$ corresponds to the appearance of a level, and $\epsilon = -1$ corresponds to its intersection with the boundary of the lower continuum, that is, to the critical depth $V = V_c$ of the potential. Let us consider the last case in more detail.

For $\kappa < 0$ we assume

$$G = ar^{-\varkappa}\cos\theta, \quad F = \frac{2a}{1-2\varkappa}(r^{1-\varkappa}\cos\theta - r^{\varkappa}\sin\theta) \qquad (3.1)$$

(this substitution is suggested by the asymptotic form of G and F outside the effective range of the potential). Substituting (3.1) into (2.1) we are led to the equation

$$\theta' = -V(r)[\beta r^{-2\varkappa}\cos^2\theta + \beta^{-1}(r^{1-\varkappa}\cos\theta - r^{\varkappa}\sin\theta)^2], \qquad (3.2)$$

where $\beta = 1/2 - \kappa$. The terms in the solutions G and F which increase as $r \to \infty$ vanish for $V = V_c$; this leads to the following condition on the asymptotic behavior of the phase shift η:

$$\eta = (n+1/2)\pi, \quad n = 0, 1, 2, \ldots \qquad (3.3)$$

For an attractive potential the function $\theta(r)$ monotonically increases with r, and η increases together with the depth of the potential. Let us illustrate this for the case of a rectangular well, $V(r) = -v$ for $r < r_0$, when the solution can be found analytically:

$$\operatorname{tg}\eta = r_0^3 + \frac{3r_0}{2v}(1 - K\operatorname{ctg}K), \quad K = r_0[v(v-2)]^{1/2} \qquad (3.4)$$

($\kappa = -1$). Condition (3.3) gives $K = n\pi$, from which it follows that

$$V_c(ns_{1/2}) = 1 + [1 + (n\pi/r_0)^2]^{1/2}.$$

The rate at which the phase $\theta(r)$ approaches its asymptotic value η is determined by the nature of the decrease of V(r) as $r \to \infty$. For example, the following result is obtained for the 1s-level at the critical point:

$$\theta(r) = \frac{\pi}{2} + \frac{2}{3}\int_r^\infty V(x)x^{-2}\,dx + \ldots. \qquad (3.5)$$

The difference $\eta - \theta(r)$ becomes negligible outside the effective range of the potential, which is very favorable for numerical calculations.

The phase equation takes the following form for states with $\kappa > 0$:

$$\theta' = -V(r)[\beta r^{-2\varkappa}\sin^2\theta + \beta^{-1}(r^{1-\varkappa}\sin\theta + r^{\varkappa}\cos\theta)^2]. \qquad (3.6)$$

Finally, for $\epsilon = 1$ the appropriate equations are obtained from (3.2) and (3.6) by the substitution $\kappa \to -\kappa$, $V \to -V$ (charge conjugation). In all of these cases $\theta(0) = 0$.

Let us briefly discuss the nonrelativistic case. Let R denote the characteristic radius of action of the potential. Let us introduce $x = r/R$; then

$$V(r) = -g^2 v(x), \quad \varkappa^2 = 2(gR)^2, \qquad (3.7)$$

where v(x) is a dimensionless function. For $l = 0$ we make the substitution

$$\chi = a(x\cos\theta + \sin\theta), \quad \chi' = a\cos\theta \qquad (3.8)$$

(i.e., the derivative of χ is taken as if a and θ do not de-

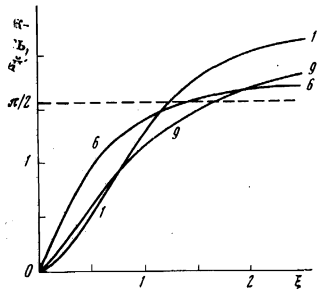

FIG. 1.

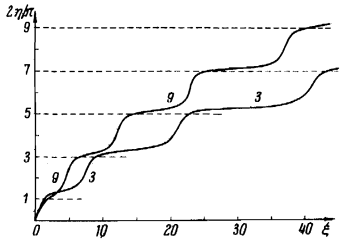

FIG. 2.

FIG. 1. The dependence of the asymptotic phase η on the parameter ξ (defined in expression (3.10) for three potentials. At the instant when the first level appears, $\eta(\xi_0) = \pi/2$. The figures on the curves correspond to the numbers used to label the potentials in Table I.

FIG. 2. The dependence of the asymptotic phase η on the parameter ξ (defined in expression (3.10)) for Gaussian and Yukawa potentials (No. 3 and No. 9 in Table I).

TABLE I. The emergence of a level in the potential

№	$v(x)$	ξ_0	γ	$\gamma_0 - \gamma$
1	$\theta(1-x)$	1.234	1/2	0
2	$(1-x^2)\theta(1-x)$	1.281	7/12	−0.018
3	$\exp(-x^2)$	1.342	3/4	−0.096
4	$(\mathrm{ch}\, x)^{-2}$	1.386	3/4	−0.043
5	$(e^x+1)^{-1}$	1.416	3/4	−0.012
6	e^{-x}	1.446	3/4	0.015
7	$x^{-1/2}e^{-x}$	1.531	5/6	0.029
8	$(e^x-1)^{-1}$	1.645	1	0
9	$x^{-1}e^{-x}$	1.680	1	0.034
10	$x^{-1/2}e^{-x}$	2.079	3/2	−0.013

pend on x) and we obtain

$$d\theta/dx = \kappa^2 v(x)\,(x\cos\theta + \sin\theta)^2. \tag{3.9}$$

The instant when the ns-level will appear is determined from condition (3.3). In contrast to the Dirac equation, here one can express the condition for the emergence of the level in terms of a unique invariant parameter:[2)]

$$\xi = -\frac{2m}{\hbar^2}\int_0^\infty V(r)\,r\,dr = b\kappa^2, \quad b = \int_0^\infty v(x)\,x\,dx. \tag{3.10}$$

Let us denote the value of ξ, corresponding to the appearance of the 1s-level, by ξ_0 (see Fig. 1). The values of ξ_0 for a series of different potentials were calculated with a computer by using the Runge-Kutta method, and the results are given in Table I. Of this example, the Yukawa potential $v(x) = e^{-x}/x$ is especially important since it is frequently encountered not only in nuclear physics, but also in solid state physics, plasma physics (Debye screening), etc. The result $\kappa_0 = \sqrt{\xi_0}$ for the Yukawa potential has been calculated by various methods in a large number of articles (see, for example, [17-22]). The result of our calculation is in good agreement with [20].

Equation (3.9) is not only applicable to the ground state, but can also be used for the excited states, and is also easily generalized to arbitrary values of l. For short-range potentials, the dependence of the phase η on ξ has a characteristic "steplike" shape (see Fig. 2). For example, we obtain the following result for a rectangular well:

$$\mathrm{tg}\,\eta = \mathrm{tg}\,\sqrt{2\xi}/\sqrt{2\xi} - 1.$$

Let us say a few words about the accuracy of the WKB method. According to the Bohr-Sommerfeld condition, the appearance of the (n + 1)s level in the attractive potential (3.7) is determined by the equation

$$\kappa_n a = (n+\gamma)\pi, \quad n = 0, 1, 2, \ldots; \qquad a = \int_0^\infty [v(x)]^{1/2}\,dx, \tag{3.11}$$

where it is usually assumed that $\gamma = 3/4$. A more detailed analysis indicates that the value of the constant γ depends on the behavior of V(r) as $r \to 0$ and as $r \to \infty$. Thus, if $V(r) \approx -g^2 r^{-\alpha}$ for small r and if the potential decreases exponentially at infinity, then the correct value of γ is as follows:

$$\gamma = (3-\alpha)/2(2-\alpha), \quad 0 \leqslant \alpha < 2 \tag{3.12}$$

(for potentials which are finite at the origin, $\alpha = 0$ and $\gamma = 3/4$). Let γ_0 denote the value determined from the exact value of κ_0 at the instant when the first level appears:

$$\gamma_0 = \frac{\kappa_0 a}{\pi} = \frac{a}{\pi}\sqrt{\frac{\xi_0}{b}}. \tag{3.13}$$

Values of γ and $\gamma_0 - \gamma$ are given in Table I. The latter quantity, characterizing the accuracy of the quasiclassical solution, does not exceed a few per cent in the cases we have investigated. Thus, the WKB method gives good results even for the ground state for the potentials which are usually applied in physics (the error associated with the WKB method naturally decreases with increasing values of n and with an increase in the depth of the level). In this connection, however, it is important in Eq. (3.11) to use the correct value of the constant γ.

4. THE INFLUENCE OF SCREENING OF THE CRITICAL NUCLEAR CHARGE

The critical charge Z_c was calculated in [8,9] for a "bare" nucleus, i.e., without taking the screening of the Coulomb field by the electron shell into account. The attraction of an electron towards the nucleus is weakened due to the screening:

$$V(r) = -\frac{Z\alpha}{r}\chi(r), \quad 0 < \chi(r) < 1, \tag{4.1}$$

and therefore the value of Z_c increases. An estimate of this effect is especially important in connection with setting up an experiment to detect the spontaneous creation of positrons in collisions between heavy nuclei. As is shown in [4,5] such an experiment can be performed not only with "bare" nuclei (i.e., with their electron shells stripped off) but also with a beam of bare nuclei Z_1 incident on an ordinary heavy target Z_2, provided the following two conditions are satisfied: $Z_1 \geq Z_2$ and $Z_1 + Z_2 > Z_c$. In this case the quasi-molecule formed when the nuclei approach each other is surrounded by an electron shell, and it is necessary to estimate the increase of Z_c due to screening. Since the total charge of the nucleus, $Z_1 + Z_2$, only exceeds the critical charge $Z_c \approx 170$ (calculated for the "bare" nucleus) by 15 to 20 units, an increase of Z_c by 10 to 20 units would markedly hinder the experimental arrangements (an experiment with the heavy elements known at the present time).

In view of the complicated nature of the calculation of Z_c in the two-center problem, in order to determine the size of the corrections due to screening let us investigate a model problem involving a spherical nucleus. The screening function $\chi(r)$ in Eq. (4.1) satisfies the conditions $\chi(0) = 1$ and $\chi(\infty) = 0$ (for the neutral atom). Let

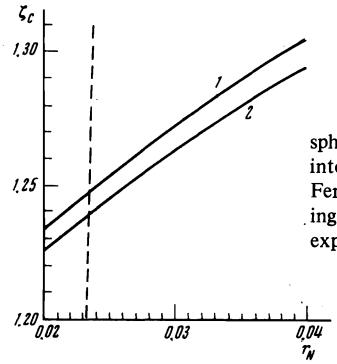

FIG. 3. The critical charge for a spherical nucleus with screening taken into account according to the Thomas-Fermi model (curve 1) and the screening (curve 2) (the nuclear radius r_N is expressed in units of $\hbar/m_e c$ = 386 F).

us consider a screening function χ which satisfies the Thomas-Fermi equation:[23]

$$\chi=\chi(\beta r), \quad \beta=\frac{Z^{1/3}}{137b}=0{,}0425\zeta^{1/3} \tag{4.2}$$

(r is measured in units of $\hbar/m_e c$; the remaining notation agrees with that adopted in[23]). At $\zeta = Z\alpha > 1$ the velocity of the inner electrons is $v \approx c$; however, the majority of the electrons is located at distances $r \sim 137\, Z^{-1/3} \gg 1$ from the nucleus and has an energy $\epsilon \sim Z^{4/3}\alpha^2 \ll 1$, which justifies the use of the nonrelativistic Thomas-Fermi model.

The results of the calculation are shown in Fig. 3. The potential inside the nucleus was taken in the form $V(r) = -\zeta[3 - (r/r_N)^2]/2r_N$. Curve 1 is constructed with screening taken into consideration; curve 2 is for the unscreened Coulomb potential. By assigning a definite dependence of r_N on Z, from here one can easily determine the critical charge of the nucleus. For example, if $r_N = r_0 A^{1/3}$, where r_0 = 1.2 F and A = 2.5 Z (see the dashed straight line shown in Fig. 3), then ζ_c = 1.247 and 1.238 respectively for curves 1 and 2. Ultimately Z_c = 171 instead of Z_c = 169 according to[8]. Taking the screening into account only increases the critical charge by an amount ΔZ_c = 1.2, and the remaining corrections ~0.6 are related to the inaccuracy of the approximation $r_N \ll 1$, which was utilized in[8] in order to solve the Dirac equation inside the nucleus. In connection with the collision of a bare nucleus with a neutral atom, the screening effects are even smaller since the electronic shell of the combined atom is only half filled.

Utilization of the phase equation simplifies the calculation of Z_c so much that it would not be difficult to further improve the determination of the screening function $\chi(r)$, for example, by using the Hartree-Fock method. In view of the smallness of the correction itself, we shall not do this.

5. THE CRITICAL CHARGE IN THE TWO-CENTER PROBLEM

It is convenient to start the calculation of Z_c for a system consisting of two nuclei ($Z_1 = Z_2 = Z$; for $Z < 137$ we shall regard the nucleus as point-like) with the simpler case of scalar particles. For $\epsilon = -1$ the Klein-Gordon equation is equivalent to finding the minimum of the following functional:[5]

$$J[\psi]=\int d^3r[\tfrac{1}{2}|\nabla\psi|^2+\psi^2 U\psi], \tag{5.1}$$

where $U = -(V + \frac{1}{2}V^2)$ is the effective potential;

$$V=-\frac{1}{2}\zeta\left(\frac{1}{r_1}+\frac{1}{r_2}\right)=-\frac{2\zeta\xi}{R(\xi^2-\eta^2)}, \quad \zeta=2Z\alpha; \tag{5.2}$$

$\xi = (r_1 + r_2)/R$ and $\eta = (r_1 - r_2)/R$ are elliptic coordinates, and R is the distance between the nuclei. If we consider $J[\psi]$ for the class of trial functions that depend only on a single variable: $\psi = \psi(x)$, $x = x(\xi, \eta)$, then

$$J[\psi]=\text{const}\cdot\int_0^\infty dx[p\psi'^2+q\psi^2],$$

and for $\psi(x)$ we obtain the equation

$$\frac{d}{dx}\left[p(x)\frac{d\psi}{dx}\right]-q(x)\psi=0, \tag{5.3}$$

to which we have already applied the phase method.

As the examples given in[10,11] indicate, in order to obtain a good approximation to Z_c it is important that the trial functions should properly reflect the nature of the singularity of the exact solution near the Coulomb centers[3)] and also as $\xi \to \infty$. The form of the singularity is known[10] and dictates the choice of the variable x: $x = (\xi^2 - \eta^2)\varphi(\xi)$. We shall consider two versions: a) $\varphi(\xi) = \xi^{-1}$ and b) $\varphi(\xi) = 1$.

Let us begin with case a). By changing to the new variables

$$x=(\xi^2-\eta^2)/2\xi, \quad y=\eta/\xi, \quad \psi=\psi(x), \tag{5.4}$$

we obtain

$$\xi=\frac{2x}{1-y^2}, \quad \eta=\frac{2xy}{1-y^2}, \quad d\xi\, d\eta=\frac{4x}{(1-y^2)^2}dx\, dy. \tag{5.5}$$

Here

$$V=-\frac{\zeta}{Rx}, \quad U=\frac{1}{R^2}\left(\frac{\zeta R}{x}-\frac{\zeta^2}{2x^2}\right), \tag{5.6}$$

i.e., the given choice of the trial function corresponds to the symmetry of the potential. The ranges of variation of the variables are as follows:

$$0\leqslant x<\infty, \quad y_1(x)<y<y_2(x),$$

where $y_1(x) = \sqrt{1-2x}$ for $0 < x < 1/2$, $y_1(x) = 0$ for $x > 1/2$, and $y_2(x) = \sqrt{1+x^2} - x$ for all x. Integrating (5.1) in the limits $y_1(x) < y < y_2(x)$, we obtain

$$J[\psi]=\text{const}\int_0^\infty dx[p(\psi')^2+q\psi^2]. \tag{5.7}$$

Hence follows Eq. (5.3) in which

$$p(x)=x^2, \quad q(x)=(\zeta Rx-\zeta^2/2)g(x). \tag{5.8}$$

For $0 < x < 1/2$ (region I) we obtain

$$g(x)=1+\frac{1}{4x}(\sqrt{1+x^2}-(1+3x)\sqrt{1-2x})+\frac{3}{4}x\ln\frac{2(1+\sqrt{1+x^2})}{(1+\sqrt{1-2x})^2}, \tag{5.9}$$

and for $x > 1/2$ (region II) we find

$$g(x)=1+\tfrac{1}{4}[\sqrt{1+x^{-2}}+3x\ln(1/x+\sqrt{1+x^{-2}})].$$

We note that the topology of the surfaces $x(\xi, \eta)$ = const changes at the point x = 1/2; they are doubly connected for $x < 1/2$, and simply connected for $x > 1/2$. The function g(x) is continuous at this point.

Equation (5.3) was solved at both ends of the interval $(0, \infty)$ and the solutions were matched at the point x = 0.5. The substitution $\psi(x) = \chi(x)/x$ reduces (5.3) to the form of the Schrödinger equation (the necessary transformation for the general case is indicated in the Appendix). Furthermore, it is convenient to change to $y = h\chi'/\chi$, having chosen h(x) such that y(x) has a constant limit for $x \to 0, \infty$. Expansions of y(x) near the singular points are found analytically and play the role of boundary conditions, thus yielding the solution we need. In the present case h(x) = x in region I, $h(x) = \sqrt{x}$ in region II, and

$$y(0)=\frac{1}{2}(1+\sqrt{1-\zeta^2}), \quad y'(0)=\frac{\zeta-R}{2\zeta}(1-\sqrt{1-\zeta^2}), \tag{5.10}$$

$$y(x)=\sum_{n=0}^{\infty} a_n x^{-n/2} \quad \text{as} \quad x\to\infty, \tag{5.11}$$

where

$$a_0=-\sqrt{2\zeta R},\quad a_1=1/4,\quad a_2=-(\zeta^2-3/16)/2a_0,\quad a_3=a_2/2a_0.$$

We obtain the equation

$$y'=Q_0+Q_1y+Q_2y^2,$$

for y(x), and this reduces to (3.2) by making the substitution y = tan θ. Here

$$Q_0=h\left[\frac{q}{p}+\left(\frac{p'}{2p}\right)^2-\frac{p''}{2p}\right],\quad Q_1=\frac{h'}{h},\quad Q_2=-\frac{1}{h}.$$

As the result of the calculation we obtain curve a shown in Fig. 4, which determines the critical distance R_c associated with a given $\zeta = 2Z/137$.

The calculation of R_c is carried out analogously for the class of trial functions b):

$$\psi=\psi(\xi^2-\eta^2). \tag{5.12}$$

The coefficients p and q of Eq. (5.5) for this case are given in [13]. Changing to the functions

$$y(x)=-(8p)^{1/4}\psi'/\psi,\quad y(0)=1-\sqrt{1-\zeta^2},\quad y(\infty)=\sqrt{2\zeta R}, \tag{5.13}$$

we obtain curve b shown in Fig. 4.

The values of $\zeta_c(R)$, calculated from the asymptotic formula (10) of article [13], are shown in Fig. 4 for purposes of comparison. For $R < 0.1$ the results of the variational calculations essentially agree with the asymptotic formula.

Having investigated the question of the form of the trial functions, let us now proceed to the case of spin s = 1/2. The generalization of the variational principle to this case does not present any problems:[11]

$$J[\psi]=\int d^3r[1/2|\nabla\psi|^2+\psi^+U\psi],$$
$$U=-V-\frac{V^2}{2}-\frac{\Delta V}{4V}+\frac{3}{8}\left(\frac{\nabla V}{V}\right)^2-\frac{1}{2V}[\nabla V,\times\mathbf{p}]\sigma \tag{5.14}$$

(here ψ is a two-component spinor). Choosing $\psi=(\psi(\xi^2-\eta^2)/2\xi)$ we note that $[\nabla V, \nabla\psi] = 0$. Therefore, for the present choice of ψ the spin structure in (5.13) is unimportant, and we arrive at Eq. (5.3) in which

$$p=x^2,\quad q=(\zeta Rx-\zeta^2/2)g(x)+3/4. \tag{5.15}$$

A qualitative analysis of this equation is performed by using the method of the effective potential (see the Appendix). The results of the numerical calculations are presented in Table II. We emphasize that these values give an upper limit on the value of $\zeta_c(R)$ in the two-center problem.

6. OTHER APPLICATIONS OF THE PHASE METHOD

Problems which reduce to the oscillator with a variable frequency,

$$\ddot{x}+\omega^2(t)x=0. \tag{6.1}$$

are encountered in various areas of physics. The one-dimensional Schrödinger equation has this same form. We change from x, $\dot{x}$ to the amplitude and phase by the following transformation:

$$x=\omega^{-1/2}a\sin\theta,\quad \dot{x}=\omega^{1/2}a\cos\theta, \tag{6.2}$$

$$\dot{\theta}=\omega+\frac{\dot{\omega}}{2\omega}\sin 2\theta, \tag{6.3}$$

$$a^2(t)=I(t)=I(t_0)\exp\left[-\int_{t_0}^{t}\frac{\dot{\omega}}{\omega}\cos 2\theta\,dt\right]. \tag{6.4}$$

FIG. 4. The critical charge for scalar particles. Curves a and b are the result of variational calculations using the trial functions (5.4) and (5.12), curves I and II are taken from the calculation for a spherical nucleus [8] of radius $r_N = R/2$ (cut-off models I and II); and curve A corresponds to the asymptotic formula given in [13].

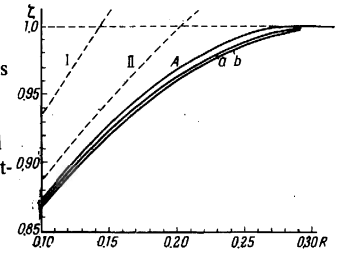

TABLE II. The Critical Distance for an Electron in the Two-Center Problem*

ζ	R_c (ζ)		
	a	b	I
1.20	0.0212	0.0215	0.0220
1.25	0.0395	0.0401	0.0406
1.30	0.0633	0.0645	0.0644
1.35	0.0921	0.0943	0.0928
1.40	0.1256	0.1291	0.1252
1.45	0.1635	0.1685	0.1608
1.50	0.2057	0.2124	0.1992
1.55	0.2519	0.2605	0.2400
1.60	0.3023	0.3130	0.2826

*Here $\zeta = 2z/137$; columns a and b correspond to the trial functions (5.4) and (5.12); column I gives the values of ζ for a spherical nucleus with radius $r_N = R/2$ and the cut-off model I.

Here $I(t) = (\dot{x}^2 + \omega^2x^2)/\omega$ is the adiabatic invariant for the oscillator. The advantage of the phase equation (6.3) lies in the fact that the solution x(t) oscillates as $t \to \pm\infty$, whereas the phase varies monotonically. As soon as the oscillator's frequency reaches its constant limit, $\theta(t) = \omega_\pm t + \text{const}$ ($\omega_\pm$ denotes the limiting values of $\omega(t)$ for $t \to \pm\infty$).

Let us denote by $\xi(t)$ the complex solution of Eq. (6.1) with the initial condition $\xi(t) \to \exp(-i\omega_- t)$ for $t \to -\infty$. Then, for $t \to +\infty$ the solution becomes

$$\xi(t)\to C_1\exp(-i\omega_+t)+C_2\exp(i\omega_+t).$$

Let us set

$$\rho=|C_2/C_1|^2. \tag{6.5}$$

From the point of view of the Schrödinger equation, ρ is the coefficient for the reflection of the wave from the barrier. One can show[26] that the parameter ρ completely determines the probability for transitions between the states $|m, \omega_-\rangle$ and $|n, \omega_+\rangle$ of a quantum oscillator with a variable frequency. In order to calculate ρ, let us find a pair of solutions, θ_1 and θ_2, of the phase equation which satisfy $\theta_1(t_0) = 0$, $\theta_2(t_0) = \pi/2$ (here we assume that $\dot{\omega} = 0$ for $t < t_0$; in the answer we let $t_0 \to -\infty$). Then we find

$$\rho=(\nu-1)/(\nu+1),\quad \nu=1/2(\nu_1+\nu_2), \tag{6.6}$$

$$\nu_k=\frac{I_k(\infty)}{I_k(-\infty)}=\exp\left[-\int_{-\infty}^{\infty}\frac{\dot{\omega}}{\omega}\cos 2\theta_k\,dt\right]$$
$$=\left|\exp\left[-\frac{1}{2}\int_{-\infty}^{\infty}\frac{\dot{\omega}}{\omega}e^{2i\theta_k}\,dt\right]\right|^2 \tag{6.7}$$

(for k = 1, 2). In order to prove this formula, let us consider the variation of the invariant I. If $x(t) = \sin(\omega_- t + \psi/2)$ as $t \to -\infty$ and $C_2^*/C_1 = \rho^{1/2}e^{i\sigma}$, then

$$\nu=\frac{I(\infty)}{I(-\infty)}=\frac{1+\rho-2\rho^{1/2}\cos(\sigma+\psi)}{1-\rho}. \tag{6.8}$$

In classical mechanics the invariant I may either in-

crease or decrease (depending on the initial phase ψ):

$$e^{-2\beta}\leqslant\nu\leqslant e^{2\beta},\quad \rho=\mathrm{th}^2\beta.$$

However, if we average ν with respect to ψ (which corresponds to the quantum oscillator), then we find

$$\nu=(1+\rho)/(1-\rho)=\mathrm{ch}\,2\beta\geqslant 1, \tag{6.9}$$

and Eq. (6.6) follows from here.

One can use formula (6.7) to calculate the probability for pair production in a homogeneous electric field $\mathbf{E}(t)$. For scalar particles $\omega^2(t) = m^2 + \mathbf{p}^2(t)$, where $\mathbf{p}(t)$ is the momentum of the classical particle. For spinor particles ($e^{\pm}$) the frequency of the equivalent oscillator turns out to be complex.[27,28] If $\omega(t)$ is slowly varying and is an analytic function of t, then it is clear from Eq. (6.7) that the ratio $(I_+ - I_-)/I_-$ is exponentially small and is determined by the contribution of the complex zeros of the function $\omega(t)$. Let us consider the opposite case when the frequency changes abruptly. Let $\omega(t)$ vary from ω_- to ω_+ during a time interval of the order of τ, where $\omega_\pm\tau \ll 1$, $\omega = \omega_-$ for $t < 0$. The functions $\theta_1(t)$ and $\theta_2(t) - \pi/2$ are small in virtue of the smallness of τ, and Eq. (6.3) can be linearized. Hence

$$\theta_1(t)\approx\omega(t)t,\quad \theta_2(t)\approx\frac{\pi}{2}+\frac{1}{\omega(t)}\int_0^t\omega^2(t')\,dt'.$$

Substituting these expressions into the integral in (6.7), we obtain

$$\rho=\rho_0+\rho_1+\ldots, \tag{6.10}$$

$$\rho_0=\left(\frac{\omega_+-\omega_-}{\omega_++\omega_-}\right)^2,\quad \rho_1=\frac{4\omega_+\omega_-}{(\omega_++\omega_-)^4}(K_1^2-K_0K_2), \tag{6.11}$$

$$K_n=\int_{-\infty}^{\infty}t^n\frac{d\omega^2}{dt}dt,\quad K_0=\omega_+^2-\omega_-^2.$$

The first term of the series (6.10) corresponds to an instantaneous change of the frequency from ω_- to ω_+, the correction ρ_1 takes the finiteness of the transition time into consideration: $\rho_1 \sim (\omega_\pm\tau)^2$. We note that the correction ρ_1 was previously investigated by Kolkunov,[29] and he obtained the expression

$$\rho_1=\frac{8\omega_+\omega_-}{(\omega_++\omega_-)^4}\int_{-\infty}^{\infty}dt_1\int_{t_1}^{\infty}dt_2[\omega^2(t_1)-\omega_-^2][\omega^2(t_2)-\omega_+^2]. \tag{6.12}$$

by using the complicated method of the multiplicative integral. With the aid of an artificial device one can transform (6.12) to the form (6.11). In order to do this we represent $\omega^2(t) - \omega_\pm^2$ in the form of integrals of the type

$$\int_{\pm\infty}^{t}(d\omega^2/dt)\,dt;$$

in the resulting four-fold integral we interchange the order of integration, and after calculating the inner integral with respect to t_1 and t_2 we symmetrize the integrand. The advantage of the phase equation is that it immediately leads to formula (6.11), which only contains one-dimensional integrals.

The phase equations considered above possess two general properties: 1) they are first-order equations, where the phase θ appears in the argument of a sine or cosine function; 2) after such a phase equation is solved, the amplitude a is determined by quadratures. These equations are extremely convenient for numerical calculations, and they are also very convenient for the development of approximate methods (the adiabatic approximation, the anti-classical approximation, etc.).

APPENDIX

The substitution $\chi = p^{1/2}\psi$ reduces (5.3) to the Schrödinger equation with zero energy:

$$\chi''-2U\chi=0, \tag{A.1}$$

$$U=\frac{1}{2}\left[\frac{q}{p}+\left(\frac{p'}{2p}\right)^2-\frac{p''}{2p}\right]. \tag{A.2}$$

From (5.8) we obtain:

$$U_a(x)=\frac{1}{4}\left(\frac{\zeta R}{x}-\frac{\zeta^2}{2x^2}\right)g(x)=\begin{cases}-\dfrac{\zeta^2}{8x^2}-\dfrac{\zeta(\zeta-R)}{4x}+\ldots, & x\to 0\\[2ex] \dfrac{\zeta R}{x}-\dfrac{\zeta^2}{2x^2}+\ldots, & x\to\infty\end{cases} \tag{A.3}$$

As $x \to 0$ the potential $\tilde{U}(x)$ corresponds to an attractive interaction, but it contains a Coulomb barrier for $x \gg 1$—that is, qualitatively it has the same form as the effective potential $U(\xi, \eta)$. However, there is an important difference between these two potentials. Comparing Eqs. (A.3) and (5.6) we see that $\tilde{U}$ differs from U by the factor $(1/4)g(x)$, which plays the role of the square of the effective charge in the "orbit" of an electron with a given x. As the value of x varies from 0 to ∞ the effective charge e(x) increases by a factor of two, whereas it is almost constant for $x > 1$.

Since a "collapse to the center" arises in the potential $\tilde{U}(x)$ for $\zeta > 1$, the first bound level appears for $\zeta < 1$, no matter what the distance R is. Thus, for the best trial function of type a) one will obtain $\zeta_c(R) < 1$ and $\zeta_c \to 1$ as $R \to \infty$, which agrees with the behavior of the exact solution.

We have the following result for the trial function (5.12)

$$U_b(x)=\begin{cases}-\dfrac{\zeta^2}{8x^2}-\dfrac{\zeta(\zeta-2R)}{16x}+\ldots, & x\to 0\\[2ex] \dfrac{\zeta R}{8x^{3/4}}-\dfrac{\zeta^2-3/4}{8x^2}+\ldots, & x\to\infty,\end{cases} \tag{A.4}$$

and for spin s = 1/2 we obtain

$$U(x)=U_a(x)+3/8x^2 \tag{A.5}$$

(see formula (5.15)). The additional repulsion leads to an increase in the value of ζ_c associated with the same value of R. Instead of (5.10) we now have

$$y(0)=\frac{1+\sqrt{4-\zeta^2}}{2},\quad y'(0)=-\frac{\zeta(\zeta-R)}{4y(0)}, \tag{A.6}$$

but the coefficients a_0 and a_1 in the expansion (5.11) are the same as before, while $a_2 = -(\zeta^2 - 15/16)/2a_0$ and $a_3 = a_2/2a_0$. The method used to calculate $\zeta_c(R)$ is broken down in Sec. 5 and gives the results presented in Table II.

Note added in proof (20 October 1973): The change of variables (2.12) was proposed by Prüfer,[30] and was used to investigate the general properties of the Sturm-Liouville equation.[31] The question of the stability of numerical methods of calculating the eigenvalues of equations of the type (2.13) is investigated in article [32]. This equation has already been applied to the calculation of the terms of the molecular hydrogen ion [33] and to the calculation of the quasinuclear states in the system consisting of two nucleons and two anti-nucleons.[34] The authors thank A. A. Abramov and B. O. Kerbikov for calling our attention to these articles.

[1)]It is assumed that $rV(r) \to 0$ as $r \to 0$; in this case $G \sim r^{-k}$, $F \sim r^{1-k}$, and $\theta \sim r$ for $k < 0$. If the potential has a singularity at zero of the form $V = -\zeta/r$ then $G/F \sim$ const and instead of Eq. (2.5) the initial condition is given by $\theta(0) = (1/2)\sin^{-1}(\zeta/k)$.

[2)]One can easily see that ξ does not vary under scale transformations, $V(r) \to \lambda^2 V(\lambda r)$.

[3)]This requirement is generally essential for variational calculations. Thus, the wave function for the ^{1}S-state of the helium atom contains a singularity of the type $ln(r_1^2 + r_2^2)$ corresponding to triple collisions.[24] Taking the logarithmic singularity into consideration in the trial function improves the rate of convergence of the variational method.[25]

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