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The Wave Functions of Continuum for the Two-Center Problem in Quantum Mechanics

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An algorithm is given for the calculation of the wave functions (to within $\sim 10^{-7}$) and the separation constants $\lambda_{mq}(k, R)$ (to within $\sim 10^{-11}$) of the continuum of the two-center problem with Coulomb interaction. The phases $\Delta_{mq}(k, R)$ of the solutions to the radial equation are found as functions of the momentum k and the intercenter spacing R. The constructed angular $\Xi_{mq}(\eta; k, R)$ and radial $\Pi_{mq}(\xi; k, R)$ Coulomb spheroidal functions are a natural generalization of the Coulomb functions $F_l(\gamma, kr)$ of the one-center problem.

INTRODUCTION

The wave functions of the continuum for the two-center problem are necessary for the solution of various quantum mechanical problems: scattering of electrons on two Coulomb centers [1], photoionization of molecules [2], three-body problem with Coulomb interaction [3], etc.

The wave functions of the continuum for the two-center problem with charges $Z_1 = Z_2 = 1$ were first found by Bates *et al.* [2]. The scattering on two Coulomb centers with different charges $Z_1 \neq Z_2$ was considered by Shimizu [4], who also tabulated the eigenvalues of the angular equation for certain values of the parameters of the problem.

The present paper contains a description of the algorithm for the calculation of the eigenvalues of $\lambda_{mq}(k, R)$ of the angular equation and the wave functions $\phi_{mq}(\xi, \eta, \varphi; k, R)$ of the continuum of the two-center problem. This paper is a direct continuation of the studies of [5] dealing with the calculation of the eigenvalues and the wave functions of the discrete spectrum of the two-center problem. The routine is written in Fortran-4 as applied to the computer CDC-6200.

The wave functions $\Phi_{\mathbf{k}}(\mathbf{r}; R)$ of the continuum of the two-center problem are defined as solutions to the Schrödinger equation

$$\left(-\frac{1}{2}\Delta_{\mathbf{r}} - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}\right)\phi_{\mathbf{k}}(\mathbf{r}; R) = E_k\phi_{\mathbf{k}}(\mathbf{r}; R), \tag{1}$$

where r_1 and r_2 are the distances of a negative particle (electron) from positive charges (nuclei) Z_1 and Z_2 spaced from each other by R, and $E_k = \mathbf{k}^2/2$ is the energy of the electron in a state with momentum $\mathbf{k}$.

In spheroidal coordinates

$$\xi = (r_1 + r_2)/R, \qquad \eta = (r_1 - r_2)/R, \qquad \varphi, \tag{2}$$

the solution $\phi_{\mathbf{k}}(\mathbf{r}; R)$ is represented in the form of the product of the functions

$$\begin{aligned}\phi_{\mathbf{k}}(\mathbf{r}; R) &= \phi_{mq}(\xi, \eta, \varphi; k, R) \\ &= N_{mq}(k, R)\, \Pi_{mq}(\xi; k, R)\, \Xi_{mq}(\eta; k, R)\, \frac{e^{\pm im\varphi}}{(2\pi)^{1/2}}\end{aligned} \tag{3}$$

where $m = |m|$ is an integer, and q is equal to the number of zeros of the function $\Xi_{mq}(\eta; k, R)$ in the interval $(-1, 1)$.

We call the functions $\Pi_{mq}(\xi; k, R)$ and $\Xi_{mq}(\eta; k, R)$ radial and angular Coulomb spheroidal functions (by analogy with the Coulomb functions $F_l(\gamma, kr)$ of the one-center problem [6]. They are defined as regular solutions of the equations

$$\begin{aligned}&\frac{d}{d\xi}\left[(\xi^2 - 1)\frac{d}{d\xi}\Pi_{mq}(\xi; k, R)\right] \\ &\quad + \left[-\lambda_{mq} + c^2(\xi^2 - 1) + a\xi - \frac{m^2}{\xi^2 - 1}\right]\Pi_{mq}(\xi; k, R) = 0, \\ &|\Pi_{mq}(1; k, R)| < \infty, \qquad \Pi_{mq}(\xi; k, R) \xrightarrow[\xi\to\infty]{} 0, \qquad 1 \leqslant \xi < \infty,\end{aligned} \tag{4a}$$

$$\begin{aligned}&\frac{d}{d\eta}\left[(1 - \eta^2)\frac{d}{d\eta}\Xi_{mq}(\eta; k, R)\right] \\ &\quad + \left[\lambda_{mq} + c^2(1 - \eta^2) + b\eta - \frac{m^2}{1 - \eta^2}\right]\Xi_{mq}(\eta; k, R) = 0, \\ &|\Xi_{mq}(\pm 1; k, R)| < \infty, \qquad -1 \leqslant \eta \leqslant 1.\end{aligned} \tag{4b}$$

The notation is as follows.

$$a = R(Z_2 + Z_1), \qquad b = R(Z_2 - Z_1), \qquad c = kR/2 = (R/2)(2E_k)^{1/2}. \tag{4c}$$

The normalization $N_{mq}(k, R)$ is determined by the condition

$$\begin{aligned}\int d\mathbf{r}\, \phi^*_{\mathbf{k}'}(\mathbf{r}; R)\, \phi_{\mathbf{k}}(\mathbf{r}; R) &= \int d\tau\, \phi^*_{m'q'}(\xi, \eta, \varphi; k', R)\, \phi_{mq}(\xi, \eta, \varphi; k, R) \\ &= \delta_{mm'}\delta_{qq'}\delta(k - k'),\end{aligned} \tag{5}$$

where

$$\int d\tau = (R^3/8) \int_1^\infty d\xi \int_{-1}^1 d\eta \int_0^{2\pi} d\varphi(\xi^2 - \eta^2). \tag{6}$$

The solution of Eqs. (4) can be considered as a generalization of certain special functions. In particular, for $a = b = 0$, Eqs. (4) turn into the ones for prolate sheroidal functions [7], for $c = b = 0$, Eq. (4b) turns into the equation for the associated Legendre polynomial, and for $c \to 0$, $a \to 0$, $a/2c \to$ const., Eq. (4a) turns into the equation determining the Coulomb functions [6].

In the general case $c \neq 0$, $a \neq 0$, $b \neq 0$, little is known about the solutions of Eqs. (4), and the algorithms for their numerical finding are not sufficiently well developed.

On the complex plane z, Eqs. (4) are identical and differ only by the domain of definition of the solutions. The solutions $u(z)$ of Eqs. (4) are analytic functions on the z-plane with the cut joining the singular points of the equation: two regular ($z = \pm 1$) and one irregular ($z = \infty$). The indices of the regular points $z = \pm 1$ are $\pm m/2$ and the regular solutions in their vicinity behave like

$$u(z) \sim (1 - z^2)^{m/2}, \qquad z \to \pm 1,$$

the asymptotic of the singular solutions for $z \to \pm 1$ is of the form

$$u(z) \sim \ln(1 - z^2), \qquad \text{for} \quad m = 0,$$
$$u(z) \sim (1 - z^2)^{-m/2}, \qquad \text{for} \quad m \neq 0.$$

The asymptotic behavior in the irregular point $z = \infty$ is of the form

$$u(z) \sim (1/z)\{\pm i(cz - (b/2c) \ln 2cz)\}, \qquad z \to \infty.$$

For $c = 0$, $b \neq 0$, the point $z = \infty$ remains irregular:

$$u(z) \sim z^{-3/4} \exp\{\pm 2(-bz)^{1/2}\}.$$

Calculation of the Eigenvalues $\lambda_{mq}(k, R)$

The eigenvalues $\lambda = \lambda_{mq}(k, R)$ are found from the angular solution of Eq. (4b) and depend on the discrete set of the quantum numbers $(m, q) = 0, 1, 2, \ldots$ and the two continuous parameters $0 \leqslant k < \infty$ and $0 \leqslant R < \infty$. To calculate them,

the solution of the Sturm–Liouville problem (4b) is sought in the form of a series

$$\Xi_{mq}(\eta;\, k,\, R) = e^{-ic(1-\eta)} \sum_{s=0} d_s(k,\, R)\, P^m_{s+m}(\eta), \qquad d_{-1} = 0, \quad d_0 = 1, \tag{7}$$

where $P^m_{s+m}(\eta)$ are the associated Legendre polynomials defined by the Rodrigues formula [7]. Inserting the expansion (7) in Eq. (4b) leads to three-term recurrent relations for the coefficients d_s

$$\rho_s d_{s+1} - \kappa_s d_s + \delta_s d_{s-1} = 0, \tag{8}$$

where

$$\begin{aligned} \rho_s &= (s + 2m + 1)[b - 2ic(s + m + 1)]/[2(s + m) + 3], \\ \kappa_s &= -\lambda + (s + m)(s + m + 1), \\ \delta_s &= s[b + 2ic(s + m)]/[2(s + m) - 1]. \end{aligned} \tag{9}$$

The eigenvalues $\lambda = \lambda_{mq}(k, R)$ are the roots of the transcendent equation $y(\lambda) = 0$, the left-hand side of which can be represented as an infinite chain fraction [5]

$$y(\lambda) = \kappa_0 - \cfrac{\rho_0\delta_1}{\kappa_1 - \cfrac{\rho_1\delta_2}{\kappa_2 - \ddots}} \tag{10}$$

The function $y(\lambda)$ is real since it depends on κ_s and $\rho_s\delta_{s+1}$ alone.

To find the roots of the equation $y(\lambda)$, we have used the Newton–Raphson method realized in the program with double accuracy. As an initial approximation for the eigenvalues $\lambda_{mq}(k, R)$, the following expansion is used.

$$\begin{aligned} \lambda_{mq}(k, R) = l(l + 1) &- \frac{(l^2 - m^2)(b^2 + 4c^2l^2)}{2l(2l + 1)(2l - 1)} \\ &+ \frac{[(l + 1)^2 - m^2][b^2 + 4c^2(l + 1)^2]}{2(l + 1)(2l + 1)(2l + 3)}, \end{aligned} \tag{11}$$

which follows from Eqs. (10) in the limit $R \to 0$. For other calculation details, see [5].

For the majority of physical applications, it is sufficient to know the $\lambda_{mq}(k, R)$ values within a relative accuracy $\epsilon \sim 10^{-8} - 10^{-10}$. Thus, the number of the terms of the chain fraction (10) does not exceed 100, while the time of calculation of $\lambda_{mq}(k, R)$ in the interval $R = 0.025$ (0.025) 20 for fixed m, q, and k is about 15 min. Figure 1 gives the results of calculations of $\lambda_{mq}(k, R)$ for different sets of m, q, and k in the case $Z_1 = 1$ and $Z_2 = 2$.

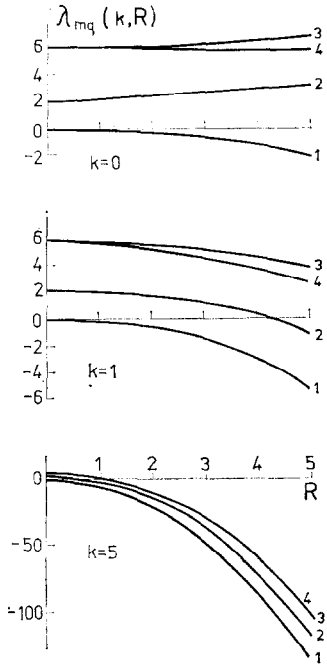

FIG. 1. The dependencies $\lambda_{mq}(k, R)$ on R at fixed values of k and different sets of quantum numbers: (1) $m = 0$, $q = 0$; (2) $m = 0$, $q = 1$; (3) $m = 0$, $q = 2$; (4) $m = 1$, $q = 1$. At $R \to 0$, $\lambda_{mq}(k, R) \to l(l + 1)$.

CALCULATION OF THE FUNCTIONS $\Xi_{mq}(\eta; k, R)$

The algorithm of calculation of the angular Coulomb spheroidal functions of the discrete spectrum of the two-center problem suggested in [5] is not efficient in the case of the continuum since at $R \gg 1$, the appropriate series representing the functions $\Xi_{mq}(\eta; k, R)$ converges very slowly. For example, in the expansion (7), at $c \sim 10$, $d_s \sim 500$ already for $s \sim 20$, and the coefficients d_s change their sign and increase rapidly in absolute value. Therefore, it is better to find the functions $\Xi_{mq}(\eta; k, R)$ by a direct integration of Eq. (4b) using, near the singular points $\eta = \pm 1$, suitable expansions. For example, near $\eta \approx -1$

$$\Xi_{mq}(\eta; k, R) = (1 - \eta^2)^{m/2} \sum_{s=0}^{s_1} \bar{d}_s (1 + \eta)^s, \tag{12}$$

where the coefficients $\bar{d}_s$ are found from the four-term recurrent relations

$$p_s\bar{d}_{s+1} + q_s\bar{d}_s + r_s\bar{d}_{s-1} + t_s\bar{d}_{s-2} = 0; \tag{13}$$

in this case, $d_{-2} = d_{-1} = 0$, $d_0 = 1$.

The following notation is introduced.

$$\begin{aligned} p_s &= 2(s + 1)(s + m + 1), \\ q_s &= -[-\lambda + b + m(m + 1) + s(s + 2m + 1)], \\ r_s &= 2c^2 + b, \\ t_s &= -c^2. \end{aligned} \tag{14}$$

To ensure a relative accuracy of calculation of the functions $\epsilon \sim 10^{-7}$, it is sufficient to take $s_1 = 4$, $1 + \eta = 10^{-6}$ and the integration step $\Delta\eta = 2^{-12}$. The normalization of the solutions naturally can be determined by the relation

$$\int_{-1}^{1} \Xi_{m'q'}(\eta; k, R)\, \Xi_{mq}(\eta; k, R)\, d\eta = \delta_{qq'}\,. \tag{15}$$

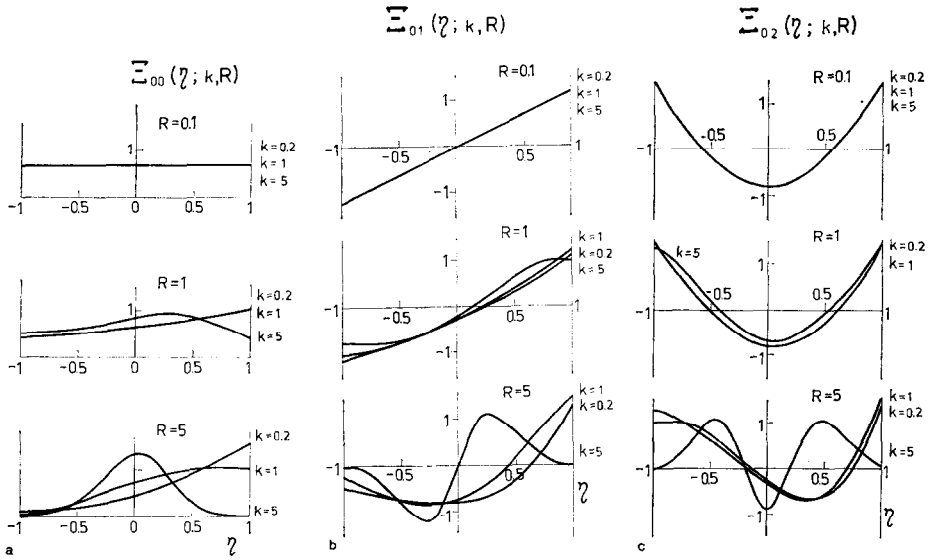

FIG. 2(a, b, c). The angular Coulomb spheroidal functions $\Xi_{mq}(\eta; k, R)$ normalized by (15) at fixed values k, R, m, q; $Z_1 = 1$, $Z_2 = 2$.

When $R \to 0$, Eq. (4b) turns to the equation for the associated Legendre polynomials $P_{m+q}(\eta)$. Thus, the following relation ($l = m + q$) takes place.

$$\Xi_{mq}(\eta; k, 0) = \left[\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\eta), \tag{16}$$

from which the sign of the functions $\Xi_{mq}(\eta; k, R)$ is determined. Figs. 2a–2c give the functions $\Xi_{mq}(\eta; k, R)$ normalized by condition (15) for different k and R and for different sets of quantum numbers m and q.

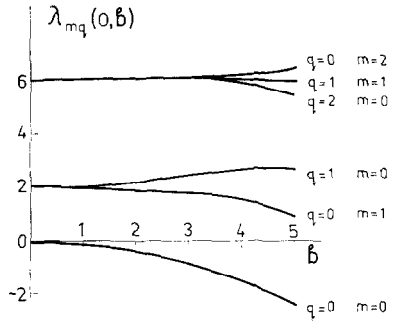

FIG. 3. The functions $\lambda_{mq}(0, b)$ at different sets of quantum numbers m and q.

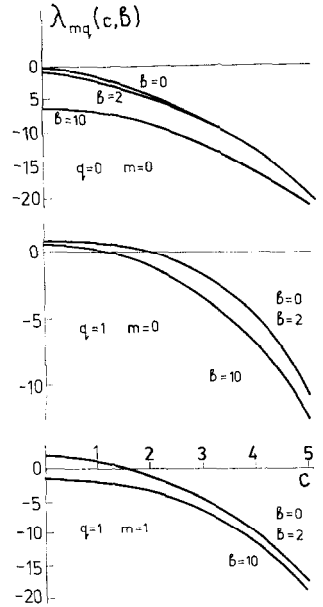

FIG. 4. Eigenvalues of $\lambda_{mq}(c, b)$ as a function of the parameter c at fixed values b, m, and q.

The Sturm–Liouville problem can be considered independently of the initial three-dimensional problem. In this case, the eigenvalues $\lambda_{mq}(k, R) = \lambda_{mq}(c, b)$ are functions of the parameters c and b. For $b = 0$, Eq. (4b) turns to the equation for prolate spheroidal functions [7] and its solutions coincide with the spheroidal functions $S_{ml}(c, \eta)$.

In the inverse extreme case, $c \to 0$, $b \neq 0$, the solutions of Eq. (4b) are used to express the wave functions of the electron in the finite dipole field [8]. Figure 3 gives the $\lambda_{mq}(c, b)$ values for $c = 0$ as functions of the parameter b. Figure 4 also gives the $\lambda_{mq}(c, b)$ values as functions of the parameter c for different b and different sets of the quantum numbers m and q.

Calculation of the Functions $\Pi_{mq}(\xi; k, R)$

Two linearly independent solutions of Eq. (4a) can be presented as follows ($t = \xi - 1$).

$$\Pi^{\text{reg}}_{mq}(\xi; k, R) = (\xi^2 - 1)^{m/2} F(t), \tag{17a}$$

$$\Pi^{\text{irreg}}_{mq}(\xi; k, R) = (\xi^2 - 1)^{m/2} G(t), \tag{17b}$$

where $F(t) \equiv F(t, 0)$. The function $F(t, m)$ obeys the equation

$$t(t+2)F'' + 2(m+1)(t+1)F' + [c^2t^2 + (2c^2 + a)t + a + m(m+1) - \lambda]F = 0, \tag{18}$$

and for $t < 1$, it is defined by the series

$$F(t, \nu) = \sum_{s=0}^{s_2} g_s(\nu)\, t^{s+\nu}, \tag{19}$$

the coefficients of which satisfy the four-term recurrent relation

$$\bar{p}_s g_{s+1} + \bar{q}_s g_s + \bar{r}_s g_{s-1} + \bar{t}_s g_{s-2} = 0, \tag{20}$$

$$g_{-2} = g_{-1} = 0, \qquad g_0 = 1, \tag{20a}$$

$$\begin{aligned} \bar{p}_s &= 2(\nu + s + 1)(\nu + s + m + 1), \\ \bar{q}_s &= (\nu + s)(\nu + s + 2m + 1) - \lambda + a + m(m+1), \\ \bar{r}_s &= 2c^2 + a, \\ \bar{t}_s &= c^2. \end{aligned} \tag{21}$$

The nonregular solution is determined by the function $F(t, \nu)$ with the aid of the formulas: For $m \neq 0$,

$$G(t) = (\partial/\partial\nu)[(\nu + m) F(t, \nu)]|_{\nu=-m}. \tag{22a}$$

For $m = 0$,

$$G(t) = F(t) \ln t + (\partial/\partial\nu) F(t, \nu)|_{\nu=0} \tag{22b}$$

The derivatives $\partial F(t, \nu)/\partial\nu$ are calculated with the account of Eqs. (19)–(21) as well as the conditions $\partial g_{-2}/\partial\nu = \partial g_{-1}/\partial\nu = \partial g_0/\partial\nu = 0$.

Using the representation (22) and the expansion (19) at the singular point $t = 0$, both solutions (17) of Eq. (4a) are found by means of direct integration. To ensure a relative accuracy of the calculation of the functions, $\epsilon \sim 10^{-7}$, it is sufficient to choose $s_2 = 4$ and $t = 10^{-6}$, and the step of integration $\Delta\xi = 0.002/c$ and $\Delta\xi = 0.02/c$. In integrating Eq. (4a), the Numerov method was used [10] which is more effective than the Runge–Kutta method. The sign of the functions $\Pi_{mq}(\xi; k, R)$ is determined from the requirement for them to be positive at $\xi \to 1$.

The normalization is fixed by the asymptotic behavior of the solution at $c\xi \gg 1$:

$$(\xi^2 - 1)\, \Pi_{mq}(\xi; k, R) = A \cdot \mathrm{Re} \left\{ \left[1 + \sum_{s=1}^{s_j} g_s (c\xi)^{-s} \right] \cdot \exp\left[-i \left(c\xi + \frac{a}{2c} \ln 2c\xi - \frac{l+1}{2} \pi + \Delta_{mq} \right) \right] \right\}. \tag{23}$$

Here, $\Delta_{mq} = \Delta_{mq}(k, R)$ is the phase of the radial Coulomb spheroidal function that is analogous to the Coulomb phase $\sigma_l = \arg \Gamma(l + 1 - i\gamma)$, $\gamma = Z/k$ in the scattering on the Coulomb attraction potential $-Z/k$. The following limiting relations take place.

$$\Delta_{mq}(k, 0) = \sigma_l = \arg \Gamma(l + 1 - i\gamma), \qquad \gamma = a/2c, \quad l = m + q. \tag{24}$$

The coefficients g_s of the expansion (23) satisfy the six-term recurrent relation ($\gamma = a/2c$)

$$\begin{aligned} & i2(s+1)\, g_{s+1} + [s(s+1) - \lambda - \gamma^2 + i(2s+1)\gamma]\, g_s \\ & \quad + 2c^2[\gamma - i2(s-1)]\, g_{s-1} \\ & \quad + c^2[-2(s-1)(s-2) + \lambda + 1 - m^2 + 2\gamma^2 - i2(2s-3)\gamma]\, g_{s-2} \\ & \quad + 2c^4[-\gamma + i(s-3)]\, g_{s-3} \\ & \quad + c^4[(s-3)(s-4) - \gamma^2 + i(2s-7)\gamma]\, g_{s-4} = 0. \end{aligned} \tag{25}$$

The normalization A and the phase Δ_{mq} are found from the condition of sewing the asymptotics of the solution (23) and its derivative at a point $\xi^* \gg 1$ with the solution $\Pi_{mq}(\xi; k, R)$ and its derivative $(\partial/\partial\xi)\, \Pi_{mq}(\xi; k, R)$ found in the numerical integration of Eq. (4a). In order to ensure a relative accuracy $\epsilon \sim 10^{-7}$, when calculating A and Δ_{mq}, it is sufficient to put $s_3 \approx 10$ for

$$c\xi^* = 50 \cdot |\, \lambda + \gamma^2 \,|.$$

Within the limit $R \to 0$, the two-center problem turns to a one-center problem with charge $Z = Z_1 + Z_2$, and Eq. (4a), after a scale transformation $r = R\xi/2$, turns to an equation defining the Coulomb functions $F_l(\gamma, kr)$ and $G_l(\gamma, kr)$ [6]. In this case, the wave function $\phi_{mq}(\xi, \eta, \varphi; k, R)$, normalized by the condition (5), transforms to a normalized solution $\psi_{klm}(\mathbf{r})$ of the one-center problem [11]

$$\psi_{klm}(\mathbf{r}) = (2/\pi)^{1/2}\,(1/r)\,F_l(\gamma, kr)\,Y_{lm}(\theta, \varphi), \tag{26}$$

where $R\xi/2 \to r$, $\eta \to \cos\theta$ and $Y_{lm}(\theta, \varphi)$ is the Legendre spherical function.

By comparing the asymptotic of the functions

$$F_l(\gamma, kr) \sim \sin[kr + \gamma \ln 2kr - (l\pi/2) + \sigma_l] \tag{27}$$

with the expansion (23), we find that $A = 1$. For such a choice of A, the normalization coefficient $N_{mq}(k, R)$ of the solution (3) is

$$N_{mq} = (2/R)(2/\pi)^{1/2}. \tag{28}$$

This result follows immediately from the comparison of expressions (3) and (26), taking into account relations (15), (16), (23), and (27).

Another derivation of the expression for N_{mq} is given in the paper by Bates *et al.* [2]. Figures 5a–5c give the regular solution $\Pi_{mq}(\xi; k, R)$ normalized by the

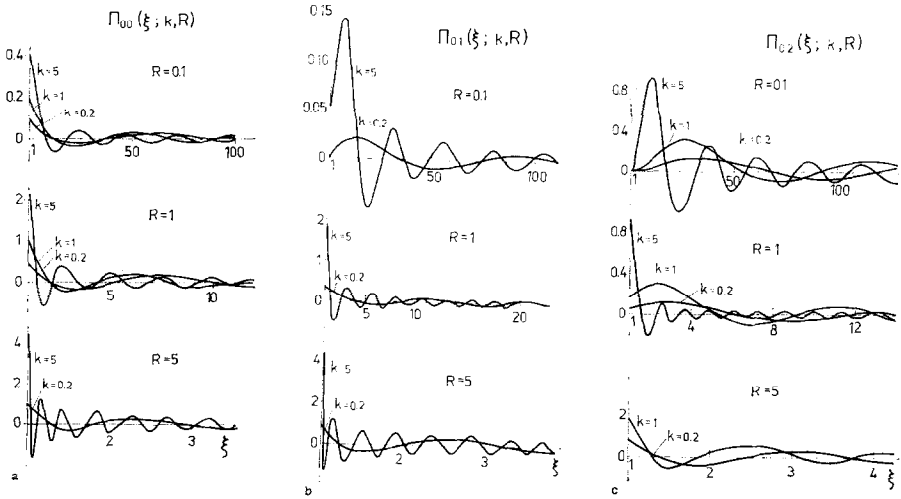

FIG. 5(a, b, c). The radial Coulomb spheroidal functions $\Pi_{mq}(\xi; k, R)$ normalized by the asymptotic condition $\Pi_{mq}(\xi; k, R) \to (1/\xi)\sin(c\xi + (a/2c)\ln 2c\xi - (l\pi/2) + \Delta_{mq})$ at fixed values k, R and different sets m and q; $Z_1 = 1$, $Z_2 = 2$.

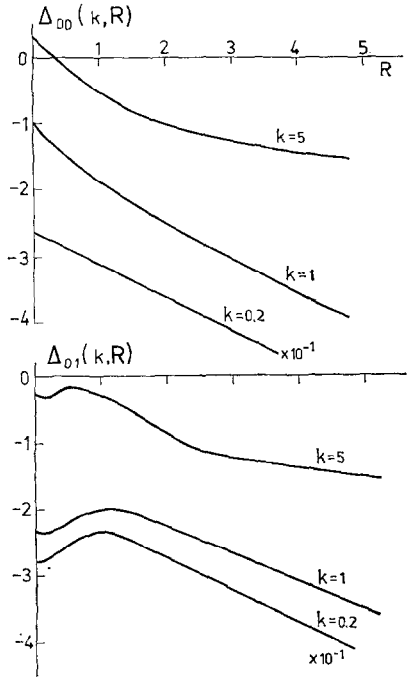

FIG. 6. The phases of solutions of the radial equation $\Delta_{mq} = \Delta_{mq}(k, R)$ as a function of R at different values of k. When $R \to 0$ Δ_{mq} coincides with the Coulomb phase of one-center problem with the charge $Z = Z_1 + Z_2$: $\Delta_{mq}(k, 0) = \arg \Gamma(l + 1 - (Z_1 + Z_2)/k)$.

condition $A = 1$ for different k and R and different sets of m and q. Figure 6 also gives the phases $\Delta_{mq}(k, R)$ as functions of the intercenter spacing R for different k-, q-, and m-values.

The cross sections for scattering of electrons on two Coulomb centers [1] are expressed in terms of these phases.

CHECKING OF THE ACCURACY OF CALCULATIONS

For an additional verification of the accuracy of calculations, the eigenvalues of $\lambda_{mq}(c, b)$ were compared with the analytic expressions $\lambda_{mq}(0, b)$ that are known for definite values (e.g., $\lambda_{00}(0, b = 1.27863) = \frac{1}{4}$.

The criterion of the accuracy of calculation of the raditional functions was the condition of constancy of the Wronskian

$$W = \bar{\Pi}_{mq}(\partial \bar{G}_{mq}/\partial \xi) - \bar{G}_{mq}(\partial \bar{\Pi}_{mq}/\partial \xi) = \text{const.}, \tag{29}$$

where $\bar{\Pi}_{mq}$ and $\bar{G}_{mq}$ are defined by the relations

$$\begin{aligned} \bar{\Pi}_{mq} &= (\xi^2 - 1)^{1/2}\, \Pi_{mq}^{\mathrm{reg}}(\xi; k, R), \\ \bar{G}_{mq} &= (\xi^2 - 1)^{1/2}\, \Pi_{mq}^{\mathrm{irreg}}(\xi; k, R). \end{aligned} \tag{30}$$

Condition (29) was satisfied in the calculations with a relative accuracy $\epsilon \lesssim 10^{-7}$. To verify the accuracy of calculations the number of the terms of the sums s_n in expansions (12), (19), and (23), and the quantity $c\xi^*$ were varied. The values of these quantities given in this paper ensure the relative accuracy of calculation of the wave functions $\epsilon \sim 10^{-7}$.

The accuracy of calculation of the angular functions $\Xi_{mq}(\eta; k, R)$ at $kR \lesssim 5$ was verified by comparing the values obtained as a result of integration of Eq. (4b) with the values given by the expansion

$$\Xi_{mq}(\eta; k, R) = (1 - \eta^2)^{m/2}\, e^{ic(1\pm\eta)} \sum_s c_s (1 \pm \eta)^s. \tag{31}$$

While for $kR > 5$ near $\eta \approx 1$, the logarithmic derivatives obtained by the integration of Eq. (4b) using the expansion (12) and those that follow from the expansion (12) after the replacement $\eta \to -\eta$ were compared.

For a global checking of the solutions constructed, the orthogonality condition

$$\int d\tau\, \phi_{mq}(\xi, \eta, \varphi; k, R)\, \Psi_{Nlm}(\xi, \eta, \varphi; R) = 0, \tag{32}$$

is used, where $\Psi_{Nlm}(\xi, \eta, \varphi; R)$ is the wave function of the discrete spectrum of the two-center problem calculated earlier in [5]. The condition (32) was fulfilled in our calculations within an accuracy $\epsilon \sim 10^{-7}$.

Note Added in Proof. Reference [12], which contains similar results, appeared while this paper was in press.

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REFERENCES

1. D. I. ABRAMOV, I. V. KOMAROV, *Teor. Mat. Fiz.* **22** (1975), 253; MING CHIANG LI, *J. Math. Phys.* **15** (1974), 570.
2. D. R. BATES AND G. POOTS, *Proc. Phys. Soc.* **66** (1953), 784; D. R. BATES, U. ŒPIK, AND G. POOTS, *Proc. Phys. Soc.* **66** (1953), 1113.

3. N. F. MOTT AND H. S. W. MASSEY, "The Theory of Atomic Collisions," Oxford Univ. Press (Clarendon) London, 1965, A. V. MATVEENKO AND L. I. PONOMAREV, *Theor. Mat. Fiz.* **12** (1972), 64.
4. MIKIO SHIMIZU, *Nat. Sci. Rep. Ochanomizu Univ.* **12** (1961), 1; *J. Phys. Soc. Japan* **18** (1963), 811.
5. L. I. PONOMAREV AND T. P. PUZYNINA, *Zh. Vychisl. Mat. Mat. Fiz.* **8** (1968), 1256; Preprints Joint Inst. Nuclear Research, P2-3009, P2-3012, Dubna, 1966, P4-5040, Dubna, 1970.
6. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," Nat. Bur. Stand., Washington D.C; A. R. CURTIS, "Coulomb Wave Functions," Cambridge Univ. Press, London, 1964.
7. C. FLAMMER, "Spheroidal Wave Functions," Stanford Univ. Press, Stanford, Calif., 1957.
8. D. I. ABRAMOV AND I. V. KOMAROV, *Theor. Mat. Fiz.* **13** (1972), 209.
9. H. JEFFREYS AND B. SWIRLES, JEFFREYS, "Methods of Mathematical Physics," Cambridge University Press, London, 1966.
10. B. NUMEROV, *Publ. Observ. Cent. Astrophys Russ.* **2** (1933), 188.
11. D. R. HARTREE, "Numerical analysis," 2nd ed., Sect. 7.23. Oxford Univ. Press, London/New York, 1958. L. D. LANDAU AND E. M. LIFSHITZ, "Quantum Mechanics" (in Russian), Fizmatgiz, Moscow, 1963.
12. I. V. KOMAROV, L. I. PONOMAREV, AND S. YU. SLAVJANOV, "Spheroidal and Coulomb Spheroidal Functions" (in Russian), Nauka, Moscow, 1976.