ON THE BINDING ENERGY OF TWO PARTICLES WHOSE STATE IS DESCRIBED BY THE SCHRÖDINGER EQUATION WITH A SCREENED COULOMB INTERACTION POTENTIAL

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Abstract

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ON THE BINDING ENERGY OF TWO PARTICLES WHOSE STATE IS DESCRIBED BY THE SCHRÖDINGER EQUATION WITH A SCREENED COULOMB INTERACTION POTENTIAL

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The Schrödinger equation for two particles with an attractive potential of the form $\exp(-\lambda r)/r$ is applicable in many areas of physics. In those cases where such a potential is used in plasma physics or solid-state physics, it is usually called the Debye–Hückel potential; in nuclear physics it appears under the name of the Yukawa potential. There is a considerable number of works in the literature devoted to the study of bound states ($E < 0$) in the field of this potential. However, no analytic solution of this problem has been found up to the present time, and therefore all studies have been carried out by numerical or approximate methods. In this connection, the results of various authors show substantial discrepancies concerning the nature of the dependence of the binding energy E on the screening parameter λ in the region where λ is of the order of the Bohr radius and, accordingly, $E \to 0$.

In papers ([1–4]) the conclusion was drawn that, if the screening parameter λ is different from zero, then there exists only a finite number of levels corresponding to bound states. According to these data, as λ increases there is a monotonic decrease in the number of such levels, and for λ greater than some $\lambda_{\max}$ the original equation has no solutions at all corresponding to bound states. This conclusion agrees with the effect known in plasma physics, consisting in the gradual disappearance of spectral lines as the plasma concentration increases (see, for example, ([7])). However, in paper ([6]) Rogers, on the basis of detailed numerical calculations, came to the conclusion that the values of the energy levels of the Schrödinger equation with a screened Coulomb potential asymptotically approach zero as the screening parameter increases.

In the present work, for the Schrödinger equation with a screened Coulomb potential, a spherically symmetric solution is found in the form of a functional series. The properties of this solution make it possible to conclude that, at some finite value of λ, the energy of the $1s$-state becomes zero.

The initial Schrödinger equation for a spherically symmetric wave function $\psi(r)$, by means of the standard substitution $\psi(r) = r^{-1}\varphi(r)$, is reduced to the form

$$\varphi''(r) + \frac{2\mu}{\hbar^2}E\varphi(r) = -\frac{2\mu e^2}{\hbar^2}\frac{\exp(-\lambda r)}{r}\varphi(r). \tag{1}$$

Let us introduce the notation $\alpha = \dfrac{2\mu e^2}{\hbar^2}$, $\beta^2 = -\dfrac{2\mu}{\hbar^2}E$ (μ is the reduced mass of the particles under consideration). In this notation, the unnormalized solution of equation (1) can be written in the form

$$\varphi(r) = \exp(-\beta r) + \alpha\int_{\beta+\lambda}^{\infty}\frac{\exp(-rq)}{\beta^2-q^2}\,dq + \alpha^2\int_{\beta+\lambda}^{\infty}\frac{dq}{\beta^2-q^2}\int_{q+\lambda}^{\infty}\frac{\exp(-rk)}{\beta^2-k^2}\,dk +$$

$$+\alpha^3\int_{\beta+\lambda}^{\infty}\frac{dq}{\beta^2-q^2}\int_{q+\lambda}^{\infty}\frac{dk}{\beta^2-k^2}\int_{k+\lambda}^{\infty}\frac{\exp(-rp)\,dp}{\beta^2-p^2} + \cdots \tag{2}$$

The fact that expression (2) is a solution of equation (1) is proved by direct substitution. It is easy to see that each term of expression (2), starting with the second, when substituted into the left-hand side of equation (1), gives the expression that is obtained if the preceding term is substituted into the right-hand side of this equation. The eigenvalue (the quantity β) is found from the boundary condition $\varphi(0) = 0$.

Let us pose the problem of finding the maximum value of λ for which β goes to zero. The equation for determining $\lambda_{\max}$ will have the form

$$0 = 1 + \alpha\int_{\lambda}^{\infty}\frac{dq}{-q^2} + \alpha^2\int_{\lambda}^{\infty}\frac{dq}{-q^2}\int_{q+\lambda}^{\infty}\frac{dk}{-k^2} + \cdots; \tag{3}$$

it is convenient to write this equation in the form

$$0 = 1 - x + a_2x^2 - a_3x^3 + a_4x^4 - \cdots, \tag{4}$$

where $x = \alpha/\lambda$. The constant coefficients $a_n > 0$. The values of a_2, a_3, and a_4 are

$$a_2 = 0.306853, \qquad a_3 = 0.045229, \qquad a_4 = 003906$$

The required root of equation (4) may be found approximately in the following way. Let $x_n^{(1)}$ and $x_{n+1}^{(1)}$ be, respectively, the least positive roots of the equations

$$1 - x + a_2x^2 - \cdots + a^n_{nx}(-1)^n = 0,$$

$$1 - x + a_2x^2 - \cdots + a^n_{nx}(-1)^n + a_{n+1}x^{n+1}(-1)^{n+1} = 0, \tag{5}$$

where $n \geqslant 3$. Then, if the series on the right-hand side of equation (4) is monotonically decreasing in the interval of values of x containing the points $x_n^{(1)}$ and $x_{n+1}^{(1)}$ (i.e., $a_{m+1}x/a_m < 1$), then, since this series is alternating and $a^k_{kx} \to 0$ as $k \to \infty$, its sum will vanish at some value of x lying in the interval $x_n^{(1)} < x < x_{n+1}^{(1)}$ (if n is odd) or in the interval $x_{n+1}^{(1)} < x < x_n^{(1)}$ (if n is even). This assertion follows from the well-known Leibniz theorem on the properties of alternating series possessing the indicated properties. For such series an arbitrary remainder of the series has the sign of its first term and is smaller than it in absolute value. Therefore those remainders of series (4) which correspond to equation (5) will have different signs, and, consequently, the sum of the entire series (4) must vanish in the indicated intervals.

This property of equation (4) also proves the existence of a finite value of λ for which the binding energy vanishes.

The equation $1 - x + a_2x^2 - a_3x^3 = 0$ has the unique real root $x_3^{(1)} = 1.60$. The equation $1 - x + a_2x^2 - a_3x^3 + a_4x^4 = 0$ has two real roots $x_4^{(1)} = 1.69$ and $x_4^{(2)} = 3.94$.

The condition $a_{m+1}x/a_m < 1$ is fulfilled at least for $x < 2$ (starting from $m = 1$). Indeed, since

$$\frac{a_{m+1}x}{a_m} = \left[x\int_1^\infty \frac{dk}{k^2}\int_{k+1}^\infty \frac{dk_1}{k_1^2}\,F_{m-1}(k_1+1)\right] \Big/ \left[\int_1^\infty \frac{dk_1}{k_1^2}\,F_{m-1}(k_1+1)\right], \qquad m \geqslant 1, \tag{6}$$

where $F'_{i-1}(k+1)$ is a function whose form is determined by the expression for a_i, from expression (6) it is easy to obtain the following relations for $a_{m+1}x/a_m$:

$$\frac{a_{m+1}x}{a_m} < \left[x\int_1^\infty \frac{dk}{k^2}\int_2^\infty \frac{dk_1}{k_1^2}F_{m-1}(k_1+1)\right] \Big/ \left[\int_1^\infty \frac{dk_1}{k_1^2}F_{m-1}(k_1+1)\right] =$$

$$= \left[\frac{x}{2}\int_1^\infty \frac{dt}{t^2}F_{m-1}(1+2t)\right] \Big/ \left[\int_1^\infty \frac{dk_1}{k_1^2}F_{m-1}(k_1+1)\right] <$$

$$< \left[\frac{x}{2}\int_1^\infty \frac{dt}{t^2}F_{m-1}(t+1)\right] \Big/ \left[\int_1^\infty \frac{dk_1}{k_1^2}F_{m-1}(k_1+1)\right] = \frac{x}{2}. \tag{7}$$

The condition $a_m x^m \to 0$ as $m \to \infty$ is satisfied for any x, since

$$a_m x^m = x^m \int_1^\infty \frac{dq_1}{q_1^2} \int_{q_1+1}^\infty \frac{dq_2}{q_2^2} \cdots \int_{q_{m-1}+1}^\infty \frac{dq_m}{q_m^2} < x^m \int_1^\infty \frac{dq_1}{q_1^2} \int_2^\infty \frac{dq_2}{q_2^2} \cdots \int_m^\infty \frac{dq_m}{q_m^2} = \frac{x^m}{m!}. \quad (8)$$

Thus, taking into account relations (7) and (8), one may assert that the root of equation (4) lies in the interval 1.60–1.69. For comparison, we give the values of α/λ ($\alpha = 2\mu e^2/\hbar^2$, λ is the screening parameter), obtained in works ([2], [4]), for which the energy of the $1s$-state becomes zero,

([2])	([4])	Present work
1.74	1.68	1.69–1.60

It should be noted that the Schrödinger equation with a screened Coulomb potential has only such solutions that, for each of them as $\lambda \to 0$, a definite hydrogen-like wave function corresponds. However, in the expression for $\varphi(r)$ (2), as $\lambda \to 0$ all terms (except the first) tend to infinity. Therefore the expression for the hydrogen-like wave function can be obtained from the expression for $\varphi(r)$ only by summing all terms of the series (2). To carry out such a summation explicitly does not seem possible to us. However, the assertion that expression (2) represents the wave function of the $1s$-state can be justified if one shows that the value of β at $\lambda = 0$, found from condition (3) ($\varphi(0) = 0$), corresponds to the value of the ground-state energy of a hydrogen-like atom.

For $\lambda = 0$ the expression for $\varphi(0)$ is connected with the expansion in a series of an exponential; using this circumstance, the equation $\varphi(0) = 0$ can be represented in the form

$$1 + \alpha \int_\beta^\infty \frac{dq}{\beta^2 - q^2} \exp\left[-\frac{\alpha}{2\beta} \ln\left|\frac{q+\beta}{q-\beta}\right|\right] = 0. \quad (9)$$

This equation has the solution $\beta = \alpha/2$, which is the expression for the energy of the ground state of a hydrogen-like atom.

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Note: Figure translations are in progress. See original paper for figures.