

Analytical Solution for a Yukawa-Type Potential

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We use an iterative process to get an analytical solution for a screened Thomas-Fermi (Yukawa) potential. The analytical solution is not exact, but the result agrees with the best variational and numerical integration results. The critical Thomas-Fermi wave vector q_c above which there is no bound state is obtained within 0.03% accuracy. We also show that the critical effective charge vanishes.

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Since the pioneering work of Yukawa¹ the potential

$$V(r) = -(A/r)\exp(-qr) \quad (1)$$

has been extensively investigated in the literature. In plasma physics it is known as the Debye-Hückel potential and in solid-state physics as the Thomas-Fermi potential. In both cases this potential arises from a screened Coulomb potential. Thus, $A = -e^2$, but q , the Thomas-Fermi wave vector, is given by different expressions, depending on the problem under consideration.²

The problem of finding an accurate solution for the screened Coulomb potential, Eq. (1), has received a lot of attention in the literature.³⁻¹⁰ The screened potential is also relevant in the study of hydrogen under pressure.¹¹⁻¹³ In such a problem it is desirable to have a well determined solution for the ground-state energy as a function of the screened Thomas-Fermi wave vector, i.e., $E = E(q)$.

In this work we use an iterative process to solve the Schrödinger equation in the momentum space. This scheme gives a recurrence relation which lends itself to an analytical approximate solution. We also obtain analytical expressions for the critical parameters.

We start out with the Schrödinger equation in the momentum space,

$$\chi(p) = \frac{2}{p^2 - 2E} \int \tilde{v}(p')\chi(p-p')dp', \quad (2)$$

where $\chi(p)$ is the wave function in p space and $\tilde{v}(p)$ is the Fourier transform of the potential $V(r)$.

We shall use an iterative process to solve Eq. (2). We associate an index n ($n=1,2,3,\dots$) to each quantity involved in each order of iteration. First we use a starting wave function for the ground state,

$$\chi_1(p) = B_1/(p^2 + \alpha_1^2)^2, \quad (3)$$

which is the solution of the unscreened ($q=0$) hydrogen

atom, with $\alpha_1 = (-2E_1)^{1/2}$, and $B_1 = (2\alpha_1)^{3/2}\alpha_1/\pi$ as a normalization constant. We shall assume that for all orders of iteration the energy takes the form

$$E_n = -\frac{1}{2}\alpha_n^2. \quad (4)$$

We now use the wave function (3) on the right-hand side of Eq. (2) to obtain

$$\chi_2(p) = \frac{B_2}{(p^2 + \alpha_2^2)(p^2 + \gamma_2^2)}, \quad (5)$$

where $\gamma_2 = q + \alpha_1$. By iterating again we get

$$\chi_3(p) = \frac{B_3}{(p^2 + \alpha_3^2)} \left\{ \frac{1}{p} \arctan \frac{(\gamma_2 - \alpha_2)p}{p^2 + \gamma_3^2} \right\}, \quad (6)$$

with

$$\gamma_3^2 = (\gamma_2 + q)(\alpha_2 + q). \quad (7)$$

For most cases of interest we can replace the arctan by its argument, so that Eq. (6) can be approximated by

$$\chi_3(p) = \frac{B_3}{(p^2 + \alpha_3^2)(p^2 + \gamma_3^2)}. \quad (8)$$

Notice that the form of the wave function is not changed as the order of iteration increases. This suggests that at order n the wave function can be readily expressed as

$$\chi_n(p) = \frac{B_n}{(p^2 + \alpha_n^2)(p^2 + \gamma_n^2)}, \quad (9)$$

with

$$\gamma_n^2 = (\gamma_{n-1} + q)(\alpha_{n-1} + q), \quad (10)$$

and

$$B_n = \{\alpha_n \gamma_n (\alpha_n + \gamma_n)\}^{3/2} / \pi. \quad (11)$$

Observe that by setting $\gamma_1 = \alpha_1$, and using Eqs. (9) and (10), we reproduce all the previous relations [except Eq. (6)]. We use Eq. (9) to obtain the energy and

$$\alpha_{n+1}^2 = -\gamma_n \alpha_n \left\{ 1 + \frac{4(\alpha_n + \gamma_n)}{(\gamma_n - \alpha_n)^2} \ln \left[\frac{(2\alpha_n + q)(2\gamma_n + q)}{(\alpha_n + \gamma_n + q)^2} \right] \right\}, \quad (12)$$

where in the last step we have used Eq. (4). For a given q , Eqs. (10) and (12) establish a closed system of recurrence relations for the energy. Even though after a few iterations this relation converges to fixed α and γ , an analytical result is obtained by making $n \rightarrow \infty$, $\gamma_n \rightarrow \gamma$, $\alpha_n \rightarrow \alpha$, and $E_n \rightarrow E$. Then,

$$\gamma = \{q + \alpha + [(q + \alpha)(5q + \alpha)]^{1/2}\} / 2, \quad (13)$$

$$\alpha = -\gamma \left\{ 1 + \frac{4(\alpha + \gamma)}{(\gamma - \alpha)^2} \ln \left[\frac{(2\alpha + q)(2\gamma + q)}{(\alpha + \gamma + q)^2} \right] \right\}, \quad (14)$$

and

$$\chi(p) = \frac{B}{(p^2 + \alpha^2)(p^2 + \gamma^2)}. \quad (15)$$

The above equations (13) and (14) yield $\alpha = \alpha(q)$ and $E = E(q)$. There are no adjustable parameters, and consequently they represent a simple, yet accurate analytical solution.

We now consider the inverse Fourier transform of Eq. (15),

$$\psi(r) = e^{-\alpha r} \left(\frac{1 - e^{-\lambda r}}{\lambda r} \right), \quad (16)$$

where $\lambda = \gamma - \alpha$ is the "screening parameter." Note that for small values of r , i.e., $\lambda r \ll 1$, the screening is not effective and $\psi(r)$ behaves as in the hydrogen atom, as expected. The screening parameter λ turns out to be as important as the effective charge α . From now on we shall use the screening parameter λ instead of γ since it has more physical meaning. For $\lambda \rightarrow 0$, i.e., $\gamma \rightarrow \alpha$, we

obtain

$$E = \frac{1}{2} \alpha^2 - \frac{4\alpha^3}{(2\alpha + q)^2}, \quad (17)$$

which reproduces the energy obtained with the wave function Eq. (3), which corresponds to first-order perturbation theory.³

In the limit $E \rightarrow 0$, Eqs. (13) and (14) yield the critical parameters

$$\alpha_c = 0, \quad (18)$$

$$\lambda_c = 4 \ln \rho = 1.924847, \quad (19)$$

and

$$q_c = \lambda_c / \rho = 1.189621. \quad (20)$$

Here $\rho = \gamma_c / q_c = (\sqrt{5} + 1) / 2$. These are very important results: The above equations give explicit analytical expressions for the critical effective charge α_c , the critical screening parameter λ_c , and the critical Thomas-Fermi wave vector q_c . Equation (18) shows that the effective nuclear charge is null for no binding energy. This makes more sense than the finite value of α obtained in the literature (see, e.g., Refs. 3 and 4, and also our Figs. 2 and 3). This is the expected trend of a Mott-type transition in a metal. The screening parameter λ has no correspondent in the literature. Finally, our q_c agrees with the best numerical value in the literature (see Table II). Whereas other authors determine q_c by numerical methods, our method has the advantage of determining q_c analytically.

In order to test our analytical result, we shall use Eq. (16) as a trial variational function with α and λ regarded now as free parameters. The ground-state energy with respect to that variational wave function is given by

$$E(\alpha, \lambda) = \frac{1}{2} \alpha(\lambda + \alpha) \left\{ 1 + \frac{4(\lambda + 2\alpha)}{\lambda^2} \ln \left[\frac{(2\alpha + q)(2\lambda + 2\alpha + q)}{(\lambda + 2\alpha + q)^2} \right] \right\}. \quad (21)$$

The energy obtained from the variational conditions is similar to that obtained by the analytical procedure. In Fig. 1 we plot the energy as a function of the Thomas-Fermi wave vector q . Curve 1 is the variational energy obtained with the $1s$ wave function [Eq. (17), plotted here as a reference]. Curve 2 is the analytical result, while curve 3 is the result of the variational calculation [Eq. (21)]. There is no discernible difference between them, in spite of the fact that there exist some differences between the α and λ computed by the two methods (see Fig. 2). In Table I we display the energy for some values of q . For $0 < q \leq 1$, our results agree with those of Rogers, Graboske, and Harwood⁶ and of Harris⁴ with an error which is far less than 1%. For $1.0 < q < q_c$, taking the variational result as standard, we see that our error in the analytical energy is less than that of Harris, in which there are three adjustable coefficients and three adjustable charges. In Fig. 2 we show the parameters α and λ as a function of q . Curve 1 shows α for the $1s$ wave function. Observe that for $E \rightarrow 0$, $\alpha = \frac{1}{2}$. Curves

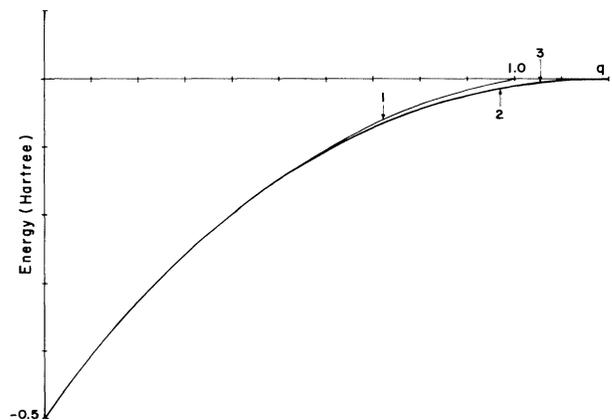


FIG. 1. Energy vs Thomas-Fermi wave vector q . Curve 1, variational hydrogenic function; curve 2, analytical result; and curve 3, variational with screening.

TABLE I. Ground-state energy (10^{-3} hartree) vs q as computed by various authors. E_{1s} : variational result with hydrogenic wave function. E_H (Harris): combination of atomic orbitals, with three adjustable coefficients and three adjustable charges; E_{RGH} (Rogers, Graboske, and Harwood): numerical integration; E_A : our analytical result; and E_V : our variational result.

Energy	E_{1s}	E_H	E_{RGH}	E_A	E_V
q					
0	500	500	500	500	500
0.1	407.5	...	407.5	407.6	407.6
0.2	326.73	...	326.8	326.80	326.81
0.25	290.75	290.92	290.9	290.91	290.92
0.5	146.51	148.12	148.1	148.07	148.11
0.8	38.471	44.70	...	44.623	44.679
1.0	0	10.225	10.285	10.217	10.261
1.05	...	5.455	...	5.4952	5.5306
1.1	...	2.115	...	2.2464	2.2715

2 and 3 are, respectively, α and λ from the analytical calculation, while curves 5 and 4 are, respectively, α and λ from the variational calculation. We notice that both curves 2 and 5 predict $\alpha_c \rightarrow 0$ as $E \rightarrow 0$. This shows that the electrons with no binding energy see a null effective nuclear charge. These results are very distinct from those obtained by combining atomic wave functions,⁴ where the effective charge never vanishes. Nevertheless, when the number of atomic orbitals is increased, the critical wave vector q_c increases while the effective charge α decreases. Hence we may expect that an infinite number of atomic orbitals might eventually produce $\alpha_c = 0$. For $q \rightarrow 0$, we see that $\alpha \rightarrow 1$, as expected, and the screening parameter $\lambda \rightarrow 0$. For small q , λ is proportional to q . In general, λ is an increasing function of q , as expected.

In the limit $E \rightarrow 0$ the variational condition together with Eq. (21) gives $\alpha_c = 0$, $\lambda_c = 1.826992$, and $q_c = 1.190213$. Even though λ_c has a difference of 5% in relation to the analytical one (given by Eq. (19)), the difference in q_c is only 0.03%. In Table II we compare our results with other authors.

The behavior of α and λ near q_c is given by

$$\alpha = \beta_1(1 - q/q_c), \quad (22)$$

and

$$\xi = 1 - \lambda/\lambda_c = \beta_2(1 - q/q_c). \quad (23)$$

TABLE II. Critical q_c for the ground state as calculated by various authors. q_S (Smith): perturbation theory; q_{SG} (Sachs and Goepfert-Mayer): numerical methods; q_{HL} (Hulthén and Laurikainen): variational; q_{LM} (Lovelace and Masson): Regge trajectories; q_{SS} (Schey and Schwartz): technique for counting the bound states as a function of q . Others as in Table I.

q_S	q_{1s}	q_{SG}	q_{HL}	q_{LM}	q_H	q_{SS}	q_{RGH}	q_A	q_V
0.998	1.0	1.1884	1.1906	1.20105	1.149	1.1905	1.1906	1.18962	1.190213

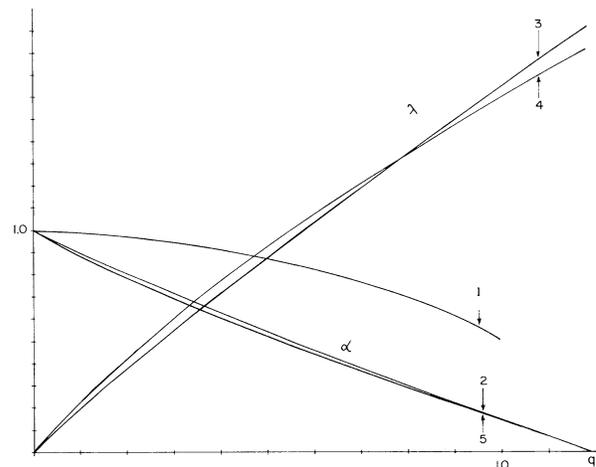


FIG. 2. The screening parameter λ and the effective charge α vs q . Curve 1, variational hydrogenic; curve 2, α analytical; curve 3, λ analytical; curve 4, λ variational; and curve 5, α variational.

Here β_1 and β_2 are numerical coefficients which can be obtained with the help of Eqs. (13) and (14) (analytical case) or from the variational condition. The coefficients are different, but the "critical behavior" follows the same law (that is not the case of the $1s$ wave function where $\alpha \rightarrow \frac{1}{2}$ when $E \rightarrow 0$). In Fig. 3 we show the behavior of α and ξ near the critical point. To our knowledge, there is not any study on the critical behavior for this problem in the literature. However, we find it very instructive to compare our analytical result with our variational calculation.

In conclusion, by using a recurrence method, we obtained an analytical expression for the ground state of a screened Yukawa potential. The recurrence relation obtained is such that the energy and wave function obtained improve at each iteration. We end up with the wave function, Eq. (16), and an analytical expression for the energy with no adjustable parameters. Conversely, by using the analytic form obtained from the iterative procedure, with α and λ now regarded as variational parameters, we have shown that the wave function obtained is a good variational one, and both results are in good agreement with the best result found in the literature. We hope this is a step in the direction of an exact solution to the problem.

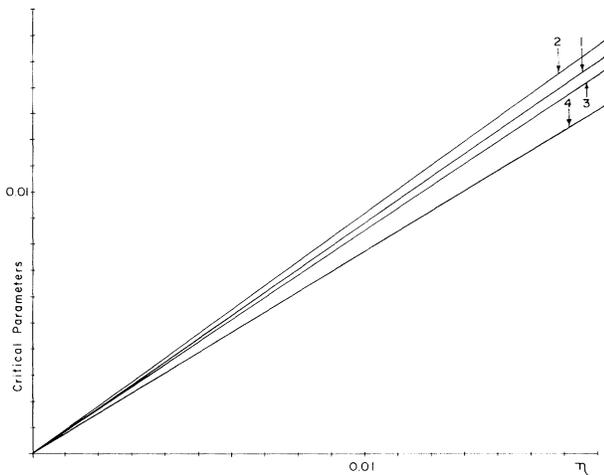


FIG. 3. Critical behavior of α and $\xi = 1 - \lambda/\lambda_c$ vs $\eta = 1 - q/q_c$. Curve 1, α analytical; curve 2, ξ analytical; curve 3, α variational; and curve 4, ξ variational.

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