

The Yukawa potential: ground state energy and critical screening

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We study the ground state energy and the critical screening parameter of the Yukawa potential in nonrelativistic quantum mechanics. After a short review of the existing literature on these quantities, we apply fifth-order perturbation theory to the calculation of the ground state energy, using the exact solutions of the Coulomb potential together with a cutoff on the principal number summations. We also perform a variational calculation of the ground state energy using a Coulomb-like radial wave function and the exact solution of the corresponding minimization condition. For not too large values of the screening parameter, close agreement is found between the perturbative and variational results. For the critical screening parameter, we devise a novel method that permits us to determine it to 10 digits. This is the most precise calculation of this quantity to date, and allows us to resolve some discrepancies between previous results.
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1. Introduction

The Yukawa potential was proposed by Yukawa in 1935 (Ref. [1]) as an effective nonrelativistic potential describing the strong interactions between nucleons. It takes the form

$$V(r) = -\alpha \frac{e^{-\mu r}}{r}, \quad (1.1)$$

and thus can be seen as a screened version of the Coulomb potential, with α describing the strength of the interaction and $1/\mu$ its range. The same potential appears under the name of the Debye–Hückel potential in plasma physics, where it represents the potential of a charged particle in a weakly nonideal plasma (Ref. [2]), as well as in electrolytes and colloids. In solid state physics it is known as the Thomas–Fermi potential, and describes the effects of a charged particle in a sea of conduction electrons.

In quantum mechanics, the physics of this potential depends strongly on the value of the screening parameter μ . While for the Coulomb case $\mu = 0$ there is an infinite number of bound states, for any positive value of μ the screening is sufficient to reduce this number to a finite one (Refs. [3–5]), and for μ larger than a certain critical value μ_c , bound states cease to exist altogether. This critical value

is proportional (Refs. [3,6–11]) to αm :

$$\mu_c \approx 1.19\alpha m. \quad (1.2)$$

Despite its superficial closeness to the Coulomb potential, the Yukawa one shares hardly any of the exceptional mathematical properties of the former. To this date, for $\mu \neq 0$ neither the energy eigenvalues, nor the eigenfunctions, nor the critical screening parameter are known in closed form. This combination of physical importance and mathematical intractability makes the Yukawa potential a natural test case for approximation methods in quantum mechanics.

The purpose of the present paper is fourfold. First, in Sect. 2 we will give an overview of the various approximation methods that have been used to date. Our emphasis here is on the ground state energy $E_0(\mu)$ and on the critical screening μ_c , since these are the quantities that we will then study ourselves in the rest of the paper. We will use the literature data to construct a literature average curve $E_0(\mu)$.

Second, in Sect. 3 we will perform a perturbative calculation of the ground state energy, taking the exactly solvable Coulomb Hamiltonian as the unperturbed one. The special properties of the Coulomb case will allow us to push this calculation to an unusual fifth order. We further improve on this calculation by including in the unperturbed Hamiltonian the contribution from the Yukawa potential that is linear in μ . We also study the dependence of the perturbative calculation for the energy on the cutoff in the principal quantum number of the Coulomb wave functions that becomes necessary starting from second order.

Third, in Sect. 4 we then compare our perturbative results with a variational calculation, using a trial function of the type of the Coulomb ground state wave function. Although this simple trial function has been used before, to the best of our knowledge the minimization condition, a third-order algebraic equation, has been solved only approximately (e.g., in the textbook [12], see problem 7.14). Here we give its exact solution, and it turns out that, remarkably, it closely matches our result from fifth-order perturbation theory in the whole range of μ except for the region close to the critical endpoint.

Fourth, in Sect. 5 we will present a novel, but simple, method to determine the critical screening parameter. We obtain for it the value

$$\frac{\mu_c}{\alpha m} = 1.190\,612\,210\,5(5), \quad (1.3)$$

which is the most precise value to date. We compare with previous results given for the screening parameter.

2. Review of the literature

A number of general theorems exist on the existence and number of bound states for a given potential. In 1951 Pais and Jost (Ref. [3]) showed that for a 3-dimensional spherical potential such that $I = 2m \int_0^\infty dr r |V(r)|$ is finite, bound states must exist for $I > 1$. One year later, Bargmann (Ref. [4]) proved that the number of bound states n_l , for a given angular momentum quantum number l , is bounded by

$$(2l + 1)n_l < I. \quad (2.1)$$

For the Yukawa potential, this relation (in our units) is $(2l+1)n_l < \frac{2m}{\mu}\alpha$. In particular, no bound state can exist for $\mu > 2m\alpha$. Inequality (2.1) was rederived and further generalized in 1960 by Schwinger (Ref. [5]).

As was mentioned in the introduction, no exact results exist to date for the wave functions and energies of the Yukawa potential. As to approximate calculations, the most widely used method has been the variational principle. In 1962, Harris (Ref. [6]) used trial wave functions constructed from the 1s, 2s, and 3s solutions of the Coulomb potential to obtain very good values for the ground state and the first 45 excited energies of the system. In 1990, Garavelli and Oliveira (Ref. [8]) applied the variational method using the 1s Coulomb solution together with a second wave function involving a screening parameter to be determined. In 1993, Gomes et al. (Ref. [9]) devised a two-step procedure where optimized few-parameter trial functions are obtained from an initial linear combination of atomic orbitals (LCAO) with up to 26 basis functions. This allowed them to obtain very precise values for $E_0(\mu)$ and μ_c , and also to demonstrate the delocalization of the ground state wave function in the bound–unbound transition, i.e., $\psi_0(r) \rightarrow 0$ for $\mu \rightarrow \mu_c$. They were also able to determine the critical exponents for $\psi_0^2(0)$ and E_0 for this transition.

Somewhat less popular in this context has been perturbation theory. The work by Harris already cited (Ref. [6]) was also the first to treat the Yukawa potential as a perturbation of the Coulomb one, although only in first-order perturbation theory. Gönül et al. (Ref. [13]) in 2006 combined the perturbative treatment with an expansion of the exponential factor $e^{-\mu r}$. In 1985, Dutt et al. (Ref. [14]) used a scaled Hulthén potential instead of the Coulomb one as the unperturbed Hamiltonian.

As to numerical approximations, in 1970, Rogers et al. (Ref. [7]) solved the Schrödinger equation numerically. For the same purpose, in 2005 Yongyao et al. (Ref. [11]) used Runge–Kutta and Numerov algorithms, as well as Monte Carlo methods.

There have also been less standard approximations to analyze the Yukawa potential. Garavelli and Oliveira (Ref. [8]) used an iterative process to solve the Schrödinger equation in momentum space. In 2012, Hamzavi et al. (Ref. [15]) used the generalized parametric Nikiforov–Uvarov method for obtaining approximate analytical solutions of the Schrödinger equation, and showed that this works well for $\mu \lesssim 0.15m\alpha$.

In Fig. 1 we show a plot of $E_0(\mu)$ obtained by averaging over the results given by various authors, based on Table I of Ref. [8] (we have not included here the results of Ref. [9], since they consider only 4 different values of μ).

The μ_c values given by a number of authors are listed in Table 1.

3. Perturbative calculation of the ground state energy

Of the many ways of finding approximate solutions to the Schrödinger equation for a system that cannot be solved exactly, probably the most widely used is perturbation theory, where one builds on the known exact solutions of some other, usually simpler system. However, the perturbative expansion becomes quickly cumbersome at higher order, so that most textbooks on quantum mechanics, e.g., Griffiths (Ref. [12]), give the explicit formulas only to second order. Exceptionally, Landau and Lifshitz (Ref. [16]) give them to third order, the fourth order is worked out in an unpublished article (N. Wheeler, *Higher-Order Spectral Perturbation, by a New Determinantal Method*, Reed College Physics Department, 2000), and Wikipedia (Ref. [17]) has the expressions for the energy levels to fifth order (for the nondegenerate case). Those expressions, whose correctness we have verified by an independent calculation, are included in Appendix for easy reference. Here we wish to apply them to the ground state energy of the Yukawa Hamiltonian, taking advantage of the fact that the Coulomb

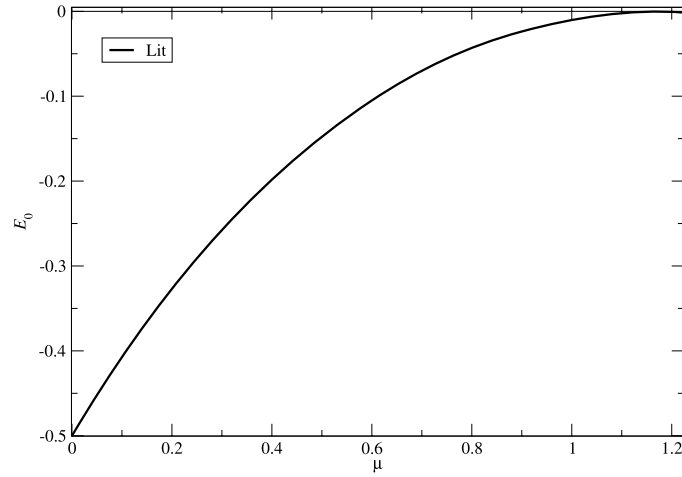


Fig. 1. A literature average of the Yukawa ground state energy $E_0(\mu)$ (for $m = \alpha = 1$).

Table 1. Comparison of (\cdot) values for different works and our results.

Study	Method ^a	Value	Study	Method ^a	Value
Harris (Ref. [6])	V	1.15	Harris (Ref. [6])	VC	1.0
Harris (Ref. [6])	P	0.828	RGH (Ref. [7])	N	1.190 607
GO (Ref. [8])	A	1.189 621	YXK (Ref. [11])	N	1.1906
GO (Ref. [8])	VC	1.0	HL (Ref. [20])		1.1906
GO (Ref. [8])	V	1.190 213	Us	VC	1.0
GCM (Ref. [9])	V	1.190 610 74	Us	P with H'_0	1.006
GCM (Ref. [9])	LCAO	1.190 612 27	Us	P with H_0	1.006

^a V=variational, VC=variational taking as trial wave function the ground state wave function of the Coulomb potential, P=perturbation theory, N=numerical, A=analytical method by Garavelli and Oliveira (Ref. [8]), LCAO=linear combination of atomic orbits by Gomes et. al. (Ref. [9]).

case is exactly solvable:

$$H_{\text{Yuk}} \equiv -\frac{1}{2m} \nabla^2 - \alpha \frac{e^{-\mu r}}{r} = \underbrace{-\frac{1}{2m} \nabla^2 - \frac{\alpha}{r}}_{H_0} + \underbrace{\frac{\alpha}{r} (1 - e^{-\mu r})}_{\Delta H}. \quad (3.1)$$

We recall that the eigenvalues of H_0 are

$$E_n = -\frac{m\alpha^2}{2} \frac{1}{n^2}, \quad (3.2)$$

with eigenfunctions

$$\psi_{nlm}(r, \theta, \phi) = \left(\left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n(n+l)!} \right)^{1/2} \exp\left(-\frac{r}{na_0}\right) \left(\frac{2r}{na_0} \right)^l L_{n-l-1}^{2l+1} \left(\frac{2r}{na_0} \right) Y_l^m(\theta, \phi), \quad (3.3)$$

where $n = 1, 2, 3, \dots$; $l = 0, 1, 2, \dots, n-1$; $m = -l, \dots, l$, and $a_0 = 1/m\alpha$ is the Bohr radius. Here $Y_l^m(\theta, \phi)$ are the spherical harmonics, and L_n^k the associated Laguerre polynomials (our convention for the latter is given in Eq. (A.6) in the Appendix and corresponds to that of MATHEMATICA). Since

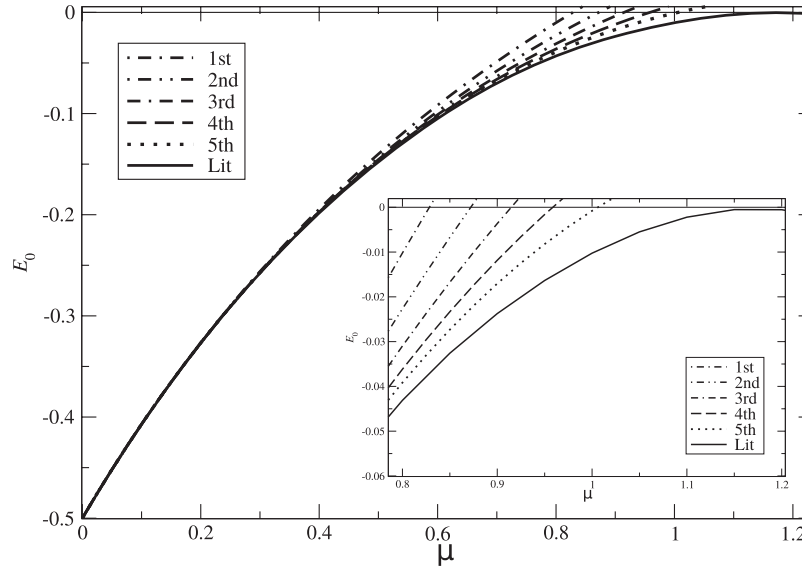


Fig. 2. The ground state energy $E_0(\mu)$ of the Yukawa Hamiltonian at various orders of perturbation theory (for $m = \alpha = 1$), with a cutoff at $n = 19$, together with the literature average curve.

both the unperturbed ground state and the perturbation ΔH are spherically symmetric, it is easily seen that the eigenstates with nonvanishing angular momentum, i.e., with $l > 0$, will not contribute to any order in the perturbative expansion. This greatly simplifies the expansion, and in particular reduces it to the nondegenerate case, so that we can use the formulas for nondegenerate perturbation theory as given in Appendix, restricting them to the spherically symmetric eigenfunctions $\psi_n \equiv \psi_{n00}$ from the beginning. They involve, apart from the energy differences $\Delta_{nm} \equiv E_n - E_m$, only the matrix elements $V_{nm} \equiv \langle \psi_n | \Delta H | \psi_m \rangle$, which we obtain in closed form in Eq. (A.8). From the second-order correction onwards the expressions involve infinite sums over the principal quantum number n , which we were unable to do in closed form. However, all these sums converge very rapidly (at least as $1/n^3$), so that a cutoff could be used on them; using C++, we were able to sum over the first 19 terms for each infinite sum.

In Fig. 2 we show a plot of the results of this calculation for the ground-state energy as a function of μ at various orders of perturbation theory (choosing $m = \alpha = 1$), together with the literature average curve obtained in the previous section. We observe that perturbation theory works well up to $\mu \simeq 0.5$ and breaks down for $\mu \gtrsim 0.8$. As one would expect, the addition of the higher-order terms delays the onset of this breakdown, but not very significantly. It is also interesting to note that, in the range where perturbation theory works, the perturbation series for fixed μ still shows apparent convergent behavior to fifth order, even though it is known that the perturbation series in quantum mechanics (as well as in quantum field theory) is generically an asymptotically divergent one (see, e.g., Ref. [18]). It would be interesting to push this calculation to even higher orders to see the onset of asymptoticity.

As a check on the cutoff that we have used for the principal number summations, let us also show in Fig. 3 the corresponding plot obtained by summing over only the first 10 terms, rather than 19, for all these sums. The plots are indistinguishable in the range of μ where perturbation theory works.

The expansion in ΔH is effectively an expansion in μ , which suggests that better results might be obtained by using the same perturbation series with a different break-up of the Yukawa Hamiltonian: instead of Eq. (3.1), let us try moving the term linear in μ contained in the Yukawa potential, which

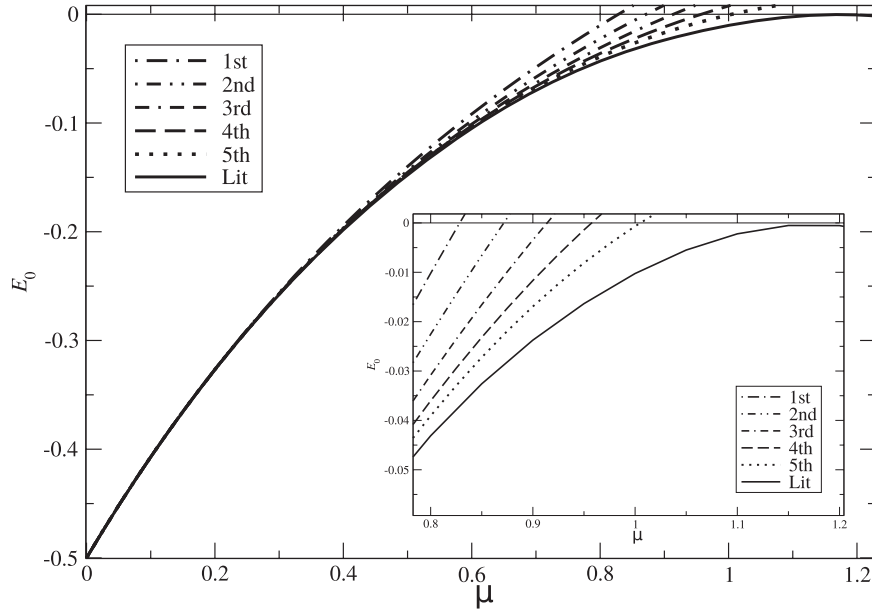


Fig. 3. The ground state energy $E_0(\mu)$ of the Yukawa Hamiltonian at various orders of perturbation theory (for $m = \alpha = 1$), with a cutoff at $n = 10$, together with the literature average curve.

corresponds to a constant term in the Hamiltonian, from ΔH to H_0 :

$$H_{\text{Yuk}} = \underbrace{-\frac{1}{2m}\nabla^2 - \frac{\alpha}{r}}_{H'_0} + \underbrace{\mu\alpha + \frac{\alpha}{r}(1 - \mu r - e^{-\mu r})}_{\Delta H'}. \quad (3.4)$$

The new H'_0 has the same eigenfunctions as H_0 and eigenvalues shifted by the constant $\mu\alpha$:

$$E'_n = -\frac{m\alpha^2}{2} \frac{1}{n^2} + \mu\alpha. \quad (3.5)$$

Redoing the perturbative calculation with this modification, up to fifth order and with the same cutoff at $n = 19$, we have obtained the results for $E_0(\mu)$ shown in Fig. 4.

Comparing with Fig. 2 we see that the new break-up does not show any improvement. An important remark is that increasing the cut-off above $n = 19$ leads to numerical instability in the fifth-order perturbation theory due to delicate cancelations between large numbers (generated by the combinatoric factorials present in the equations in the appendix). Various ad hoc modifications to the methods of calculating the summands become necessary to alleviate these problems.

4. Variational principle

For the case of the ground state energy, the variational principle provides an approximation method that is more universally applicable than perturbation theory, and often yields accurate results with relatively little effort. It states that to obtain the ground state energy of a system described by the Hamiltonian H , in the case that it is not possible to solve the Schrödinger equation exactly, then one can pick any normalized wave function ψ whatsoever and, using the spectral representation of the Hamiltonian, it is easily seen that one always has

$$E_0 \leq \langle \psi | H | \psi \rangle. \quad (4.1)$$

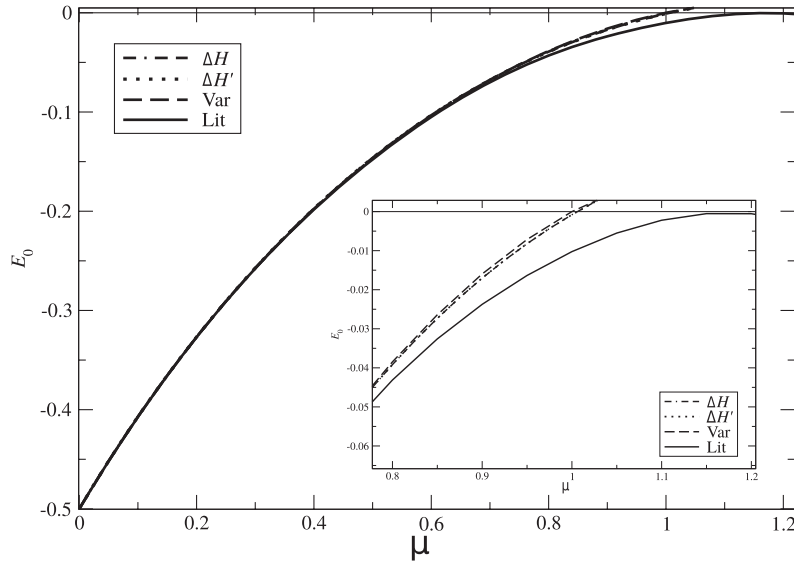


Fig. 4. The ground state energy $E_0(\mu)$ of the Yukawa Hamiltonian using H'_0 (for $m = \alpha = 1$), together with the literature average curve, with a cutoff at $n = 19$.

That is, unless ψ is the true ground state, the expectation value of H in the state ψ is certain to overestimate the ground state energy (Ref. [12]).

For the Yukawa Hamiltonian (1.1), the simplest possible choice is a trial wave function $\psi_t(r)$ that mimics the ground state wave function of the Coulomb potential, that is the ψ_{100} of Eq. (3.3):

$$\psi_t(r) \equiv \frac{1}{\sqrt{\pi b^3}} \exp\left(-\frac{r}{b}\right). \quad (4.2)$$

This wave function is normalized, and b is the variational parameter that needs to be adjusted to minimize the expectation value of the Hamiltonian (3.3). Since there is only radial dependence, the calculations are simple and lead to

$$E_t \equiv \langle \psi_t(r) | H | \psi_t(r) \rangle = \frac{1}{2mb^2} - \frac{4}{a_0 mb(2 + b\mu)^2}, \quad (4.3)$$

where we have also used the relation $\alpha = 1/(ma_0)$.

The minimization of the expression (4.3) leads to an algebraic third-order equation. Curiously, although the variational method has been applied to the Yukawa potential by a number of authors, and the trial function (4.2) was used in Ref. [12] (in problem 7.14), the exact solution of this equation does not seem to be in the literature. MATHEMATICA gives it as

$$\begin{aligned} b_0(\mu) = & \frac{1}{3a_0\mu^3} \left[-6\mu(-2 + a_0\mu) \right. \\ & + \frac{i6^{2/3}(i + \sqrt{3})\mu^2(-6 + 5a_0\mu)}{\left(-36\mu^3 + 45a_0\mu^4 - 9a_0\mu^5 + a_0\mu^4\sqrt{3}(-9 - 20a_0\mu + 27a_0\mu^2) \right)^{1/3}} \\ & \left. + 6^{1/3}(1 + i\sqrt{3}) \left(-36\mu^3 + 45a_0\mu^4 - 9a_0\mu^5 + a_0\mu^4\sqrt{3}(-9 - 20a_0\mu + 27a_0\mu^2) \right)^{1/3} \right]. \end{aligned} \quad (4.4)$$

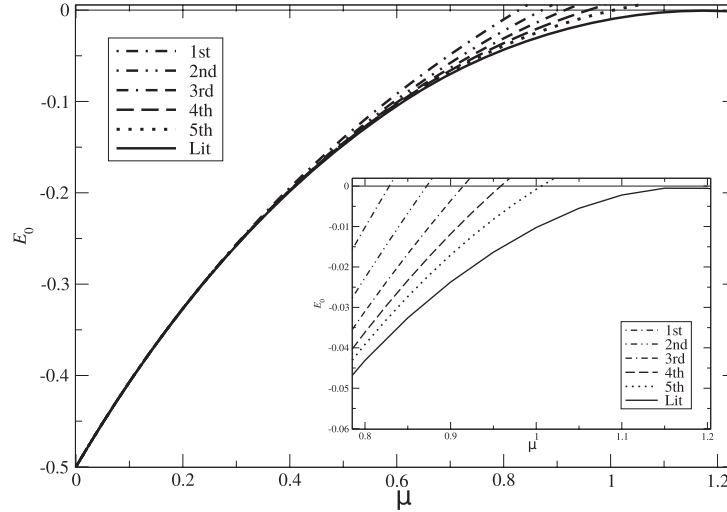


Fig. 5. Variational solution to the ground state energy of the Yukawa potential, together with the literature average curve and the fifth-order perturbative ones.

This solution is real, although it is not obviously so. The physically relevant one among the 3 solutions of the third-order equation was determined by assuming that $b_0(\mu)$ should go to the Coulomb value a_0 for $\mu \rightarrow 0$. Thus for $\mu \ll 1$ it expands out as a_0 plus perturbations in powers of μ :

$$b_0 = a_0 + \frac{3}{4}a_0^3\mu^2 - a_0^4\mu^3 + \frac{21}{8}a_0^5\mu^4 - 6a_0^6\mu^5 + \mathcal{O}(\mu^6). \quad (4.5)$$

In Fig. 5 we show the result of using Eq. (4.4) in Eq. (4.3), together with the literature average curve and the curves from both versions of fifth-order perturbation theory (the curves for H_0 and H'_0 are practically indistinguishable at the scale of the figure). Note that, for very small μ , the numerical evaluation of the variational curve becomes unstable; a smooth result can be obtained by replacing the exact $b_0(\mu)$ of Eq. (4.4) by its small μ approximation (4.5). Remarkably, the variational and the fifth-order perturbative curves are in close agreement.

5. The critical screening parameter μ_c

As we mentioned in the introduction, an important difference between the Coulomb and Yukawa cases is that, for the latter, bound states cease to exist if μ becomes larger than a critical value μ_c . Such a transition in quantum mechanics holds important information on the dynamics of the system. For example, in solid state physics the existence of bound states makes it possible to condense electrons around protons and get an insulating system, while in their absence the system is a metal (Ref. [19]). The transition between both regimes is called Mott transition. The value of $\mu_c = (\cdot)m\alpha$ is not known exactly. In Table 1 we give some values for (\cdot) found in the literature, together with the ones that follow from our approximate calculations above, determined by the intersection of the $E_0(\mu)$ curve with the $E_0 = 0$ axis.

Further, we will now present a method for the calculation of μ_c that is quite simple, but which we have not been able to find in the literature. For $\mu = \mu_c$ we have the lowest eigenvalue $E_0 = 0$ with corresponding radial Schrödinger equation

$$-\frac{1}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) \psi_0(r) - \frac{\alpha}{r} e^{-\mu r} \psi_0(r) = 0. \quad (5.1)$$

In terms of $g(r) \equiv r\psi_0(r)$, this can be written as

$$g''(r) + \alpha m \frac{2}{r} e^{-\mu r} g(r) = 0. \quad (5.2)$$

According to Eq. (1.2) the critical value μ_c is proportional to αm , so that we can also set $\alpha m = 1$. Equation (5.2) describes, for μ just below the critical value μ_c , a bound state solution, and for μ just above μ_c a scattering solution (here we neglect an infinitesimal contribution to the right-hand side of Eq. (5.2), $-2mE_0g(r)$, that is present whilst $\mu \neq \mu_c$). In either case we must have $g(0) = 0$, for regularity of the wave function at the origin, and in the bound state case also $g(\infty) = 0$, since the wave function must decrease (much) faster than $1/r$ for large r to be square integrable. This suggests (Ref. [20]) that one could distinguish between $\mu < \mu_c$ and $\mu > \mu_c$ by checking numerically whether Eq. (5.2) can be solved with the boundary conditions

$$g(0) = g(\infty) = 0. \quad (5.3)$$

However, these boundary conditions are not the most convenient ones for numerical purposes. It is thus important to observe that we can also replace them by the conditions

$$g(0) = 0, \quad g'(0) = g_1, \quad (5.4)$$

where g_1 is an arbitrary nonzero number, and check whether the numerical solution of Eq. (5.2) leads to $g(\infty) = 0$ or not. These procedures are equivalent, since the boundary conditions (5.3) are homogeneous, so that a solution of Eq. (5.2) fulfilling them can be rescaled to make $g'(0)$ take any given nonzero value g_1 (nonzero, since $g'(0) = g(0) = 0$ leads to the trivial solution $g(0) \equiv 0$). Moreover, it is easy to check the behavior of $g(r)$ at large r , since Eq. (5.2) implies that $g'(r)$ rapidly converges to a constant for large r . Thus, the critical μ_c can be found by starting with a μ somewhat below it, and then hiking it up little by little, each time solving Eq. (5.2) numerically with some arbitrary $g_1 > 0$, and checking whether the slope of $g(r)$ still becomes negative for large r , as it must for $g(r)$ to represent a bound state solution (in the bound state case, the slope of $g(r)$ ultimately must go to zero for very large r ; in an exact calculation, this would be ensured by the tiny positive contribution to the right-hand side of Eq. (5.2) that is present whilst $\mu < \mu_c$).

In Figs. 6 and 7 we show plots obtained by setting $g_1 = 1$ and using the `NDSolve` command of MATHEMATICA 10. Since $r = 0$ cannot be used in the numerical evaluation, here we have replaced the exact conditions (5.4) by the approximate ones

$$g(r_0) = g(0) + r_0 g'(0) = r_0 g_1, \quad g'(r_0) = g'(0) = g_1, \quad (5.5)$$

with $g_1 = 1$ and the small radial cutoff $r_0 = 10^{-10}$.

From these plots we conclude that $\mu_c/\alpha m$ lies between 1.190 612 210 and 1.190 612 211. This is compatible with the LCAO result of Ref. [9], $\mu = 1.190\,612\,27(4)$ (except for their last digit) and Ref. [11], but not with Refs. [7] and [8]. We have also checked that this result is stable under a further reduction of the radial cutoff r_0 .

6. Conclusions

In this paper, we have summarized the existing literature on the ground state energy E_0 and the critical screening parameter μ for the Yukawa potential, and we have performed 3 calculations that, although

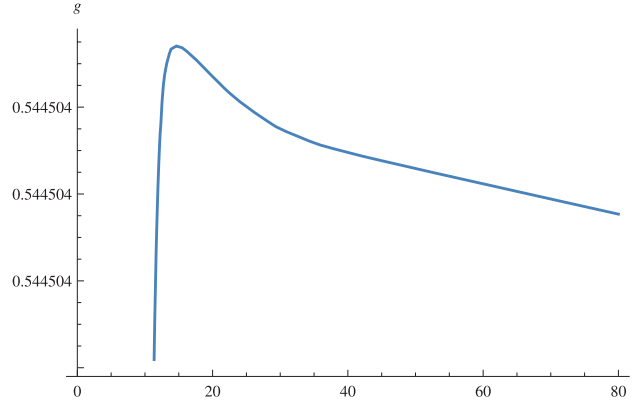


Fig. 6. MATHEMATICA plot of $g(r)$ for $\mu = 1.190\,612\,210$, just below its critical value.

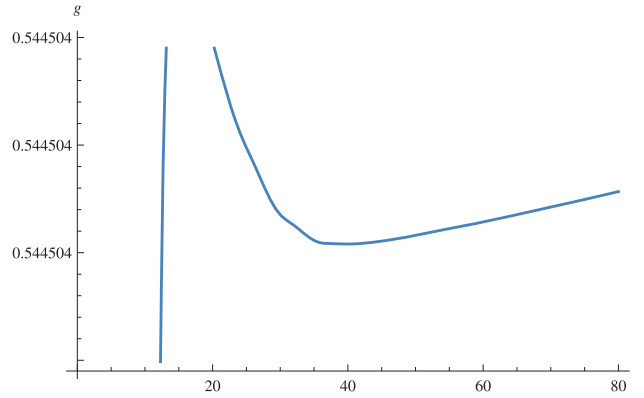


Fig. 7. MATHEMATICA plot of $g(r)$ for $\mu = 1.190\,612\,211$, just above its critical value.

straightforward, to the best of our knowledge have not been done before: (i) a fifth-order perturbative calculation of E_0 using the exact solutions of the Coulomb potential together with a cutoff on the principal number summations; (ii) a variational calculation of E_0 using a simple Coulomb-like radial wave function and the exact solution of the corresponding minimization condition, a third-order equation; (iii) a high-precision determination of μ_c by numerical integration of the radial Schrödinger equation with appropriate boundary conditions. Our main findings are the close agreement between the fifth-order perturbative result with the variational one, and a calculation of μ_c to 10 significant digits. This is one digit more than was obtained in the LCAO calculation of Ref. [9], previously the most precise determination of this parameter available in the literature, with an incomparably greater effort. Our calculation essentially confirms their value, and shows the inaccuracy of some other values found in the literature. Moreover, since our new approach essentially amounts to a form of interval bisection, its rate of convergence, being linear, is an improvement on the computational complexity of many other approaches, making it easier—and less time consuming—to increase the accuracy of our determination of μ_c to greater numbers of decimal places. The result presented here should also become useful as a benchmark for future approximative calculations. Moreover, the method proposed here for the calculation of μ_c may find generalizations to other spherically symmetric potentials.

Appendix A. Formulas needed for the fifth-order perturbation expansion

For easy reference, let us list here the expressions given in Wikipedia (Ref. [17]) for the energy level corrections up to fifth order in (nondegenerate) perturbation theory:

$$\Delta E_n^1 = V_{nn}, \quad (\text{A.1})$$

$$\Delta E_n^2 = \sum_{m \neq n} \frac{V_{nm}^2}{\Delta_{nm}}, \quad (\text{A.2})$$

$$\Delta E_n^3 = \sum_{m \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rm} V_{mn}}{\Delta_{nm} \Delta_{nr}} - V_{nn} \sum_{m \neq n} \frac{V_{nm}^2}{\Delta_{nm}^2}, \quad (\text{A.3})$$

$$\begin{aligned} \Delta E_n^4 = & \sum_{l \neq n} \sum_{m \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rm} V_{ml} V_{ln}}{\Delta_{nr} \Delta_{nm} \Delta_{nl}} - V_{nn} \sum_{l \neq n} \sum_{m \neq n} \frac{V_{nm} V_{ml} V_{ln}}{\Delta_{nm}^2 \Delta_{nl}} - V_{nn} \sum_{l \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rl} V_{ln}}{\Delta_{nr} \Delta_{nl}^2} \\ & + V_{nn}^2 \sum_{l \neq n} \frac{V_{nl}^2}{\Delta_{nl}^3} - \sum_{l \neq n} \sum_{m \neq n} \frac{V_{nm}^2 V_{nl}^2}{\Delta_{nm} \Delta_{nl}^2}, \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} \Delta E_n^5 = & \sum_{s \neq n} \sum_{l \neq n} \sum_{m \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rm} V_{ml} V_{ls} V_{sn}}{\Delta_{ns} \Delta_{nm} \Delta_{nl} \Delta_{nr}} - \sum_{s \neq n} \sum_{l \neq n} \sum_{m \neq n} \frac{V_{nm}^2 V_{nl} V_{ls} V_{sn}}{\Delta_{nm} \Delta_{nl}^2 \Delta_{ns}} \\ & - \sum_{s \neq n} \sum_{l \neq n} \sum_{r \neq n} \frac{V_{nl}^2 V_{nr} V_{rs} V_{sn}}{\Delta_{nr} \Delta_{ns}^2 \Delta_{nl}} - \sum_{s \neq n} \sum_{m \neq n} \sum_{r \neq n} \frac{V_{ns}^2 V_{nr} V_{rm} V_{mn}}{\Delta_{ns}^2 \Delta_{nm} \Delta_{nr}} \\ & - V_{nn} \sum_{s \neq n} \sum_{l \neq n} \sum_{m \neq n} \frac{V_{nm} V_{ml} V_{ls} V_{sn}}{\Delta_{nm}^2 \Delta_{nl} \Delta_{ns}} - V_{nn} \sum_{s \neq n} \sum_{l \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rl} V_{ls} V_{sn}}{\Delta_{nr} \Delta_{nl}^2 \Delta_{ns}} \\ & - V_{nn} \sum_{s \neq n} \sum_{m \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rm} V_{ms} V_{sn}}{\Delta_{nr} \Delta_{nm} \Delta_{ns}^2} + V_{nn} \sum_{s \neq n} \sum_{m \neq n} \frac{V_{nm}^2 V_{ns}^2}{\Delta_{nm}^3 \Delta_{ns}} + V_{nn} \sum_{s \neq n} \sum_{m \neq n} \frac{V_{nm}^2 V_{ns}^2}{\Delta_{nm} \Delta_{ns}^3} \\ & + V_{nn} \sum_{s \neq n} \sum_{m \neq n} \frac{V_{nm}^2 V_{ns}^2}{\Delta_{nm}^2 \Delta_{ns}^2} + V_{nn}^2 \sum_{s \neq n} \sum_{l \neq n} \frac{V_{nl} V_{ls} V_{sn}}{\Delta_{nl}^3 \Delta_{ns}} + V_{nn}^2 \sum_{s \neq n} \sum_{m \neq n} \frac{V_{nm} V_{ms} V_{sn}}{\Delta_{nm}^2 \Delta_{ns}^2} \\ & + V_{nn}^2 \sum_{s \neq n} \sum_{r \neq n} \frac{V_{nr} V_{rs} V_{sn}}{\Delta_{nr} \Delta_{ns}^3} - V_{nn}^3 \sum_{s \neq n} \frac{V_{ns}^2}{\Delta_{ns}^4}. \end{aligned} \quad (\text{A.5})$$

Here we have used the short-hand notation $V_{nm} \equiv \langle \psi_n | \Delta H | \psi_m \rangle$ and $\Delta_{nm} \equiv E_n - E_m$.

Using the formula for the associated Laguerre polynomials

$$L_n^b(x) = \sum_{i=0}^n \binom{n+b}{n-i} \frac{(-x)^i}{i!}, \quad (\text{A.6})$$

we can write

$$\psi_{n00}(r) = \frac{1}{n^2 \sqrt{n\pi a_0^3}} \exp\left(-\frac{r}{na_0}\right) \sum_{i=0}^{n-1} \binom{n}{n-1-i} \frac{1}{i!} \left(-\frac{2r}{na_0}\right)^i. \quad (\text{A.7})$$

Considering first the case of $\Delta H' = \frac{\alpha}{r}(1 - \mu r - e^{-\mu r})$, here we find

$$\begin{aligned}
 & \langle \psi_{n00} | \Delta H' | \psi_{p00} \rangle \\
 &= \frac{4\pi\alpha}{n^2 p^2 \sqrt{n p} a_0^3} \sum_{i=0}^{n-1} \sum_{j=0}^{p-1} \binom{n-1}{n-1-i} \binom{p-1}{p-1-j} \frac{1}{i!} \frac{1}{j!} \\
 & \quad \times \int_0^\infty dr r \exp\left(-\frac{r}{na_0}\right) \exp\left(-\frac{r}{pa_0}\right) (1 - e^{-\mu r} - \mu r) \left(-\frac{2r}{na_0}\right)^i \left(-\frac{2r}{pa_0}\right)^j \\
 &= \frac{4\alpha}{n^2 p^2 \sqrt{n p} a_0^3} \sum_{i=0}^{n-1} \sum_{j=0}^{p-1} \binom{n}{n-1-i} \binom{p}{p-1-j} \frac{1}{i!} \frac{1}{j!} \left(-\frac{2}{na_0}\right)^i \left(-\frac{2}{pa_0}\right)^j \\
 & \quad \times \int_0^\infty dr r^{i+j+1} \left[\exp\left(-r\left(\frac{1}{na_0} + \frac{1}{pa_0}\right)\right) - \exp\left(-r\left(\frac{1}{na_0} + \frac{1}{pa_0} + \mu\right)\right) \right. \\
 & \quad \left. - \mu r \exp\left(-r\left(\frac{1}{na_0} + \frac{1}{pa_0}\right)\right) \right] \\
 &= \frac{4\alpha}{n^2 p^2 \sqrt{n p} a_0^3} \sum_{i=0}^{n-1} \sum_{j=0}^{p-1} \binom{n}{n-1-i} \binom{p}{p-1-j} \left(-\frac{2}{na_0}\right)^i \left(-\frac{2}{pa_0}\right)^j \frac{(i+j+1)!}{i!j!} \\
 & \quad \times \left[\frac{1}{\left(\frac{1}{na_0} + \frac{1}{pa_0}\right)^{i+j+2}} - \frac{1}{\left(\frac{1}{na_0} + \frac{1}{pa_0} + \mu\right)^{i+j+2}} - \mu(i+j+2) \frac{1}{\left(\frac{1}{na_0} + \frac{1}{pa_0}\right)^{i+j+3}} \right] \\
 &= \frac{4m\alpha^2}{\sqrt{n p}} \sum_{i=0}^{n-1} \sum_{j=0}^{p-1} \binom{n}{n-1-i} \binom{p}{p-1-j} \frac{(i+j+1)!}{i!j!} \left[\frac{1}{(p+n)^2} \left(\frac{-2p}{p+n}\right)^i \left(\frac{-2n}{p+n}\right)^j \right. \\
 & \quad - \frac{m^2\alpha^2}{[(p+n)m\alpha + pn\mu]^2} \left(\frac{-2pm\alpha}{(p+n)m\alpha + pn\mu}\right)^i \left(\frac{-2nm\alpha}{(p+n)m\alpha + pn\mu}\right)^j \\
 & \quad \left. - \frac{\mu}{m\alpha} \frac{np}{(p+n)^3} (i+j+2) \left(\frac{-2p}{p+n}\right)^i \left(\frac{-2n}{p+n}\right)^j \right], \tag{A.8}
 \end{aligned}$$

where in particular cases the sums over i and j can be calculated in closed form:

$$\langle \psi_{100} | \Delta H' | \psi_{100} \rangle = -\frac{\mu^2\alpha(3m\alpha + \mu)}{(2m\alpha + \mu)^2}, \tag{A.9}$$

$$\begin{aligned}
 \langle \psi_{n00} | \Delta H' | \psi_{100} \rangle &= 4m\alpha^2 \frac{\sqrt{n}}{(n+1)^2} \left[\left(\frac{n-1}{n+1}\right)^{n-1} \right. \\
 & \quad \left. - \left(\frac{(n+1)m\alpha}{(n+1)m\alpha + n\mu}\right)^2 \left(\frac{(n-1)m\alpha + n\mu}{(n+1)m\alpha + n\mu}\right)^{n-1} + n(n+1)^2 \frac{\mu}{8m\alpha} s(n) \right], \tag{A.10}
 \end{aligned}$$

where

$$s(n) \equiv \begin{cases} -2, & n = 1, \\ 0, & n > 1. \end{cases} \tag{A.11}$$

With these expressions in hand, the corrections to any order to the ground state energy could be calculated in principle. The remaining task is to deal with the infinite sums.

To get the respective expressions for $\Delta H = \frac{\alpha}{r}(1 - e^{-\mu r})$, we just have to ignore the last term in the square brackets in Eq. (A.8). The particular cases (A.9), (A.10) become

$$\langle \psi_{100} | \Delta H | \psi_{100} \rangle = m\mu\alpha^2 \left[\frac{4m\alpha + \mu}{(2m\alpha + \mu)^2} \right], \quad (\text{A.12})$$

$$\begin{aligned} \langle \psi_{n00} | \Delta H | \psi_{100} \rangle &= 4m\alpha^2 \frac{\sqrt{n}}{(n+1)^2} \\ &\times \left[\left(\frac{n-1}{n+1} \right)^{n-1} - \left(\frac{(n+1)m\alpha}{(n+1)m\alpha + n\mu} \right)^2 \left(\frac{(n-1)m\alpha + n\mu}{(n+1)m\alpha + n\mu} \right)^{n-1} \right]. \end{aligned} \quad (\text{A.13})$$

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