Complete analytical solution to the quantum Yukawa potential

M. Napsuciale(1), S. Rodríguez(2)

(1) Departamento de Física, Universidad de Guanajuato, Lomas del Campestre 103, Fraccionamiento Lomas del Campestre, León, Guanajuato, México, 37150, and  
(2) Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Coahuila, Edificio A, Unidad Campusol, 25000, Saltillo, Coahuila, México.

We present a complete analytical solution to the quantum problem of a particle in the Yukawa potential, using supersymmetry and a systematic expansion of the corresponding super-potentials.

The Yukawa potential, given by
\begin{equation}
V(r) = -\alpha \frac{e^{-r/D}}{r}, \quad (1)
\end{equation}
was proposed in Ref. [1] by H. Yukawa as an effective non-relativistic description of the strong interactions between nucleons. It appears in many areas in physics and chemistry like atomic physics, plasma physics, electrolytes, colloids, and solid state physics. It is known as Debye-Hückel potential in plasma physics, Thomas-Fermi potential in solid state physics or generically as screened Coulomb potential.

The quantum Yukawa potential has a long history, in spite of which, to the best of our knowledge, there is no complete analytical solution, either in closed form or as a perturbative expansion. It is well known that for a finite screening there is a finite number of bound states [6] [8]. The corresponding energy levels depend on the value of the screening distance \( D \), and approximate calculations for some of them are available in the literature, based on variational methods at different sophistication levels [9] [10] [11].

More recently, Yukawa potential has regained interest as a possibility to solve the problem of the core-cusp problem of dark matter density profiles. The formation of darkonium is possible for some gauge interactions like the Hulén potential [15] or closely related potentials like the logarithmic perturbation theory [18] or closely related potentials like the Hulén potential [15] or closely related potentials like the logarithmic perturbation theory [18] and other methods [20] [21] [22] [23] [24] [25] [26].

The intractability of the Yukawa potential and its importance in different fields of physics triggered the numerical studies of this problem [37] [38] [39], which shows that Coulomb degeneracy is broken and for a given \( n \), states with higher \( l \) have a higher energy than lower \( l \) states. At some point, there is a crossing of levels i.e., states of a given \( n \) have a higher energy than states with \( n + 1 \). The critical screening values (those for which a given state goes to the continuous) have been also estimated numerically solving the Yukawa potential for \( n = 0 \) to \( n = 9 \) [37].

In this work, we present a complete analytical solution to the quantum Yukawa problem. The solution is based on the hidden supersymmetry (SUSY) of this potential and on a perturbative expansion of the superpotentials.

The radial Schrodinger equation for a particle of mass \( m \) in the Yukawa potential can be reduced to
\begin{equation}
H_l u_l = \left[ -\frac{d^2}{dx^2} + v_l(x) \right] u_l(x) = \epsilon_l u_l, \quad (2)
\end{equation}
with the effective potential
\begin{equation}
v_l(x) = \frac{l(l+1)}{x^2} - \frac{2}{x} e^{-\delta x}, \quad (3)
\end{equation}
where \( x = r/a_0 \) and \( \delta = a_0/D \), with \( a_0 = \frac{\hbar}{m c} \) standing for the Bohr radius. The energy levels are given by
\begin{equation}
E_l = \frac{1}{2} \mu c^2 \alpha^2 \epsilon_l. \quad (4)
\end{equation}
where \( \mu \) is the reduced mass of the system. We factorize the Yukawa Hamiltonian as
\begin{equation}
H_l = a_l a_l^\dagger + C(l, \delta), \quad (5)
\end{equation}
where
\begin{equation}
a_l = -\frac{d}{dx} + W_l(x), \quad a_l^\dagger = \frac{d}{dx} + W_l(x). \quad (6)
\end{equation}
The superpotential \( W_l \) must satisfy
\begin{equation}
W_l^2(x, \delta) - W_l'(x, \delta) + C(l, \delta) = \frac{l(l+1)}{x^2} - \frac{2}{x} e^{-\delta x}. \quad (7)
\end{equation}
If we succeed in solving the Ricatti equation (7) we also generate a factorization for the partner Hamiltonian defined as
\begin{equation}
\tilde{H}_l = a_l^\dagger a_l + C(l, \delta) = -\frac{d^2}{dx^2} + \tilde{v}_l(x). \quad (8)
\end{equation}
where
\begin{equation}
\tilde{v}_l(x) = W_l^2(x) + W_l'(x) + C(l, \delta) = v_l(x) + 2W_l'(x). \quad (9)
\end{equation}
The two-component Hamiltonian
\begin{equation}
H = \begin{pmatrix} a_l^\dagger a_l & 0 \\ 0 & a_l a_l^\dagger \end{pmatrix}, \quad (10)
\end{equation}
can be written in terms of the charges
\[ Q_1 = \begin{pmatrix} 0 & -ia_l \\ ia_l & 0 \end{pmatrix}, \quad Q_2 = \begin{pmatrix} 0 & a_l \\ a_l & 0 \end{pmatrix}. \] (11)

These operators satisfy the N = 2 supersymmetry algebra \[ \{Q_i, Q_j\} = 2\delta_{ij}H, \quad [Q_i, H] = 0. \] (12)

Explicitly, the Hamiltonian is given by
\[ H = \left( -\frac{d^2}{dx^2} + U_+ (x, l) \right) \begin{pmatrix} 0 & 0 \\ 0 & -\frac{d^2}{dx^2} + U_- (x, l) \end{pmatrix}, \] (13)

with the associated potentials
\[ U_{\pm} (x, l) = W_2 (x) \pm W_l (x). \] (14)

Expanding the effective potential in powers of \( \delta \) we get
\[ W_l^2 (x, \delta) - W_l (x, \delta) + C(l, \delta) = \frac{l(l + 1)}{x^2} - \frac{2}{x} + 2\delta - \delta^2 x + 1 - \frac{5}{3} \delta^3 x^2 + .... \] (15)

The expansion on the right hand side (r.h.s.) of this equation is also an expansion in powers of \( \delta \). The \( \delta \)-independent terms correspond to the Coulomb potential. The \( O(\delta^0) \) term on the r.h.s. is \( O(x^{n-1}) \). Working to \( O(\delta^n) \), we find polynomial solution in \( x \) for the \( \delta \)-dependent part of \( W_l (x, \delta) \), with the advantage that powers of \( \delta \) and \( x \) are correlated. The general solution can be written as
\[ W_l (x, \delta) = w_c (x, l) + a_1 \delta + (a_2 \delta^2 + a_3 \delta^3 + a_4 \delta^4 + ..) x \\
+ (b_1 \delta^4 + b_1 \delta^5 + b_2 \delta^6 + ...) x^2 \\
+ (c_1 \delta^6 + c_6 \delta^7 + c_6 \delta^8 + ...) x^3 + .... \] (16)

\[ C(l, \delta) = c(l) + y_1 (l) \delta + y_2 (l) \delta^2 + y_3 (l) \delta^3 + .... \] (17)

Here, \( w_c (x, l) \) is the \( \delta \)-independent part which corresponds to the Coulomb problem. The coefficients required to a given order in \( \delta \), can be fixed matching powers of \( x \) on both sides of this equation.

We find that to \( O(\delta^2) \), Yukawa problem is factorizable in the sense of Ref. [32]. A family \( \{ H^0 (l) \equiv H_l, H_1^1, H_2^2, .., H_l^l \} \) of SUSY Hamiltonians with “shape invariant” potentials as described in [33] can be built and the spectrum can be straightforwardly obtained as
\[ \epsilon_{r,l} = - \frac{1}{(l + r + 1)^2} + 2\delta \]
\[ - [(l + 1)(l + 3/2) + 3r(r + 2(l + 1))] \delta^2, \] (18)

which when written in terms of the principal quantum number \( n = l + r + 1 \) reads
\[ \epsilon_{n,l} = - \frac{1}{n^2} + 2\delta - \frac{1}{2} [3n^2 - l(l + 1)] \delta^2. \] (19)

The angular momentum quantum number takes the values \( l = n - 1, n - 2, .., 0 \). The eigenstate \( u_{n,n-1} (x) \) satisfies \( \delta_{l-1} \, u_{n,n-1} = 0 \), a condition that can be used to obtain its explicit form as
\[ u_{n,n-1} (x, \delta) = N_{n,n-1} e^{-\int W_{n-1} (x, \delta) dx} \\
= N_{n,n-1} x^ne^{-\delta/2 + \frac{1}{4} \delta \delta^2 x^2}. \] (20)

States with lower values of \( l \) can be obtained iteratively with the aid of the operator \( a_l \)
\[ u_{n, n-k} (x) = N_{n, n-k} a_n a_{n-k} u_{n, n-k+1}, \] (21)

where \( N_{n, n-k} \) are \( \delta \)-dependent normalization factors.

To \( O(\delta^3) \) and beyond we loose shape invariance. However, SUSY is still there and can be used to solve the problem. First, we expect the condition \( \delta_{l-1} \, u_{n,n-1} = 0 \) to be satisfied, which yields
\[ u_{n,n-1} (x, \delta) = N_{n,n-1} e^{-\int W_{n-1} (x, \delta) dx} \\
= N_{n,n-1} x^ne^{-\delta/2 + \frac{1}{4} \delta \delta^2 x^2}. \] (22)

Using this function in Eq. (2) we can check that it is indeed an eigenfunction with eigenvalue
\[ \epsilon_{n,n-1} = - \frac{1}{n^2} + 2\delta - n(n + 1) \delta^2 \\
+ \frac{1}{3} n^2 (n + 1)(n + 1) \delta^3. \] (23)

Since \( H_l \) and \( H_{l-1} \) are not longer connected by SUSY, states with lower \( l \) cannot be obtained simply applying the lowering operator \( a_l \). In order to surmount this difficulty, we solve the SUSY partner
\[ \tilde{H}_l = \tilde{H}_l^{(1)} \equiv a_l^{(1)} a_{l-1} + C(l, \delta) = -\frac{d^2}{dx^2} + \tilde{V}_l^{(1)} (x), \] (24)

following the same procedure used to solve \( H_l \) for \( l = n - 1 \). First we re-factorize \( \tilde{H}_l^{(1)} \) as
\[ \tilde{H}_l^{(1)} = \tilde{a}_l^{(1)} (\tilde{a}_l^{(1)})^\dagger + \tilde{C}^{(1)} (l, \delta), \] (25)

where
\[ \tilde{a}_l^{(1)} = - \frac{d}{dx} + \tilde{W}_l^{(1)} (x), \quad (\tilde{a}_l^{(1)})^\dagger = \frac{d}{dx} + \tilde{W}_l^{(1)} (x). \] (26)

The new superpotential \( \tilde{W}_l^{(1)} (x) \) must satisfy an equation similar to Eq. (15), but with \( \tilde{V}_l^{(1)} \) on the right hand side. Solving this equation we obtain the solution of this potential for \( l = n - 2 \) as
\[ \tilde{u}_{n,n-2}^{(1)} (x) = e^{\int \tilde{W}_{n-2}^{(1)} (x) dx} x^n e^{-\delta/2} \\
\times e^{\frac{1}{4} \delta \delta^2 x^2 - \frac{1}{4} n^2 \delta \delta^2 x^2 - \frac{1}{4} n \delta^2 x^2}. \] (27)

The corresponding energy is
\[ \epsilon_{n,n-2} = - \frac{1}{n^2} + 2\delta - (n - 1) \delta^2 \\
+ \frac{1}{3} (n - 1) n^2 (n + 3) \delta^3. \] (28)
Now we can find the eigenstate of $H_l$ for $l = n - 2$ using the SUSY connection and the double factorization

$$\hat{H}_{n-2}^{(1)} = a_{n-2}^{(1)}(\hat{a}_{n-2}^{(1)})^\dagger + \delta C(n-2, \delta),$$

$$= a_{n-2}^{(1)}(\hat{a}_{n-2}^{(1)})^\dagger + C(n-2, \delta). \quad (29)$$

The state $\hat{a}_{n-2}^{(1)}(x)$ satisfy

$$[a_{n-2}^{(1)}, C(n-2, \delta)]\hat{u}_{n-2}^{(1)} = \hat{\epsilon}_{n, n-2}^{(1)} \hat{u}_{n-2}^{(1)}. \quad (30)$$

Acting on the last equation with $a_{n-2}$ we realize that

$$u_{n, n-2} = N_{n, n-2} a_{n-2} \hat{u}_{n, n-2}^{(1)} \quad (31)$$

is an eigenstate of $H_l$ with eigenvalue

$$\epsilon_{n, n-2} = \hat{\epsilon}_{n, n-2}. \quad (32)$$

Eigenstates and eigenvalues for $l = n - 3$ can be calculated applying now this procedure to $\hat{H}_l^{(1)}$. Continuing this process we will eventually reach the lowest $l = 0$ level, completely solving the Yukawa problem to order $O(\delta^3)$. The complete set of eigenvalues to $O(\delta^3)$ is given by

$$\epsilon_{n,l}(\delta) = -\frac{1}{n^2} + 2\delta - \frac{1}{2}[5n^2 - l(l + 1)]\delta^2$$

$$+ \frac{n^2}{6}(5n^2 + 1 - 3l(l + 1))\delta^3. \quad (33)$$

The algorithm used to order $\delta^3$ can be applied to any order of the expansion of the Yukawa potential. We find that the energy levels depend in general of $n^2$ and $L^2 = l(l + 1)$ and can be written as

$$\epsilon_{n,l}(\delta) = \sum_{k=0}^{\infty} \epsilon_k(n^2, L^2)\delta^k. \quad (34)$$

The coefficient $\epsilon_k(n^2, L^2)$ for $k = 0, 1, 2, 3$ are given in Eq. (33). The next four coefficients in the series are

$$\epsilon_4(a, b) = -\frac{a}{96}(77a^2 + 55a - 30ab - 15b^2 - 6b),$$

$$\epsilon_5(a, b) = \frac{a^2}{160}(171a^2 + 245a - 70ab - 45b^2 - 50b + 4),$$

$$\epsilon_6(a, b) = \frac{a^2}{2880}(4763a^3 - 2070a^2b + 11580a^2 - 945ab^2 - 2940ab + 1057a - 340b^3 - 205b^2 - 306),$$

$$\epsilon_7(a, b) = \frac{a^3}{8064}(22763a^3 - 10857a^2b + 84700a^2 - 4095ab^2 - 26145ab + 19677a - 2163b^3 - 3843b^2 - 2058b + 36). \quad (35)$$

One of the most important physical parameters of the Yukawa potential for practical applications is the ground state critical screening $\delta_{10}$. The numerical solution to the Yukawa problem yields $\delta_{10} = 1.1906 \pm 0.0002$, a value in the large $\delta$ region. The calculation of this observable requires us the compute of a large number of terms for $\epsilon_{n, m}$. We find that the corresponding series is not convergent and the same happens for the series of all $\epsilon_{n, m}$.

The appearance of divergent Taylor series is an old problem in quantum mechanics and quantum field theory [43 45 46 47 48], and several methods are available to sum them up [49]. We choose to work with the Padé approximants method [50], which is by now a standard technique to analytically continue Taylor series beyond their convergence radii. For the series in Eq. (34), to a given order $k = M + N$ we can always find a rational function

$$[N/M](\delta) = \frac{P_N(\delta)}{Q_M(\delta)}, \quad (36)$$

where $P_N(\delta)$ and $Q_M(\delta)$ are polynomials of order $N$ and $M$ respectively, such that its Taylor expansion coincides with the Taylor expansion of $\epsilon_{n, m}(\delta)$ to order $k = M + N$. The coefficients of these polynomials are fixed by the coefficients $\epsilon_k(n^2, L^2)$. Beyond the order $k = M + N$, the actual value of the series is bounded from above and below by the values of the $[(N + 1)/N]$ and $[N/N]$ approximants respectively [49]. The required precision in the determination of the energy levels dictates the order $k = 2N + 1$ at which is necessary to calculate the Taylor series. A calculation with $N = 10$ yields the energy levels $\epsilon_{n, m}$ with a precision of the order of $10^{-7}$ near the critical screening and higher precision in the small $\delta$ region. Results based on the numerical solution in [37] are improved in several figures at this stage.

The most difficult task is the precise determination of the ground state critical screening because of the form of the curves for the $[(N + 1)/N]$ and $[N/N]$ approximants in the critical region shown in Fig. 1. Using $N = 35$ (meaning a calculation of the ground state to order $\delta^{71}$) we obtained the value

$$\delta_{10} = 1.19061242(2). \quad (37)$$

Another important parameter of the quantum Yukawa potential is the value of the wavefunction at the origin. It appears in the calculation of the decay rates of the Yukawa bound states determining the corresponding linewidths. In our formalism it can be confidently calculated since the $r = 0$ limit is well behaved. Using the expansion to order $\delta^3$ is enough for this purpose. For the ground state, the wave function at this order is given by

$$\psi_{10}(r) = \frac{e^{-x + \frac{1}{2}x^2(3 + 2\delta) - \frac{1}{4}\pi^2x^3}}{\sqrt{\pi a_0^3(1 + \frac{3}{2}\delta^2 - \frac{1}{6}\delta^3)}}, \quad (38)$$

where $x = r/a_0$, such that at the origin, to order $\delta^3$, its square has the value

$$|\psi_{10}(0)|^2 = \frac{1}{a_0^3(1 - \frac{3}{2}\delta^2 + \frac{11}{6}\delta^3)}. \quad (39)$$
Comparing this result with estimates from variational calculations in [16][34], we see that variational techniques yield the right sign in the corrections to the Coulomb result but, to order $\delta^3$, screening effects in this observable are underestimated by a factor $\pi^4/432$.

Details of the calculations and a thorough study of the phenomenology of the Yukawa potential based on the present solution will be published elsewhere.

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