

Supplementary Material: Comments on “Non-relativistic treatment of a generalized inverse quadratic Yukawa potential”

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In the article titled “Non-relativistic treatment of a generalized inverse quadratic Yukawa potential”,^[1] Oluwadare and Oyewumi examine the conventional Schrödinger wave equation with a new potential energy form given as their Eq. (6) and introduced by their Ref. [37] (Ikhdaïr, Hamzavi and Falaye^[2]):

$$V(r) = -V_0(1 + e^{-\alpha r}/r)^2 \quad (1)$$

$$= -(A'e^{-2\alpha r}/r^2) - (B'e^{-\alpha r}/r) - C', \quad (2)$$

$$A' = C' = V_0, \quad B' = 2V_0. \quad (3)$$

A basic principle of physics is that dimensional consistency is always required,^[3] dimensional inconsistency is a *sufficient* condition for an equation to be *incorrect*. Equation (1) cannot be valid for dimensional reasons as follows. The variable r is radial distance from the origin. This is clear from Eq. (7) of Ref. [1] which is the usual radial Schrödinger equation in conventional form; additionally, the screening parameter α is stated in units of fm^{-1} several times later in the article,^[1] and the exponent product αr must be dimensionless. Therefore, in the parenthesis of Eq. (1) above, the first term is unity and so is clearly dimensionless, yet the second term has dimensions $1/[\text{L}]$ (inverse length) which fundamentally cannot be added to a dimensionless quantity. Similarly, while C' is equal to V_0 and has dimensions of energy or $[\text{W}]$, A' must have dimensions of $[\text{W}][\text{L}]^2$ and so A' cannot equal C' as stated in Eq. (3). Additionally, B' must have dimensions of $[\text{W}][\text{L}]$ and therefore cannot equal $2V_0$ as stated. Equation (1) and the constitutive relations of Eq. (3) should be ignored entirely; the definitive statement of the potential energy form used is Eq. (2) above. Alternatively, the original potential energy form may be written as

$$V(r) = -V_0(W + e^{-\alpha r}/r)^2 \quad (4)$$

where V_0 has dimensions of $[\text{W}][\text{L}]^2$, and W is a constant (an inverse length), with constitutive relations

$$A' = V_0, \quad B' = 2V_0W, \quad C' = V_0W^2. \quad (5)$$

The presentation of this potential energy form by Ikhdaïr, Hamzavi and Falaye^[2] is erroneous for exactly the same reason; the subsequent development in their article appears to be mostly correct although some amendments are necessary.^[4]

Subsequently, while A' , B' , and C' appear correctly in Eq. (9) of Ref. [1], Oluwadare and Oyewumi then introduce in Eq. (11) of Ref. [1] a new dimensionless variable $y = 1/(e^{2\alpha r} - 1)$ and the Pekeris approximation for small r :

$$\frac{e^{-\alpha r}}{r} \approx \frac{e^{-\alpha r}}{\sinh(\alpha r)/\alpha} = \frac{2\alpha e^{-2\alpha r}}{1 - e^{-2\alpha r}} = 2\alpha y. \quad (6)$$

After writing $V_{\text{eff}}(y) = V(r) + l(l+1)\hbar^2/2\mu r^2 = P + Qy + Ry^2$, equating the coefficients of powers of y relates the new parameters P , Q , and R to the original parameters A' , B' , and C' . Ref. [1] gives P and Q

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correctly in its Eq. (12). However, the expression given^[1] for R is incorrect (as is immediately clear from dimensional analysis). The correct expression for R is readily obtained as

$$R = 4\alpha^2 l(l+1)\hbar^2 / 2\mu - 4\alpha^2 A'. \quad (7)$$

In transforming the radial Schrödinger equation to the new variable y , it is necessary to transform also the second derivative according to

$$\frac{d^2}{dr^2} = \frac{d}{dr} \left(\frac{d}{dr} \right) = \frac{d}{dr} \left(\frac{dy}{dr} \cdot \frac{d}{dy} \right) = \left(\frac{dy}{dr} \right)^2 \frac{d^2}{dy^2} + \frac{d^2 y}{dr^2} \cdot \frac{d}{dy} \quad (8)$$

so that the transformed radial Schrödinger equation for wave function $U(y)$ is:

$$\left(\frac{dy}{dr} \right)^2 \frac{d^2 U(y)}{dy^2} + \frac{d^2 y}{dr^2} \cdot \frac{dU(y)}{dy} + \frac{2\mu}{\hbar^2} (E - V_{\text{eff}}(y)) U(y) = 0 \quad (9)$$

or

$$\frac{d^2 U(y)}{dy^2} + \frac{2y+1}{y(y+1)} \cdot \frac{dU(y)}{dy} + \frac{2\mu}{\hbar^2} \cdot \frac{E - P - Qy - Ry^2}{4\alpha^2 y^2 (y+1)^2} U(y) = 0. \quad (10)$$

This equation corresponds to Eq. (11) of Ref. [1] but it is corrected here by the insertion of the entire first-derivative term and the factor arising from the reciprocal squared differential in the third term (as originally written, Eq. (11) of Ref. [1] is not dimensionally consistent).

Next, Oluwadare and Oyewumi^[1] calculate the positions y_A and y_B of the inflection points of the wave function $U(y)$ (the outer turning points or extreme positions of the corresponding classical motion, though *not* analytic turning points of the wave function), defined by $d^2U(r)/dr^2 = 0$, by equating $(E - V_{\text{eff}}(y))$ to 0. Then they calculate the local wavenumber k (strictly not momentum $\hbar k$ as stated) using

$$k^2 = \left(-i \frac{d}{dx} \right)^2 = \left(-i \frac{d}{dr} \right)^2 = -\frac{d^2}{dr^2} = \frac{2\mu}{\hbar^2} (E - V_{\text{eff}}(y)) = \frac{2\mu}{\hbar^2} (E - P - Qy - Ry^2) \quad (11)$$

giving

$$k = \sqrt{\frac{2\mu R}{\hbar^2}} (y - y_A)^{1/2} (y_B - y)^{1/2}, \quad (12)$$

which corresponds to Eq. (15) of Ref. [1] *except* that the exponents are corrected here.

Oluwadare and Oyewumi^[1] now introduce variable $\phi(y)$ in Eq. (16) of Ref. [1], which is a recast version of Eq. (7) of Ref. [1], but they do not define ϕ in terms of previously defined or otherwise well-known quantities; it is not clear how they transform their Eq. (7)^[1] to their Eq. (16)^[1] or what is the relation between $\phi(y)$ and the wave function $U(r)$. One possibility presumably^[5] is $\phi = -2\alpha y(y+1)(dU/dy)/U$, as this is the solution to the Riccati equation that is homomorphic to Eq. (10):

$$\frac{d\phi}{dy} = \frac{2\mu}{\hbar^2} \cdot \frac{E - P - Qy - Ry^2}{2\alpha y(y+1)} + \frac{\phi^2}{2\alpha y(y+1)} \quad (13)$$

which may be rewritten as Eq. (16) of Ref. [1]. This equation must be solved to find $\phi(y)$ valid for all values of y . Oluwadare and Oyewumi propose $\phi_0 = A + By$ as a *trial solution* (but note that A and B here are *not* the same variables that appear in their Eqs. (1), (2) and (5)). They substitute this trial solution into their Eq. (16) which reduces to a quadratic equation in y (Eq. (17) of Ref. [1]) that must be valid for *all* values of y . The only way to satisfy this condition is for the coefficients of *each* power of y independently

to be equal on both sides of the equation. To this end, they equate the corresponding coefficients of y^0 and separately those of y^2 from their Eq. (17), yielding respectively their expressions for A and B (their Eq. (18)). However, their selection of y^0 and y^2 is a completely arbitrary choice that ignores the coefficients of y^1 , requiring that A and B satisfy also

$$(A - \alpha)B = \frac{\mu Q}{\hbar^2} \quad (14)$$

which the specified values^[1] of A and B do not (Q is quadratic in l and is independent of P and R that determine the specified values^[1] of A and B ; also B has higher-order dependence upon l). There is no *a priori* reason not to choose, for example, the equations from y^0 and y^1 , which give A as in Ref. [1] but the different value $B = \frac{\mu Q / \hbar}{\pm \sqrt{2\mu(P - E) - \alpha\hbar}}$. Or, the different value $A = \alpha + \frac{\mu Q / \hbar}{\alpha\hbar \pm \sqrt{\alpha^2\hbar^2 + 2\mu R}}$ with B as in

Ref. [1] are given if the equations from y^1 and y^2 are arbitrarily chosen instead. The fundamental point is that *the solution to a well-posed problem cannot depend upon the method used to solve it.*

The underlying reason for these differences in the expressions for A and B is that the suggested trial solution is unsatisfactory; it contains only *two* unknown parameters (A and B) and is therefore inadequate for satisfying simultaneously all *three* equations from the exponents, i.e. for y^0 , y^1 , and y^2 , as required. (It is well-known that finding n variables requires precisely n independent simultaneous equations; with fewer equations the problem is under-determined and some or all variables can only be found in terms of others, and with more independent equations the problem is over-determined and has no solution that simultaneously satisfies all the equations.) Arbitrarily ignoring one of those equations such as the y^1 equation, for expediency in finding A and B as in Ref. [1], cannot correctly solve this ill-posed problem; the original Authors' trial solution^[1] for ϕ_0 *does not satisfy* Eq. (16)^[1] for *all* values of y , even though the y^1 equation is employed later in the analysis.^[1] In other words, the problem is overdetermined, and $\phi_0 = A + By$ is not a valid solution unless it can be established that the present Eq. (14) above is satisfied at least approximately over a range of values of y having physical significance.

This is clear explicitly by calculating the numerical values of the two sides of the y^1 equation, $\mu Q/\hbar^2$ and $(A - \alpha)B$, using the original expressions^[1] for A and B . These values are shown in Table 1 for the same parameter values μ and \hbar used in Table 1 of Ref. [1]. In every case examined, the left and right sides of the y^1 equation have markedly different values, demonstrating that that the y^1 equation (the present Eq. (14)) is not satisfied. The same is true when a more realistic value of reduced mass μ and the correct value of Planck's constant \hbar are used. Any analysis (such as the evaluation of the energy levels in Ref. [1]) using this formalism is seriously flawed.

This calls into question the validity of the subsequent analysis. However, even if the trial solution $\phi_0 = A + By$ is deemed an acceptable approximation, there are further issues raised. To use the proposed quantization rule,^[6] the phase-change integral $\int_{r_A}^{r_B} k dr = \int_{y_A}^{y_B} \sqrt{2\mu R/\hbar^2} (y - y_A)^{1/2} (y_B - y)^{1/2} \frac{dr}{dy} dy$ (Eq. (19)

of Ref. [1]) is evaluated, in preparation for equating the total phase difference to $n\pi$. (Note that the standard integral used, $\int_{y_A}^{y_B} \frac{\sqrt{(y - y_A)(y_B - y)}}{y(y + 1)} dy = \pi \left[+\sqrt{(y_A + 1)(y_B + 1)} - 1 - \sqrt{y_A y_B} \right]$ obtained by

contour integration, is valid only for $0 < y_A \leq y_B$, which is the case here.) Oluwadare and Oyewumi go on to relate $(A - B)^2$ to $(R - Q + P - E)/R$ in their Eq. (22) obtained using Eq. (14) above (from equating the coefficients of y^1 in their Eq. (16)). Since this is inconsistent with the specified values^[1] of A and B for the trial solution ϕ_0 , their Eq. (22) and subsequent analysis dependent upon it (including their Eqs. (23) and (24)) are therefore not correct.

Table 1. Computed values of $\mu Q/\hbar^2$ and $(A - \alpha)B$ for $\mu = 1\text{kg}$ and $\hbar = 1\text{J s}^{[1]}$ (*n.b.*, Table 1 of Ref. [1] erroneously fails to state units for any parameters except the results for E_{nl}).

| | | $\alpha = 0.001\text{m}^{-1}$ $A' = 0.5\text{J m}^2$ $B' = 1.0\text{J m}$ $C' = 0.5\text{J}$ | | $\alpha = 0.001\text{m}^{-1}$ $A' = 1.0\text{J m}^2$ $B' = 2.0\text{J m}$ $C' = 1.0\text{J}$ | | $\alpha = 0.01\text{m}^{-1}$ $A' = 0.5\text{J m}^2$ $B' = 1.0\text{J m}$ $C' = 0.5\text{J}$ | | $\alpha = 0.01\text{m}^{-1}$ $A' = 1.0\text{J m}^2$ $B' = 2.0\text{J m}$ $C' = 1.0\text{J}$ | |
|-----|-----|---|--|---|--|--|--|--|--|
| n | l | $\mu Q/\hbar^2$ (m^{-2}) | $(A - \alpha)B$ (m^{-2}) | $\mu Q/\hbar^2$ (m^{-2}) | $(A - \alpha)B$ (m^{-2}) | $\mu Q/\hbar^2$ (m^{-2}) | $(A - \alpha)B$ (m^{-2}) | $\mu Q/\hbar^2$ (m^{-2}) | $(A - \alpha)B$ (m^{-2}) |
| 0 | 1 | -0.00200 | 0.00199 | -0.00400 | 0.00399 | -0.01960 | 0.01895 | -0.03960 | 0.03920 |
| 1 | 1 | -0.00200 | 0.00122 | -0.00400 | 0.00199 | -0.01960 | 0.01107 | -0.03960 | 0.01920 |
| 2 | 1 | -0.00200 | 0.00088 | -0.00400 | 0.00132 | -0.01960 | 0.00736 | -0.03960 | 0.01240 |
| 3 | 1 | -0.00200 | 0.00068 | -0.00400 | 0.00099 | -0.01960 | 0.00512 | -0.03960 | 0.00890 |
| 0 | 2 | -0.00199 | 0.00198 | -0.00399 | 0.00398 | -0.01880 | 0.01768 | -0.03880 | 0.03778 |
| 1 | 2 | -0.00199 | 0.00144 | -0.00399 | 0.00285 | -0.01880 | 0.01190 | -0.03880 | 0.02614 |
| 2 | 2 | -0.00199 | 0.00113 | -0.00399 | 0.00222 | -0.01880 | 0.00830 | -0.03880 | 0.01939 |
| 3 | 2 | -0.00199 | 0.00093 | -0.00399 | 0.00181 | -0.01880 | 0.00575 | -0.03880 | 0.01488 |
| 0 | 3 | -0.00198 | 0.00196 | -0.00398 | 0.00396 | -0.01760 | 0.01606 | -0.03760 | 0.03612 |
| 1 | 3 | -0.00198 | 0.00154 | -0.00398 | 0.00310 | -0.01760 | 0.01121 | -0.03760 | 0.02696 |
| 2 | 3 | -0.00198 | 0.00126 | -0.00398 | 0.00254 | -0.01760 | 0.00775 | -0.03760 | 0.02075 |
| 3 | 3 | -0.00198 | 0.00106 | -0.00398 | 0.00215 | -0.01760 | 0.00508 | -0.03760 | 0.01617 |
| 0 | 4 | -0.00196 | 0.00194 | -0.00396 | 0.00394 | -0.01600 | 0.01405 | -0.03600 | 0.03409 |
| 1 | 4 | -0.00196 | 0.00159 | -0.00396 | 0.00324 | -0.01600 | 0.00970 | -0.03600 | 0.02628 |
| 2 | 4 | -0.00196 | 0.00134 | -0.00396 | 0.00274 | -0.01600 | 0.00634 | -0.03600 | 0.02049 |
| 3 | 4 | -0.00196 | 0.00115 | -0.00396 | 0.00237 | -0.01600 | 0.00358 | -0.03600 | 0.01594 |

To calculate the final result for the energy levels (notwithstanding the unsuitable trial solution used), the procedure is to take the original Authors' Eq. (21)^[1] for the phase-change integral, and impose the quantization rule^[6] $\int_{r_A}^{r_B} k dr - \int_{r_A}^{r_B} k_0 dr = n\pi$ (where the second integral is evaluated in Eq. (23) of Ref. [1]

and is therefore not accurate). This gives $X = +\sqrt{Z} - \sqrt{Z - Y}$, where $X = 2\alpha\sqrt{\frac{\hbar^2}{2\mu}\left(\frac{B}{2\alpha} + n\right)}$, $Y = Q - R$,

and $Z = -C' - E$, to be solved for Z to give $E = -C' - Z$. Equation (24) of Ref. [1] corresponds to $Z = \left[(X^2 + Y)/2X\right]^2$, but strictly this is the solution to $X = +\sqrt{Z} + \sqrt{Z - Y}$ as can be verified by back-substitution. In addition, Eq. (24) of Ref. [1] cannot be correct because V_0 reappears from Eq. (1) and is ill-defined, and also its term in $(\alpha - 1)$ is clearly erroneous (unity is dimensionless and fundamentally cannot be subtracted from α , an inverse length as discussed above). The correct solution should strictly be written $Z = \frac{1}{4}(Y/X - X)^2 + Y$, giving the corrected result written using the present notation

$$E = -C' - \frac{2\mu}{\hbar^2} \left[\frac{A' \left(\alpha - \frac{B'}{2A'} \right)}{\frac{B}{2\alpha} + n} - \frac{\alpha \hbar^2 \left(\frac{B}{2\alpha} + n \right)}{2\mu} \right]^2 + 4\alpha A' \left(\alpha - \frac{B'}{2A'} \right). \quad (15)$$

The alternate expression for B given just after Eq. (24) of Ref. [1] is also incorrect because it, too, is stated using V_0 . The correct equivalent expression for B , obtained by substituting Eq. (7) above into Eq.

(18) of Ref. [1], is $B = \alpha \left[1 \pm \sqrt{(2l+1)^2 - 8\mu A' / \hbar^2} \right]$. With these corrections, Eq. (15) is now the same as

Eq. (45) of Ref. [2] obtained using different approximations (parametric Nikiforov-Uvarov and asymptotic iteration methods). (The result for the energy levels in Eq. (24) of Ref. [1] only agrees with

the result in Ref. [2] if the incorrect constitutive relations, the present Eq. (3), are used to convert between A' , B' , C' , and V_0 .) The wave function, Eq. (25) of Ref. [1], also requires correction and should be replaced^[7] by

$$U(y) = N_{n,l} \cdot y^{i\delta/2} (1+y)^{(1+\varepsilon)/2} \cdot {}_2F_1(-n, n+i\delta+2+\varepsilon; 1+i\delta; -y), \quad (16)$$

where $\delta = \sqrt{2\mu(E+C')/\hbar^2}/\alpha$ and $\varepsilon = \sqrt{2\mu}\sqrt{2\alpha(B'-2\alpha A')-E-C'}/\alpha\hbar-1$. (Equation (3) of Ref. [1] is copied inaccurately from Eq. (2b) of Ref. [7] in which the first parenthesis is equivalent to $(1-k_3z)^{k_5}$.)

Finally, in Table 1 of Ref. [1] it seems inappropriate to list numerical values to 16 significant figures.^[8] This is roughly six orders of magnitude more precise than most fundamental physical constants are known. At most, three or four significant figures are justified by the differences between final results, and fewer would probably be adequate considering the three main approximations made in this work (the Pekeris approximation of Eq. (6), the failure to satisfy Eq. (14) as a result of using an imperfect trial solution, and the approximate quantization rule^[6] itself), and the very unphysical parameter values used.

In conclusion, the analysis of Ref. [1] has been corrected as far as possible. The originally proposed simple solution of the correct equations is unsatisfactory, even though the final result for the energy levels apparently agrees with the result obtained using different approximations. In the original article,^[1] Eqs. (1, 2, 3, 5, 6, 11, 12, 15, 18, 22, 23, 24, 25) and conclusions based upon them, Table 1, and the definitions of δ and ε are all faulty for various reasons including errors of notation, typography or transcription, or more serious technical errors.

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