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No Need for the Quasiclassical Approximation to be Applied to All Degrees of Freedom: the Solution for the Spherically Symmetric States of Singular Attractive Potentials

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ABSTRACT: The Quasiclassical Approximation (QA) is widely used in theoretical atomic physics. For the spherically symmetric potentials V(r), the QA is commonly applied as follows. For the φ-motion, the QA is not applied: instead, the exact solution is used. The QA is then applied to both the θ-motion and the r-motion. The resulting QA wave function for the θ-motion is valid for some, but not all values of θ. Besides, the resulting QA wave function for the θ-motion is valid only with the substitution of L(L+1) by $(L+1/2)^2$, where L is the angular momentum quantum number. Then the QA is applied to the r-motion, but again with the substitution of L(L+1) by $(L+1/2)^2$ in the centrifugal energy term. As a result of the above standard procedure, the obtained QA wave functions are valid only for (L + 1/2) greater or of the order of $N^{1/2}$, where N is the principal quantum number. Besides, for potentials having the pole of the order 3 or higher at r = 0 or for relatively large r, it would be preferable to have L(L + 1) without the substitution by $(L+1/2)^2$. This is yet another restriction of the QA validity in this procedure. In the first part of the present paper, we provide a better alternative. This alternative can also be applied to some potentials whose geometrical symmetry is not spherical. In the second part of the present paper, we focus on the attractive singular spherically-symmetric potentials $V(r) = -a_n/r^n$, where $a_n > 0$ and the integer n > 2. They are encountered in many physical systems. There exists a paradigm that "*singular attractive potentials do not lead to physically reasonable results*" because eigenfunctions depend on the chosen cutoff at small r. In the present paper we disprove this paradigm. We demonstrate that while the *unnormalized* eigenfunctions of singular attractive potentials do depend on the cutoff at small r, there is no such problem for the corresponding *normalized* eigenfunctions. Namely, the normalized eigenfunctions, corresponding to any two different sufficiently small cutoffs (all other parameters being the same), are equal to each other or differ just by the sign. The sign difference does not affect the probability density: the latter is invariant to the variations of the cutoff. Thus, we prove that singular attractive potentials actually do lead to physically reasonable results. In doing so, we also demonstrated that a divergent integral can lead to physically meaningful results independent of the cutoff. This is a *counterintuitive* result of the importance from the fundamental point of view both for physics and mathematics.

Keywords: alternative quasiclassical approximation; singular attractive potentials; bound states of nonzero energies; van der Waals interaction; Casimir-Polder retarded regime

1. INTRODUCTION

The Quasiclassical Approximation (QA) is widely used in theoretical atomic physics. For the spherically symmetric potentials V(r), the QA is commonly applied as follows (see, e.g., textbook [1]). For the φ-motion, the QA is not applied: instead, the exact solution is used. The QA is then applied to both the θ-motion and the r-motion. The resulting QA wave function for the θ-motion is not valid for any θ: it is valid only for

$$\theta L >> 1, (\pi - \theta)L >> 1 \tag{1}$$

(see Eq. (49.4) from textbook [1]), where L is the angular momentum quantum number. Besides, the resulting QA wave function for the θ-motion is valid only with the substitution of L(L+1) by $(L+1/2)^2$. Then the QA is applied to the r-motion, but again with the substitution of L(L+1) by $(L+1/2)^2$ in the centrifugal energy term.

As a result of the above standard procedure, the obtained QA wave functions are valid only for (L + 1/2) greater or of the order of $N^{1/2}$, where N is the principal quantum number – see, e.g., book [2]. This is yet another restriction of the QA validity in this procedure – in addition to the restrictions from Eq. (1).

In the first part of the next section, we provide a better alternative. This alternative can also be applied to some potentials whose geometrical symmetry is not spherical.

Next, let us discuss the singular spherically-symmetric potentials

$$V(r) = -a_n/r^n,\ n > 2, \tag{2}$$

where a_n can be positive or negative and n is an integer. These potentials were analyzed for many decades – see, e.g, papers [3-14] and references therein. The importance of these studies is due to the fact that the singular potentials are encountered in many physical systems, such as: 1) for n = 3, the tensor force between nucleons [12], as well as two identical atoms that are in two different states, the atoms having different parities and the difference of their angular momenta is $L_2 - L_1 = \pm 1$ or zero, but $L_1L_2 > 0$ ([1], Eq. (86.3)); 2) for n = 4, electron or ions traveling through a gas of relatively small molecules, thus exhibiting the interaction between an induced dipole and a charge [6], as well as the interaction of a perfectly conduction wall with a neutral atom [4]; 3) for n = 5, perturbative corrections to the tensor force between nucleons [12], as well as two atoms, being in the states where their orbital and total angular momenta are not zeros, thus coupled by the quadrupole-quadrupole interaction ([1], Eq. (86.2)); 4) for n = 6, two atoms in the ground states coupled by the "standard" van der Waals interaction ([1], Eq. (86.1)); 5) for n = 7, Casimir-Polder regime of retarded van der Waals forces [4].

Exact wave functions for the singular potentials are available only for the *zero-energy states* (to the best of our knowledge). For L = 0, the corresponding unnormalized wave function $u(r) = \psi(r)/r$ for the *attractive* potential from Eq. (1) with $a_n > 0$ can be found in paper [11]

$$u(r) = r^{1/2} J_{1/(n-2)}[a_n^{1/2} r^{1-n/2} /(1 - n/2)] \tag{3}$$

(in Eq. (3), $J_g[\ldots]$ is the Bessel function). For arbitrary L, the corresponding unnormalized wave for the *repulsive* potential from Eq. (1) with $a_n < 0$ was given in paper [7]

$$u_{repuls}(r) = r^{1/2} K_{1/(n-2)}[a_n^{1/2} r^{1-n/2} /(n/2 - 1)] \tag{4}$$

(in Eq. (4), $K_g[\ldots]$ is the modified Bessel function of the second kind). In paper [15], for any L, first the corresponding unnormalized wave function u(r) for the *attractive* potential from Eq. (1) with $a_n > 0$ was presented

$$u(r) = r^{1/2} J_{(2L+1)/(n-2)}[a_n^{1/2} r^{1-n/2}/(1 - n/2)], \tag{5}$$

followed by calculations of the Normalization Integral (NI):

$$NI = \int_0^\infty dr\, r\{J_{(2L+1)/(n-2)}[a_n^{1/2} r^{1-n/2}/(1 - n/2)]\}^2. \tag{6}$$

The normalizing integrals turned out to converge. In this way, in paper [15] there was broken the existing paradigm, according to which in negative interaction potentials vanishing at infinity, only bound states of the negative energies can exist – see, e.g., the statement from Sect. 18 of textbook [1] that for attractive singular potentials (such as given by Eq. (1) of the present paper), the highest discrete level of the energy E_{max} is negative, so that the E = 0 state cannot be bound.

As for states of negative energy in attractive singular potentials, the only complete results were obtained for n = 4, the solutions being expressed via modified Mathieu functions that are functions of imaginary argument [6, 16]. These solutions were reproduced in detail in review [8] where the authors noted that "the solutions involve three-term recursion relations for the coefficients appearing in the infinite Bessel series solutions." They emphasized that these recursion relations contain the Floquet parameter that is a complicated function of two other parameters. They wrote that determining the Floquet parameter "is a major problem and can be done only by approximation for certain ranges" of the two other parameters.

In paper [5], the author considered the S-states in attractive singular potentials. The starting Schrödinger equation contained the dependence on the energy. However, the only solution presented in paper [5] was obtained by dropping the dependence on the energy, meaning that the solution was actually for zero energy. Besides, the solution was obtained by keeping just the leading term of the 1/r expansion, so that it was the approximate solution valid only for sufficiently small r.

In the second part of the next section, we present a quasiclassical solution of the Schrödinger equation for the S-states of any attractive singular potential (given by Eq. (2)): the solution valid in the entire range of r from zero to infinity and showing the explicit dependence on the binding energy. We also calculate the corresponding NI.

It is important to emphasize the following. There exists a paradigm that "*singular attractive potentials do not lead to physically reasonable results*". This is a quote from the review by Frank et al [8] where it says that Case [5] was the first to notice this. This view was later echoed by Beane et al [11] with the reference to both [8] and [5].

Case [5] wrote: "… the Coulomb interaction between an electron and a nucleus is not strictly proportional to 1/r down to r= 0. The finite size of the nucleus sets one limit. Even for a single proton there is the probable finite radius of the proton. The important point is, however, that if the 1/r law holds down to sufficiently small distances the eigenvalues and eigenfunctions are essentially independent of exactly when or how the power law breaks down. *For potentials as singular as $1/r^2$ or greater, this is no longer true. The eigenvalues and eigenfunctions do depend on the nature of the cut-off.*"

In the second part of the present paper we disprove this paradigm. We demonstrate that while the *unnormalized* eigenfunctions of singular attractive potentials do depend on the cutoff at small r, the corresponding *normalized* eigenfunctions do not depend on the cutoff. Namely, the normalized eigenfunctions, corresponding to any two different sufficiently small cutoffs (all other parameters being the same), are equal to each other or differ just by the sign. Of course, the sign difference does not affect the probability density: the latter is invariant to the variations of the cutoff. Thus, we prove that singular attractive potentials actually do lead to physically reasonable results.

2. NEW RESULTS

2.1. Alternative QA for multidimensional separable systems

We use, as an example, systems of three degrees of freedom described by spherically symmetric potentials. As noted in the Introduction, the standard QA is applied both to the θ-motion and the r-motion (while for the φ-motion the exact solution is used). As a result, first, the validity of the QA wave function for the θ-motion is limited by angles θ that are not to close to 0 or to π – see Eq. (1). Second, in the QA wave function for the r-motion (i.e., in the radial wave function R(r)), there is the substitution of L(L+1) by $(L+1/2)^2$ (the substitution inherited from the QA wave function for the θ-motion) and the resulting R(r) is invalid for

$$(L + 1/2) << N^{1/2}, \tag{7}$$

as stated in book [2]. In the same book, it was emphasized that modifying L(L+1) to $(L+1/2)^2$ improves the QA for small r only for potentials having the pole of the 1st or 2nd order at r = 0 (with some additional requirement), so that for other potentials (such as, e.g., the potentials given by Eq. (2)) or for larger r, it is preferable to have L(L + 1) without the substitution by $(L+1/2)^2$. The latter is true because in book [2] it was shown that for large r, the error of the QA with L(L + 1) is ~ $O(1/r^3)$, while the error of the QA with $(L+1/2)^2$ is ~ $O(1/r^2)$.

For the above reasons we suggest the following *alternative* QA for spherically symmetric potentials. Namely, not only for the φ-motion, but also for the θ-motion one can use the well-known exact solution, yielding the spherical harmonics $Y_{Lm}(\theta, \varphi)$. Then the QA can be applied for the r-motion without the need to substitute L(L+1) by $(L+1/2)^2$.

There are two advantages of this alternative QA. First, the wave function for the θ-motion is valid for any θ – in distinction to the standard QA where the corresponding wave function is invalid for the angles θ that are close to 0 or to π. Second, the radial wave function in this alternative QA is more accurate (than the one obtained in the standard QA) for *larger values of r* for *any* spherically symmetric potential or *for all values of r* for potentials given by Eq. (2).

This alternative QA can be applied not only to potentials, whose geometrical symmetry is spherical: it can be also applied, e.g., to potentials, whose geometric symmetry is axial, but whose algebraic symmetry is spherical, such as potentials of the form

$$V(r, \theta) = -a/r + b(3\cos^2\theta - 1)/r^3, \ a = \text{const} > 0, \ b = \text{const}. \tag{8}$$

This kind of potentials characterize systems, such as, e.g., hydrogenic atoms/ions in a high frequency laser field that is polarized either linearly or circularly [17, 18], hydrogenic atoms/ions having ellipsoid-shape nuclei [19], muon-electronic helium or helium-like ions [20], negative hydrogen ions [21]. For potentials given by Eq. (9), not only the projection L_z of the angular momentum is conserved (what follows from the geometric symmetry), but also the square of the angular momentum is conserved, manifesting the "hidden" spherical symmetry. Therefore, for these potentials, both for the φ-motion and for the θ-motion one can use the well-known exact solution, yielding the spherical harmonics $Y_{Lm}(\theta, \varphi)$. Then the QA can be applied for the r-motion without the need to substitute L(L+1) by $(L+1/2)^2$.

Generally, this alternative QA can be applied to any separable multidimensional system, such that some (but not all) degrees of freedom allow an exact solution of the Schrödinger equation. Then one can use the latter exact solutions and apply the QA only to the remaining degrees of freedom. In other words, there is no need to apply the QA to the degrees of freedom that allow the exact solution.

2.2. Quasiclassical solution of the Schrödinger equation for the S-states of any attractive singular potential (given by Eq. (2)) for the entire range of r from zero to infinity with the explicit dependence on the binding energy

For spherically symmetric potentials V(r), the motion is restricted (by the geometry) to $r \geq 0$. This is equivalent to having an impenetrable wall at r = 0. In this situation, the quasiclassical unnormalized wave function can be written as follows (see, e.g., Eq. (47.6) from textbook [1]):

$$\Psi(r) = [\text{const}/p(r)^{1/2}] \sin[(1/\hbar) \int_0^r dx\, p(x)], \tag{9}$$

where

$$p(r) = [2m(E - V(r)]^{1/2}. \tag{10}$$

In Eq. (10), m is either the mass of the particle moving in the potential V(r) or the reduced mass of the pair of particles, whose interaction is described by V(r). For attractive potentials given by Eq. (2) with $a_n > 0$, Eq. (9) becomes

$$\Psi(r) = \{\text{const}/[2m(E + a_n/r^n]^{1/4}\} \sin[(1/\hbar) \int_0^r dx\, [2m(E + a_n/x^n)]. \tag{11}$$

Here E < 0 since we look for possible bound states.

We denote:

$$b = 2ma_n/\hbar^2, \quad c = |E|/a_n, \tag{12}$$

so that c is the scaled binding energy. Then Eq. (11) can be represented in the form:

$$\Psi(r) = \{\text{const}/[b(1/r^n - c)]^{1/4}\} \sin[b^{1/2}\, I(r)], \tag{13}$$

where

$$0 \leq r \leq 1/c^{1/n}. \tag{14}$$

(For $r > 1/c^{1/n}$, the corresponding wave function is exponentially small, as it is well-known.) In Eq. (13),

$$I(r) = \int_0^r dx\ (1/x^n - c)^{1/2}. \tag{15}$$

Here and below, we use units where ħ = 1. In these units, the energy E has the same dimension as the frequency (s^{-1}), the angular momentum M is dimensionless, the distance r has the dimension $(s/g)^{1/2}$ (since $M^2/(mr^2)$ has the dimension of the energy (s^{-1}), m being the mass in units of gram (g)), the parameter c has the dimension $(g/s)^{n/2}$ (since c has dimension of $1/x^n$ according to Eq. (15)), and the parameter b has the dimension $(s/g)^{n/2-1}$.

For the integral in Eq. (15), we find analytically the following antiderivative A(x):

$$A(x) = -i\ c^{1/2}x\ {}_2F_1[-1/2, -1/n, 1 - 1/n, 1/(cx^n)], \tag{16}$$

where

$$0 \le x \le 1/c^{1/n}. \tag{17}$$

In Eq. (15), ${}_2F_1[\ldots]$ is the hypergeometric function, which in the range of x from Eq. (17) has both the real and imaginary parts. It turns out that in the range (17), the imaginary part of A(x) is:

$$\mathrm{Im}[A(x)] = -c^{1/2-1/n}\ {}_2F_1[-1/2, -1/n, 1 - 1/n, 1]. \tag{18}$$

It does not depend on x: in particular, it is the same at both limits of the integration in Eq. (15), so that it cancels out while calculating the definite integral in Eq. (15).

As for the real part of A(x), it is easy to find that at x → 0, one has

$$\mathrm{Re}[A(x)] \to -2/[(n - 2)x^{n/2-1}]. \tag{19}$$

Thus, the integral in Eq. (15) diverges at the lower limit. Therefore, we introduce the cutoff r_m (i.e., the minimum value of r):

$$I(r_m, r) = \int_{r_m}^{r} dx\ (1/x^n - c)^{1/2} = \mathrm{Im}[c^{1/2}r\ {}_2F_1[-1/2, -1/n, 1 - 1/n, 1/(cr^n)]] + 2/[(n - 2)r_m^{n/2-1}], \tag{20}$$

so that the unnormalized wave function becomes

$$\Psi(r_m, r) = \{\mathrm{const}/[b(1/r^n - c)]^{1/4}\}\ \sin[b^{1/2}\ I(r_m, r)]. \tag{21}$$

Now we study the dependence of the wave function on the integration cutoff r_m as we make r_m smaller and smaller. Figure 1 shows the unnormalized wave functions for n = 3, b = 10^{-6}, c = 10^{-2} for the following three values of r_m: 10^{-20} (solid blue line), 10^{-50} (dashed brown line), and 10^{-90} (red dash-dotted line).

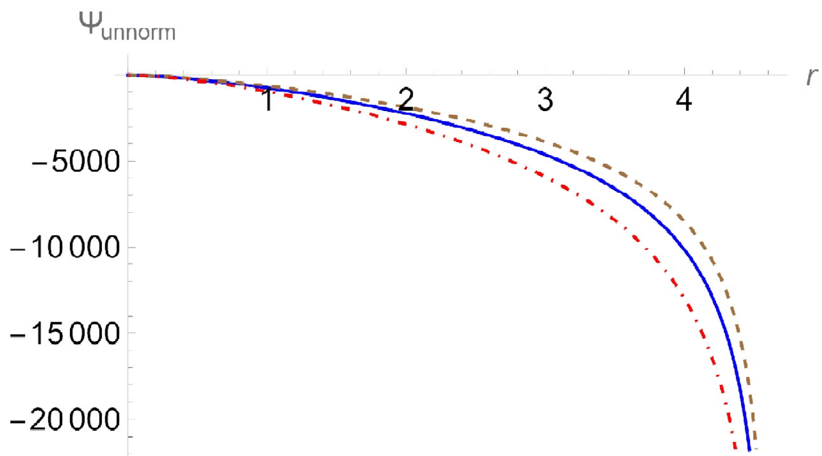

Fig. 1. Unnormalized wave functions for n = 3, b = 10^{-6}, c = 10^{-2} for the following three values of r_m: 10^{-20} (solid blue line), 10^{-50} (dashed brown line), and 10^{-90} (red dash-dotted line).

From Fig. 1 it is seen that different values of the integration cutoff r_m yield different unnormalized wave functions. However, the corresponding normalized wave functions turned out to be identical to each other. First, this is shown in Fig. 2, where it seen that all the three wave functions coincide. Second, it is demonstrated in Fig. 3 presenting the ratio of the normalized wave functions corresponding to the following two values of the integration cutoff r_m: 10^{-50} and 10^{-90}.

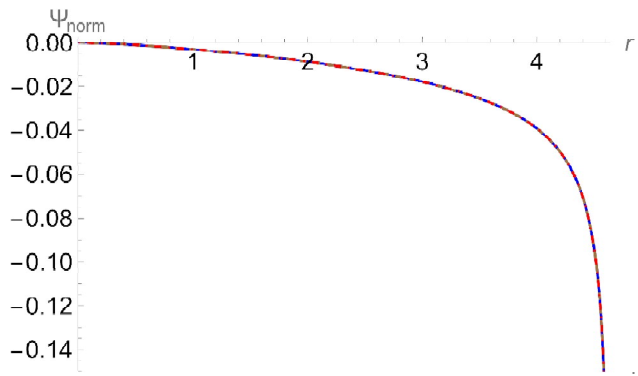

Fig. 2. The same as in Fig. 1, but for the normalized wave functions.

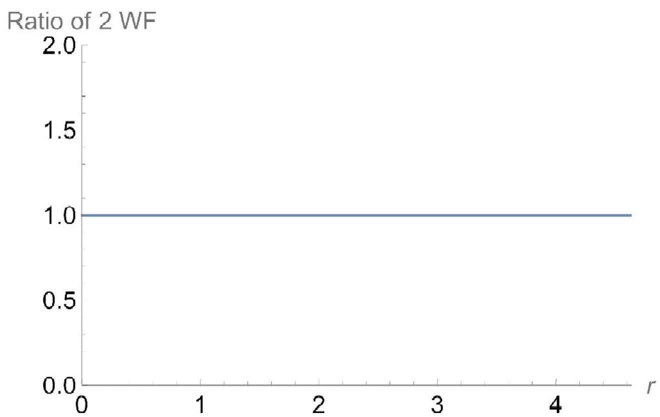

Fig. 3. The ratio of the normalized wave functions for n = 3, b = 10^{-6}, c = 10^{-2}, corresponding the two different values of the integration cutoff r_m: 10^{-50} and 10^{-90}.

Figure 4 shows that the normalized wave functions, corresponding to two different values of the integration cutoff – in this case, 10^{-35} (solid blue line) and 10^{-80} (dashed red line) – can differ by sign. However, their squared values are identical for each r, as demonstrated in Fig. 5.

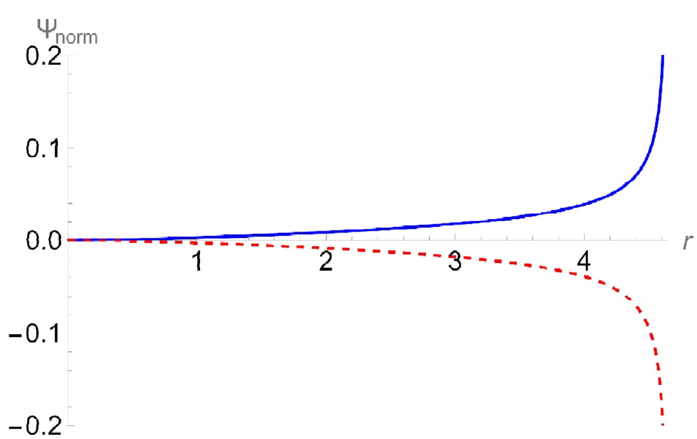

Fig. 4. Normalized wave functions for n = 3, b = 10^{-6}, c = 10^{-2} for the following two values of the integration cutoff r_m: 10^{-35} (solid blue line) and 10^{-80} (dashed red line).

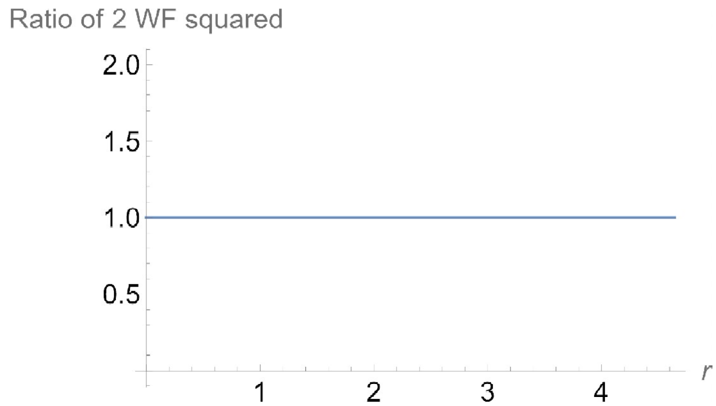

Fig. 5. The ratio of the squares of the two normalized wave functions from Fig. 5.

So, the squares of the normalized wave functions (and thus the probability densities) do not depend on the integration cutoff r_m, as the latter is chosen smaller and smaller. In other words, for a given set of n, b, and c, the square of the normalized wave function is determined unambiguously, unequivocally – regardless of the choice of the integration cutoff (as long as the latter is relatively small). This is a *counterintuitive* result.

Now we demonstrate that this finding does not depend on the choice of n, b, or c. First, we vary the parameter b. Figure 6 shows the normalized wave functions for $n = 3$, $b = 10^{-3}$, $c = 10^{-2}$ for the following three values of the integration cutoff r_m: 10^{-20} (solid brown line), 10^{-30} (dashed blue line), and 10^{-90} (dash-dotted red line). It is seen that all the three normalized wave functions coincide at any r.

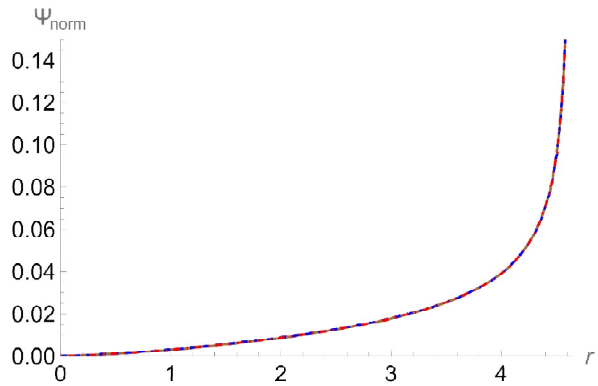

Fig. 6. Normalized wave functions for $n = 3$, $b = 10^{-3}$, $c = 10^{-2}$ for the following three values of the integration cutoff r_m: 10^{-20} (solid brown line), 10^{-30} (dashed blue line), and 10^{-90} (dash-dotted red line).

Now we vary the parameter c, which is the scaled binding energy (see, Eq. (12)). Figure 7 shows the normalized wave functions for $n = 3$, $b = 10^{-3}$, $c = 10^{-5}$ for the following three values of the integration cutoff r_m: 10^{-20} (solid brown line), 10^{-30} (dashed blue line), and 10^{-90} (dash-dotted red line). It is seen again that all the three normalized wave functions coincide at any r.

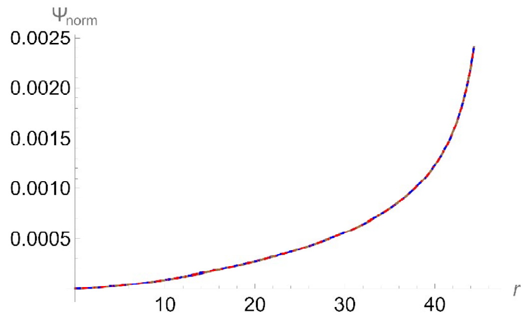

Fig. 7. Normalized wave functions for $n = 3$, $b = 10^{-3}$, $c = 10^{-5}$ for the following three values of the integration cutoff r_m: 10^{-20} (solid brown line), 10^{-30} (dashed blue line), and 10^{-90} (dash-dotted red line).

Finally, we vary the parameter n. Figure 8 shows the normalized wave functions for n = 5, b = 10^{-3}, c = 10^{-5} for the following two values of the integration cutoff r_m: 10^{-50} (solid brown line) and 10^{-80} (dashed red line). It is seen that these two normalized wave functions differ by sign. However, their squared values are identical for each r, as demonstrated in Fig. 9.

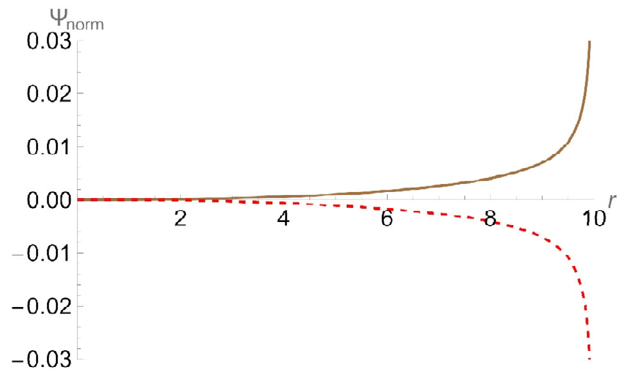

Fig. 8. Normalized wave functions for n = 5, b = 10^{-3}, c = 10^{-5} for the following two values of the integration cutoff r_m: 10^{-50} (solid brown line) and 10^{-80} (dashed red line).

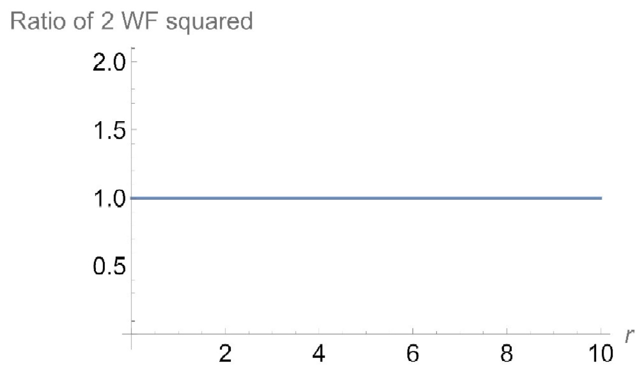

Fig. 9. The ratio of the squares of the two normalized wave functions from Fig. 8.

Thus, it is true that for a given set of n, b, and c, the square of the normalized wave function is determined unambiguously, unequivocally – regardless of the choice of the integration cutoff (as long as the latter is relatively small).

3. CONCLUSIONS

We re-analyzed the Quasiclassical Approximation (QA) commonly used in theoretical atomic physics. We started by discussing the QA for the spherically symmetric potentials V(r). We emphasized that the wave functions, obtained by the QA in the standard way, are valid for some, but not all values of θ, and not for (L + 1/2) << $N^{1/2}$ (where (L + 1/2) corresponds to the substitution of L(L+1) by $(L+1/2)^2$, the latter substitution being mandatory in the standard QA). Besides, for potentials having the pole of the order 3 or higher at r = 0 or for relatively large r, it would be preferable to have L(L + 1) without the substitution by $(L+1/2)^2$. This is yet another restriction of the QA validity in this procedure.

In the first part of the present paper, we provided a better alternative. For spherically symmetric potentials, not only for the φ-motion, but also for the θ-motion one can use the well-known exact solution, yielding the spherical harmonics $Y_{Lm}(\theta, \varphi)$. Then the QA can be applied for the r-motion without the need to substitute L(L+1) by $(L+1/2)^2$.

There are two advantages of this alternative QA. First, the wave function for the θ-motion is valid for any θ – in distinction to the standard QA where the corresponding wave function is invalid for the angles θ that are close to 0 or to π. Second, the radial wave function in this alternative QA is more accurate (than the one obtained in the standard QA) for *larger values of r* for *any* spherically symmetric potential or *for all values of r* for potentials $V(r) = -a_n/r^n$ given by Eq. (2).

This alternative QA can be applied not only to potentials, whose geometrical symmetry is spherical. Namely, it can be also applied, e.g., to potentials, whose geometric symmetry is axial, but whose algebraic symmetry is spherical, such as, e.g., such potentials of the form $V(r, \theta) = -a/r + b(3\cos^2\theta - 1)/r^3$ (where a = const > 0, b = const) arising in many applications.

In the second part of the present paper, we focused on the attractive singular spherically-symmetric potentials V(r), given by Eq. (2) with $a_n > 0$: the potentials encountered in many physical systems. There existed a paradigm that "*singular attractive potentials do not lead to physically reasonable results*" because eigenfunctions depend on the chosen cutoff at small r. In the present paper we disprove this paradigm. We showed that while the *unnormalized* eigenfunctions of singular attractive potentials do depend on the cutoff at small r, there is no such problem for the corresponding *normalized* eigenfunctions. Namely, the normalized eigenfunctions, corresponding to any two different sufficiently small cutoffs (all other parameters being the same), are equal to each other or differ just by the sign. The sign difference does not affect the probability density: the latter is invariant to the variations of the cutoff. We obtained the normalized eigenfunctions for any binding energy. Thus, we disproved the above paradigm by showing that singular attractive potentials actually do lead to physically reasonable results.

The results obtained in both parts of the present paper have not only fundamental but also practical importance. This is because they are applicable to a variety of real physical systems.

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