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A PECULIAR PROPERTY OF THE WAVE FUNCTIONS
FOR CONFINING POTENTIALS

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ABSTRACT

We show that in contradiction with what could be expected superficially from classical considerations, the probability for the presence of a particle, at any given place inside a confining potential extending to infinity, does not necessarily go to zero as the excitation energy goes to $+\infty$. Furthermore we observe a non-uniform behaviour when we consider the square well as a limit of power potentials.

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In studying properties of wave functions for confining potentials, inspired by the recent successes of non-relativistic models for the quark-antiquark system¹⁾, we come across a property of those wave functions which seems somewhat paradoxical and opposite to simple intuitive reasoning. The study of the particular property was inspired by a suggestion by Morgan²⁾ that the reduced wave function $u_n = r\psi_n$ for the n^{th} bound S state (or, similarly, for the bound states in one dimension) in a confining potential should satisfy:

$$\lim_{n \rightarrow \infty} \left[\sup_r |u_n(r)| \right] = 0, \text{ where } \int_0^\infty |u_n(r)|^2 dr = 1, \quad (1)$$

for almost any form of the potential. The exceptions should be hard wall potentials like the square well, where this limit is known to be a finite constant. This suggestion is supported by the following facts:

i) It is true for the simple solvable cases, the harmonic oscillator and the linear potential.

ii) It seems to follow from the following physical argument: The probability to find the particle, bound in the potential well, at a particular radius r is proportional to $|u_n(r)|^2$. Since the size in space of the bound state increases with energy, and thus with n , for any potential without hard walls, this probability, and thus $u_n(r)$, can be expected to go to zero as n goes to infinity.

The last point can be made more quantitative in the following way: Assume for simplicity that

$$V(r) = r^\beta, \quad \beta > 0. \quad (2)$$

(We shall use this potential for all the calculations, and discuss at the end what can be said for more general potentials.) Then the radius of the bound state is approximately equal to r_0 , the classical turning point, which is given by

$$V(r_0) = k^2 \Rightarrow r_0 = k^{\frac{2}{\beta}} \quad (3)$$

(We use units such that $\hbar$ and the quark mass are 1.) The quantization condition is approximately

$$k r_0 \cong n \pi \Rightarrow k_n \cong \text{const} \cdot n^{\frac{\beta}{2+\beta}} \quad (4)$$

giving the growth rate of the classical radius of the n^{th} state

$$r_0^n \cong r_0^1 n^{\frac{2}{2+\beta}}. \quad (5)$$

This implies that the mean value of $|u_n(r)|^2$ should decrease like

$$\text{mean}_r |u_n(r)|^2 \cong \text{const} \times n^{-\frac{2}{2+\beta}}. \quad (6)$$

If we let $r_{n,j}$ denote the position of the j^{th} of the n maxima of $|u_n(r)|^2$, counting outwards, we also have

$$|u_n(r_{n,j})| \cong \text{const} \times n^{-\frac{1}{2+\beta}}, \quad j \text{ fixed}, \quad (7)$$

since the maxima have a tendency to become equal as n increases. This formula could also be proved by standard WKB techniques.

However, as we shall show below, the supremum of the wave function does not decrease in the way indicated by Eq. (7). It can even increase with n for some β .

In the scaled variable s ,

$$s = \frac{r}{r_0}, \quad \varphi_n(s) = u_n(r), \quad (8)$$

the radial Schrödinger equation for $\ell = 0$ becomes

$$\varphi_n''(s) = \nu_n^2 (s^\beta - 1) \varphi_n(s), \quad (9)$$

where

$$\nu_n = k_n r_0 = k_n \frac{r_0^{\frac{2+\beta}{\beta}}}{r_0^{\frac{2+\beta}{\beta}}} = r_0^{\frac{2+\beta}{2}} \quad (10)$$

is a large parameter for large n .

Equation (9) has exactly one turning point in $0 < s < \infty$. Such second order differential equations with large parameters are well known, and in particular

there exists a method to obtain approximations to their solutions, valid uniformly in s , with controllable accuracy. (See, for example, Olver³⁾. The present author has used this method in another connection⁴⁾.) The method can be considered a generalized WKB method.

We do not want to get into details here, so we just state the result. By using the theorem on p. 399 of Ref. 3) we find for the solution of Eq. (9) that goes to zero at infinity the formula

$$\varphi_n(s) = Q_n^{-1} \left(\frac{z}{s^\beta - 1} \right)^{\frac{1}{4}} [Ai(\nu_n^{2/3} z) + \varepsilon(\nu_n, z)] \quad (11)$$

where

$$\frac{2}{3} z^{\frac{3}{2}} = \int_1^s (s^\beta - 1)^{1/2} ds, \quad (12)$$

Ai is the Airy function, Q_n is a normalization factor, and an explicit bound exists for the function ε . This bound is (for $\beta \geq 1$) finite on $0 \leq \beta < \infty$ and goes to zero a factor $1/\nu_n$ faster than the Airy function as $\nu_n \rightarrow \infty$. Thus

$$u_n(r) = \varphi_n(s) \underset{\nu_n \rightarrow \infty}{\sim} Q_n^{-1} \left(\frac{z}{s^\beta - 1} \right)^{\frac{1}{4}} Ai(\nu_n^{2/3} z) \quad (13)$$

is an approximation that is valid uniformly in r and becomes better and better the larger ν_n is. Outside the neighbourhood of the turning point Eq. (13) coincides with the usual WKB approximation, but as we have already stressed, it is valid uniformly and thus also at and near this point. This implies that Eq. (13) is good enough to estimate the supremum of the wave function, at least for large ν_n .

The integral in Eq. (12) can be expressed as an incomplete beta function, and thus as a hypergeometric function⁵⁾

$$z = (s^\beta - 1) \left\{ \frac{1}{\beta} F\left(\frac{3}{2}, 1 - \frac{1}{\beta}; \frac{5}{2}; 1 - s^\beta\right) \right\}^{2/3}. \quad (14)$$

For $s = 0$ we get a beta function, and

$$z_0 = z_{s=0} = - \left\{ \frac{\Gamma(\frac{5}{2}) \Gamma(1 + \frac{1}{\beta})}{\Gamma(\frac{3}{2} + \frac{1}{\beta})} \right\}^{2/3}. \quad (15)$$

The boundary condition at $r = 0$

$$u_n(0) = 0 \Rightarrow Ai(\nu_n^{2/3} z_0) = 0 \quad (16)$$

now plays the role of a quantization condition

$$\nu_n^{2/3} z_0 = a_n \Rightarrow \nu_n = \left(\frac{a_n}{z_0} \right)^{3/2} \underset{n \rightarrow \infty}{\sim} C_\beta (4n-1). \quad (17)$$

Here, a_n are the zeros of the Airy function

$$a_1 \approx -2.338, \quad a_2 \approx -4.088, \quad a_n = -\left[\frac{3\pi}{8} (4n-1) \right]^{2/3} + O(n^{-4/3}) \quad (18)$$

and C_β the constant

$$C_\beta = \frac{\sqrt{\pi}}{2} \frac{\Gamma(\frac{3}{2} + \frac{1}{\beta})}{\Gamma(1 + \frac{1}{\beta})}. \quad (19)$$

We also have to normalize our wave function. To the same approximation as in Eq. (13), that is with a relative error of the order $1/\nu_n$, we have

$$Q_n^2 = \int_0^\infty dr \left(\frac{r}{s^{\beta-1}} \right)^{\frac{1}{2}} Ai^2(\nu_n^{2/3} z). \quad (20)$$

Now

$$\frac{dz}{dr} = \frac{1}{r_0} \frac{dz}{ds} = \frac{1}{r_0} \left(\frac{s^{\beta-1}}{z} \right)^{\frac{1}{2}} \quad (21)$$

and therefore

$$Q_n^2 = r_0 \nu_n^{-2/3} \int_{a_n}^\infty dx \left(\frac{x}{s^{\beta-1}} \right) Ai^2(x). \quad (22)$$

Here, the function

$$f(s) \equiv \left(\frac{z}{s^{\beta-1}} \right)^{\frac{1}{4}} = \left\{ \frac{1}{\beta} F\left(\frac{3}{2}, 1-\frac{1}{\beta}; \frac{5}{2}; 1-s^{\beta}\right) \right\}^{\frac{1}{6}} \quad (23)$$

is smooth, positive, and does not vary much in the part of the integration interval where the Airy function is essentially different from zero. Thus we can use a mean value theorem and write

$$Q_n^2 = r_0 \nu_n^{-2/3} \bar{f}^4 Ai'^2(a_n), \quad (24)$$

where $\bar{f}^4$ denotes the appropriate mean value of $f^4(s)$. We neglect the possible n dependence of $\bar{f}$, since it must be weak.

We have now obtained the following approximation to the wave function, valid asymptotically for large n , uniformly in r :

$$u_n(r) \underset{n \rightarrow \infty}{\sim} \nu_n^{\frac{1}{3} - \frac{1}{2+\beta}} \frac{f(s) Ai(\nu_n^{2/3} z)}{\bar{f}^2 Ai'(a_n)} \quad (25)$$

Now

$$\sup_x Ai(x) \equiv Ai(-1.019) \equiv 0.536 \quad (26)$$

and because of the smoothness of $f(s)$

$$\sup_n |u_n(r)| \underset{n \rightarrow \infty}{\sim} \nu_n^{\frac{1}{3} - \frac{1}{2+\beta}} \frac{f(1) \cdot 0.536}{\bar{f}^2 |Ai'(a_n)|}. \quad (27)$$

This supremum is attained at

$$z \cong -1.019 \cdot \nu_n^{-2/3}, \quad (28)$$

which, for large n , corresponds to s just below 1 and r below but near to the turning point r_0 . Since^{3),5)}

$$Ai'(a_n) \underset{n \rightarrow \infty}{\sim} (-1)^{n-1} \pi^{-\frac{1}{2}} \left[\frac{3\pi}{8} (4n-1) \right]^{\frac{1}{6}} \quad (29)$$

we finally obtain the n dependence explicitly

$$\sup_r |u_n(r)| \underset{n \rightarrow \infty}{\sim} \text{const} \cdot n^{\frac{1}{6} - \frac{1}{2+\beta}}. \quad (30)$$

This is to be compared to Eq. (7). The difference is due to the fact that the supremum is attained for $r = r_{n,n}$ in the notation of Eq. (7), that is for $j = n$, not for a fixed j . The relation between Eqs. (7) and (30) can be better understood by using Eq. (25). Take in this equation a particular maximum of $|u_n|$, that is of the Airy function, say $r_{n,j}$ in the notation of Eq. (7). Denoting in the usual way the zeros of Ai' by An' , we get that

$$z(r_{n,j}) = \nu_n^{-\frac{2}{3}} a'_{n-j+1}, \quad j = 1, 2, \dots, n, \quad (31)$$

are the z values at the n maxima of $|u_n|$. Since

$$Ai(a'_{n-j+1}) \cong (-1)^{n-j} \pi^{-\frac{1}{2}} \left[\frac{3\pi}{8} (4(n-j+1)-1) \right]^{-\frac{1}{6}} \quad (32)$$

we obtain

$$|u_n(r_{n,j})| \underset{n \text{ large}}{\cong} \text{const} (n-j+1)^{-\frac{1}{6}} n^{\frac{1}{6} - \frac{1}{2+\beta}}, \quad (33)$$

which contains both Eqs. (7) and (30).

Obviously, Eq. (30) implies that

$$\lim_{n \rightarrow \infty} \left[\sup_r |u_n(r)| \right] = \begin{cases} 0 & \text{for } \beta < 4 \\ \text{const} & \text{" } \beta = 4 \\ \infty & \text{" } \beta > 4 \end{cases} \quad (34)$$

for pure power potentials, Eq. (2), and our earlier intuitive reasoning, as well as the standard WKB method, obviously fails for $\beta \geq 4$. Moreover, since Eq. (34) is concerned only with the very high energy states, it should not depend on the inner parts of the potential, and thus should be valid for any reasonable potential, behaving at infinity like

$$V(r) \underset{r \rightarrow \infty}{\sim} \alpha r^\beta, \quad \alpha > 0, \beta > 0. \quad (35)$$

For Eq. (11) to be valid, and thus the above proof to apply, $V(r)$ should be twice continuously differentiable.

One might at this point worry about the connection to the square well potential, which might be thought of as the limit $\beta \rightarrow \infty$ in Eq. (2). However, our proof does not apply in this limit, since the error term in Eq. (11) depends on β in a complicated way and may become large if $\beta \rightarrow \infty$ for a finite v_n .

In this limit Eq. (17) gives

$$v_n \underset{\beta \rightarrow \infty}{\sim} \frac{3}{2} (-a_n)^{3/2} \underset{n \rightarrow \infty}{\sim} \pi (n - \frac{1}{4}) \quad (36)$$

and

$$\left(\frac{z}{5\beta-1}\right)^{\frac{1}{4}} Ai(v_n^{2/3} z) \underset{\substack{\beta \rightarrow \infty \\ n \text{ large}}}{\longrightarrow} \text{const.} \sin[(n - \frac{1}{4})\pi r], \quad r < 1-\delta, \delta > 0. \quad (37)$$

This is almost the square well wave function. The difference illustrates the non-uniformity of the limits $n \rightarrow \infty$ and $\beta \rightarrow \infty$; they must not be interchanged!

The last point might, however, be explained as a non-uniformity in our asymptotic approximation Eq. (13), and, after all, we expect the exact wave function to fulfil

$$\lim_{\beta \rightarrow \infty} u_n(r) = \sqrt{2} \sin(n\pi r), \quad (38)$$

for fixed n and r .

However, there is a deeper, physical reason why the limits $n \rightarrow \infty$ and $\beta \rightarrow \infty$ may not be interchanged! For any fixed β , however large, you come in the limit $n \rightarrow \infty$ to a point where the classical radius

$$r_0 = \nu_n^{\frac{2}{2+\beta}} \cong [C_\beta (4n-1)]^{\frac{2}{2+\beta}} \quad (39)$$

is $\gg 1$. You only have to take

$$n^{\frac{1}{\beta}} \gg 1. \quad (40)$$

On the other hand, in the limit $\beta \rightarrow \infty$ the classical radius is always strictly $= 1$, for any fixed n , however large. Thus our result Eqs. (30) and (34) is not contradicted by the square well example.

That the peculiar n dependence of Eq. (30) is not just a property of our asymptotic approximation can be checked by solving the Schrödinger equation numerically for different power potentials. Such a test shows clearly that $\beta = 4$ is a limit case, with decrease for $\beta < 4$ and increase for $\beta > 4$ ⁶⁾.

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