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AND THE WAVEFUNCTION AT THE ORIGIN

By

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Abstract

We derive an exact quantization condition for the energy levels of a particle in a radial potential assumed finite at the origin. This is used to derive corrections to the semiclassical JWKB quantization condition. We further relate the normalization integral of the wavefunction to the energy derivative of wavefunction at origin and use this expression to derive the corrections to the semiclassical JWKB expressions for the wavefunction at origin. An application to ϵ leptonic decay width is also given.

I. INTRODUCTION

Methods of non-relativistic quantum mechanics have been extensively used recently to study many of the properties of heavy quarkonium systems.¹ Although the quark anti-quark potential is, presumably, of the confining type, the potential is not known in detail. Thus for example, while the Cornell group² has obtained a satisfactory explanation of many of the properties of the charmonium system with a Coulomb plus linear potential, Martin³ on the other hand has obtained a successful fit to the charmonium spectra with a potential of the type

$$V(r) = A + Br^\epsilon \quad (1.1)$$

with $\epsilon \approx 0.1$.

Although given any $V(r)$, one can at least numerically compute to arbitrary accuracy, any quantity of interest, it is worthwhile to ask how much one can learn about the system from a knowledge of the energy levels alone as these are directly accessible from the experiment. Typical quantities of interest are $|r^{-\ell} R_{n\ell}(r)|^2_{r=0}$ where $R_{n\ell}(r)$ is the n^{th} radial wavefunction of the Schrödinger equation for the ℓ^{th} partial wave. For example the value of the S-wave function at the origin $|R_{n0}(0)|$ is needed to find the decay rates of orthocharmonium into lepton pairs or into 3 gluons. Similarly the derivative of the p-wave function is needed to compute the decay ratio of 0^{++} , 1^{++} and 2^{++} states, then gluon-production rates in hadron collisions, as well as in diffraction production of the 1^{++} in neutrino reactions.

The lowest order JWKB approximation already provides a good estimate of these quantities. In this approximation one has for the S-wave function at the origin⁴

$$|R_{n0}|^2 = \frac{1}{\pi} \left(\frac{2mE_{n0}}{\hbar^2} \right) \frac{\partial(2mE_{n0})/\hbar^2}{\partial n} \quad (1.2)$$

which, generalized to all partial waves reads as⁵

$$|r^{-\ell} R_{n\ell}(r)|_{r=0}^2 = \frac{1}{\pi} \left| \frac{\ell!}{(2\ell+1)!!} \right|^2 \left(\frac{2mE_{n\ell}}{\hbar^2} \right)^{\ell+1/2} \frac{\partial(2mE_{n\ell})/\hbar^2}{\partial n} \quad (1.3)$$

As is well known Eq. (1.2) and (1.3) become quite accurate in the short wavelength or large n limit.⁶

One of the aims of this paper is to provide a more accurate version of Eq. (1). We derive an exact relation between $|R_{n0}(0)|^2$ and $\frac{\partial E}{\partial n}$ which when expanded in a JWKB series yields Eq. (1.2) as the leading term. The successive terms of the series can be easily evaluated when the potential is analytic at $r=0$.

Apart from its relevance to the questions discussed above the JWKB method is of intrinsic interest by itself. For this reason, we have also found it worthwhile to write down the higher order correction to the energy levels and evaluate them explicitly, as an illustration, for potentials of the type $V = Ar^k$ with k an integer.

When the potential is non-analytic at the origin like e.g. $V = Ar^k$ with $k > 0$ but non-integral, the various integrals that occur in the calculation need suitable regularization. To make the procedure rigorous,

we develop an alternate expansion based on integral equation for the exact eigenfunction. This is discussed in Section IV. In Section V we comment on leptonic decay widths of the epsilon levels.

II. HIGHER JWKB APPROXIMATIONS

Introducing $u(r) = r\psi(r)$ we can write the S-wave Schrödinger equation as

$$\frac{d^2 u}{dr^2} + [\lambda - V(r)]u(r) = 0 \quad 0 \leq r < \infty \quad (2.1)$$

with $\lambda = 2mE/\hbar^2$, $V = 2m/\hbar^2 U(r)$ where $U(r)$ is the potential energy.

Defining $V(R) = \lambda$ the solution to Eq. (2.1) in the inside region $r < R$ can be written as

$$u(r) = \left[\exp \pm \frac{i}{\hbar} \int_R^r a(r, \lambda) dr \right] / \sqrt{a(r, \lambda)} \quad (2.2)$$

where $a(r, \lambda)$ satisfies the equation

$$a^2 - \frac{3\hbar^2}{4a^2} \left(\frac{da}{dr} \right)^2 + \frac{\hbar^2}{2a} \frac{d^2 a}{dr^2} = 2m[E - U(r)] \quad (2.3)$$

The general solution for $r < R$ is then

$$u(r) = \frac{C_1}{\sqrt{a(r, \lambda)}} \exp \left\{ \frac{i}{\hbar} \int_R^r a(r, \lambda) dr \right\} + \frac{C_2}{\sqrt{a(r, \lambda)}} \exp \left\{ -\frac{i}{\hbar} \int_R^r a(r, \lambda) dr \right\} \quad (2.4)$$

while the outside solution for $r > R$, vanishing at infinity is

$$u(r) = \frac{C}{2\sqrt{b}} \exp \left(-\frac{1}{\hbar} \int_R^r h(r, \lambda) dr \right) \quad (2.5)$$

where b satisfies the equation

$$b^2 - \frac{\hbar^2}{2b} b'' + \frac{3\hbar^2}{4} \left(\frac{db}{dr} \right)^2 = 2m[E - U(r)] \quad (2.6)$$

The inside and outside solutions Eq. (2.4) and Eq. (2.5) can be matched⁷ by continuing them in the complex r -plane for large enough $|R - r|$, with

$$C_1 = \frac{1}{2} C e^{i\pi/4} \quad C_2 = \frac{1}{2} C e^{-i\pi/4} \quad (2.7)$$

Hence the solution near the origin ($R > r \geq 0$) is

$$u(r, \lambda) = \frac{C}{\sqrt{a(r, \lambda)}} \sin \left(\frac{1}{\hbar} \int_r^R a(r, \lambda) dr + \frac{\pi}{4} \right) \quad (2.8)$$

The eigenvalue condition $u(0, \lambda) = 0$ reads

$$\frac{1}{\hbar} \int_0^R a(r, \lambda_n) dr + \frac{\pi}{4} = n\pi \quad (2.9)$$

We may emphasize here that the expressions (2.8) - (2.9) are exact.

One of our interests is to calculate the value of the normalized wave function at the origin

$$|\psi(0)|^2 = \frac{|u'(0, \lambda)|^2}{\int_0^\infty (u(r, \lambda))^2 dr} \quad (2.10)$$

where prime denotes differentiation with respect to r . Consider now

solutions of the Schrödinger equation corresponding to arbitrary energy values λ and λ' which satisfy the boundary condition at infinity but not at the origin

$$u''(r, \lambda) + (\lambda - v)u(r, \lambda) = 0 \quad (2.11)$$

$$u''(r, \lambda') + (\lambda' - v)u(r, \lambda') = 0 \quad (2.12)$$

From Eq. (2.11) and Eq. (2.12) we deduce

$$\frac{d}{dr} \{u(r, \lambda)u'(r, \lambda') - u'(r, \lambda)u(r, \lambda')\} = (\lambda - \lambda')u(r, \lambda')u(r, \lambda) \quad (2.13)$$

Integrating Eq. (2.13) from $0 \leq r < \infty$ and letting $\lambda' - \lambda = \lambda_m$ an eigenvalue we find⁸

$$|\psi_m(0)|^2 = \frac{1}{4\pi} \frac{[u'(0, \lambda_m)]^2}{\int_0^\infty [u(r, \lambda_m)]^2 dr} = \frac{1}{4\pi} \frac{u'(0, \lambda_m)}{\left. \frac{\partial u(0, \lambda)}{\partial \lambda} \right|_{\lambda = \lambda_m}}$$

This again is an exact equation.⁹ It takes a particularly simple and form when we substitute the formal solution Eq. (2.8) in Eq. (2.14) and use the eigenvalue condition Eq. (2.9).

$$|\psi_m(0)|^2 = \frac{1}{4\pi^2} \frac{2m}{(\hbar)^3} a(0, \lambda) \cdot \frac{\partial E}{\partial n} \quad (2.15)$$

If $\frac{\partial E}{\partial n}$ is determined from the energy spectrum, the only unknown quantity is $a(0, \lambda)$ which can be written as JWKB series as follows. Returning to Eq. (2.3), we solve for $a(r, \lambda)$ as a power series in $\hbar^2$ writing

$$a(r, \lambda) = a_0(r, \lambda) - \hbar^2 a_2(r, \lambda) + \dots \quad (2.16)$$

and substituting in Eq. (2.3) we find

$$a_0(r, \lambda) = p(r, \lambda) = +\sqrt{2m[E - V(r)]} \quad (2.17)$$

$$a_2(r, \lambda) = -\frac{3}{8a_0^3(r, \lambda)} \left(\frac{da_0(r, \lambda)}{dr} \right)^2 + \frac{1}{4a_0^2(r, \lambda)} \frac{da_0^2(r, \lambda)}{dr^2} \quad (2.18)$$

Substituting Eq. (2.17) we get

$$a_2(r, \lambda) = -\frac{U''}{8\sqrt{2m} [E - U(r)]^{3/2}} - \frac{5}{32} \frac{(U')^2}{\sqrt{2m} [E - U(r)]^{5/2}} \quad (2.19)$$

It follows then to order $\hbar^2$

$$|\psi(0)|^2 = \frac{1}{4\pi^2} \frac{(2m)}{\hbar^3} \frac{\partial E}{\partial n} \sqrt{2mE} \left[1 + \frac{\hbar^2 U''(0)}{16 m E^2} + \frac{5\hbar^2}{32} \cdot \frac{(U'(0))^2}{2mE^3} \right] \quad (2.20)$$

It is illuminating to rewrite Eq. (2.20) as

$$|\psi(0)|^2 = \frac{1!}{4\pi} \frac{2m}{\hbar^3} \frac{\partial E}{\partial n} \sqrt{2mE} \cdot \frac{1}{2} \left[\left(1 - \frac{U\left(\frac{\hbar}{\sqrt{2mE}}\right)}{E} \right)^{-1/4} + \left(1 - \frac{U\left(-\frac{\hbar}{\sqrt{2mE}}\right)}{E} \right)^{-1/4} \right] \quad (2.21)$$

This implies that the corrections to $|\psi(0)|^2$ are determined by the value of the potential at one de Broglie wavelength on either side of the origin.¹⁰ This is in conformity with the physical interpretation¹¹ that Eq. (1.2) corresponds to free particle behavior over short time intervals.

III. ENERGY EIGENVALUES

We now return to the quantization condition

$$\frac{1}{\hbar} \int_0^R a(r, \lambda_n) dr = (n - \frac{1}{4})\pi \quad (2.9)$$

and substitute the JWKB series Eq. (2.16) - (2.19). We get

$$\begin{aligned} (n - \frac{1}{4})\pi\hbar = & \int_0^R \sqrt{2m[E - U(r)]} dr + \hbar^2 \int_0^R dr \left\{ \frac{U''}{8\sqrt{2m} [E - U(r)]^{3/2}} \right. \\ & \left. + \frac{5}{32} \frac{(U')^2}{\sqrt{2m} [E - U(r)]^{5/2}} \right\} + O(\hbar^2) \end{aligned} \quad (3.1)$$

As an illustration example consider $U = Ar^k$ ($k =$ positive integer). It is evident that the integrand in the correction term is ill-defined at the classical turning point $r = R$. An elementary way to regularize the integrals is to use the identity

$$\frac{\partial^t}{\partial E^t} [E - U(r)]^\alpha = \alpha(\alpha - 1) \cdots (\alpha - t + 1) [E - U(r)]^{\alpha-t} \quad (3.2)$$

in Eq. (2.10). For large enough integer t , perform the integrals over r and then differentiate t times. We will show, in Section IV, that the correct regularized expression is given by

$$(n - \frac{1}{4})\pi\hbar = \int_0^R \sqrt{2m(E - U(r))} dr + \frac{\hbar^2}{\sqrt{2m}} \delta \quad (3.3)$$

where

$$\delta = -\frac{5}{72} \frac{1}{\int_0^R \sqrt{E-U(r)} dr} + \frac{1}{4} \int_0^R f(r') \sqrt{E-U(r')} dr' [h(r', E)]^2 + \dots \quad (3.4)$$

$$f(r) = \frac{U''(r)}{4(E-U(r))^2} + \frac{5}{32} \frac{[U'(r)]^2}{[E-U(r)]^3} - \frac{5}{72} \frac{1}{\left[\int_0^R (E-U)^{\frac{1}{2}} dr \right]^2}$$

and

$$h(r, E) = \sqrt{\frac{2\pi z}{3}} \{J_{1/3}(z) + J_{-1/3}(z)\} \quad (3.5)$$

$$z(r, E) = \frac{1}{\hbar} \int_r^R \sqrt{2m(E-U(r'))} dr' \quad (3.6)$$

For potentials $U(r)$ analytic at $r = 0$ we can replace $[h(r', E)]^2$ inside the integrand in (3.4) by its average value 2. Doing that we obtain for $U = ar^k$ ($k = 1, 2, \dots$) and

$$E = \lambda a (\hbar^2/2ma)^{k/k+2}$$

$$\lambda^{\frac{1}{2} + \frac{1}{k}} = \frac{2 \left(n - \frac{1}{2}\right) \sqrt{\pi} \Gamma\left(\frac{3}{2} + \frac{1}{k}\right)}{\Gamma\left(1 + \frac{1}{k}\right)} \left\{ 1 + \frac{(k-2)}{96\pi} \frac{\Gamma\left(1 + \frac{1}{k}\right) \Gamma\left(2 - \frac{1}{k}\right)}{\Gamma\left(\frac{3}{2} + \frac{1}{k}\right) \Gamma\left(\frac{3}{2} - \frac{1}{k}\right)} \frac{1}{\left(n - \frac{1}{4}\right)^2} + \dots \right\}$$

for $k \geq 2$

and

$$\lambda = \left[\frac{3\pi}{2} \left(n - \frac{1}{4}\right) \right]^{2/3} \left\{ 1 + \frac{5}{48} \frac{1}{\left[\frac{3\pi}{2} \left(n - \frac{1}{4}\right) \right]^2} + \dots \right\} \quad \text{for } k = 1$$

IV. INTEGRAL EQUATION METHOD

It is evident that, the singular behavior of the integrals in Eq. (3.1) is related to the non-analyticity of $a_0(r, \lambda)$ at $r = R$. Further if we consider potentials of the type $U(r) = Ar^k$ ($k = \text{non-integral}$), $a_0(r, \lambda)$ is non-analytic at the origin as well, so that both Eq. (2.20) and Eq. (3.1) become meaningless. Since this difficulty is artificial due to the failure of the expansion Eq. (2.16) at $r = 0$ and $r = R$ we now consider the integral equation form of the Schrödinger equation which is free from these troubles.

Adopting the procedure due to Langer¹² and Titchmarsh¹³ setting $2m = \hbar = 1$ and defining

$$\zeta(r) = \int_R^r [E - V(r)]^{\frac{1}{2}} dr \quad (4.1)$$

$$\eta(r) = [E - U(r)]^{\frac{1}{4}} u(r) \quad (4.2)$$

the Schrödinger equation can be written as

$$\frac{d^2 \eta}{d\zeta^2} + \left[1 + \frac{5}{36\zeta^2} \right] \eta = \hbar^2 f(r) \eta \quad (4.3)$$

where

$$f(r) = \frac{5}{36} \frac{1}{\left[\int_R^r (E - U(r))^{\frac{1}{2}} dr \right]^2} - \frac{1}{4} \frac{U''}{(E - U)^2} - \frac{5}{16} \frac{(U')^2}{(E - U)^3} \quad (4.4)$$

To solve (4.3) let

$$h(z) = \sqrt{\frac{2\pi z(r)}{3}} \left\{ J_{1/3}(z) + J_{-1/3}(z) \right\}$$

$$j(z) = \sqrt{\frac{\pi z(r)}{2}} J_{1/3}(z)$$

and

$$z(r, E) = \frac{1}{\hbar} \int_r^R \sqrt{2m(E - V(r))} dr \quad (4.4)$$

Then the solution which satisfies the boundary condition at infinity is

$$\eta(r, E) = h(z(r, E)) + \int_r^\infty G(r, r'; E) f(r') \eta(r', E) \sqrt{E - V(r')} dr' \quad (4.5)$$

Note that $h(z(r, E)) \rightarrow 0$ exponentially in r as $r \rightarrow \infty$. The Green's function $G(r, r')$ is given by

$$G(r, r'; E) = h(z(r', E)) j(z(r, E)) - (r \leftrightarrow r') \quad (4.6)$$

The first order solution of the integral equation (4.5) is given by

$$\eta(r, E) = h(z(r, E)) + \int_r^\infty G(r, r'; E) f(r') h(z(r', E)) \sqrt{E - V(r')} dr' \quad (4.7)$$

and should be used in calculation of the energy eigenvalues as well as the calculation of the wavefunction behavior near $r = 0$. The eigenvalue condition is obtained by imposing the boundary condition at $r = 0$, namely the vanishing of the wavefunction there, i.e.

$$\eta(0, E) = 0 \quad (4.8)$$

This leads to the regularization mentioned earlier in the previous section. Note that the integrand in the expression (4.7) has only integrable singularities at $r = 0$ or $r = R$ and is thus perfectly well behaved. The major contribution to the integrals is, of course, from the classically accessible region $R \geq r \geq 0$ as the integrand vanishes exponentially outside that region.

V. LEPTONIC WIDTHS OF τ STATES

As a simple but all the same quite useful application of Eq. (1.2), consider the leptonic widths of the 1S, 2S, 3S and 4S states of the τ resonances. According to recent experimnts¹⁴ the median energy values of these states is given by

$$\begin{aligned} M(\tau) &= 9.4345 \text{ GeV} & \Delta M(2S - 1S) &= 559 \text{ MeV} \\ \Delta M(3S - 1S) &= 889 \text{ MeV} & \Delta M(4S - 1S) &= 1114 \text{ MeV} \end{aligned} \quad (5.1)$$

we shall need only the relative leptonic widths of these states which are known more accurately than their absolute values. We have

$$\begin{aligned} \tilde{\Gamma}_2 &= \frac{\Gamma_2}{\Gamma_1} = 0.39 \pm 0.06 & \tilde{\Gamma}_3 &= \frac{\Gamma_3}{\Gamma_1} = 0.32 \pm 0.04 \\ \tilde{\Gamma}_4 &= \frac{\Gamma_4}{\Gamma_1} = 0.25 \pm 0.07 \end{aligned} \quad (5.2)$$

Now the leptonic width of a vector meson is given by the Van-Röyen Weisskopf formula

$$\Gamma_n = |\psi_n(0)|^2 \cdot \frac{16\pi\alpha^2 e_Q^2}{M_n^2} \cdot K \quad (5.3)$$

where k is a gluonic radiation correction factor presumed to be independent of n . Using Eq. (1.2) we can therefore write if the potential is finite at the origin

$$\tilde{\Gamma}_n = B \frac{k_n}{M_n^2} \frac{dE}{dn} \quad (5.4)$$

where B is a constant whose value we shall not need here, with

$$M_n = 2m_q + E_n \quad k_n^2 = m_q(E_n - V(0)) \quad (5.5)$$

where $V(0)$ is the value of the potential at the origin and m_q is the quark mass ($m_q/2$ is the reduced mass). We calculate the derivation $\frac{dE}{dn}$ at $n = 2, 3, 4$ from

$$\begin{aligned} \frac{dE_2}{dn} &= \frac{1}{2}(E_3 - E_1) & \frac{dE_3}{dn} &= \frac{1}{2}(E_4 - E_2) \\ \frac{dE_4}{dn} &= E_4 - E_3 - \frac{1}{2}(E_4 - E_2 + 2E_3) \end{aligned} \quad (5.6)$$

According to Eq. (5.4) through (5.6)

$$\left(\frac{\tilde{\Gamma}_n M_n^2}{\frac{dE}{dn}} \right)^2 = B^2 (E_n - \text{constant}) \quad (5.7)$$

using for $\tilde{\Gamma}_2$ and $\tilde{\Gamma}_3$ their median values given in (5.2) we predict $\tilde{\Gamma}_4$ to be 0.23, in satisfactory agreement with experiment. Note that the only assumption made about the potential is that it is smooth and finite at the origin.

When data on higher energy levels as well as precise measurements of the leptonic widths become available, it will become necessary to take into account the higher JWKB corrections, especially for small n values. Besides it would be necessary to take into account the Coulombic corrections, as discussed in ref. (15).

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FOOTNOTES AND REFERENCES

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6. For smooth potentials the formulae seem to be good even for small n values. See ref. 5. For an illustrative application of Eq. (1.2) to the T system see Section V of the present paper.
7. Cf. L. D. Landau and E. M. Lifshitz, "Quantum Mechanics Non-Relativistic Theory." Translated by J. B. Sykes and J. S. Bell. Second edition 1965, Pergamon Press, Chapter VII §47.
8. The extra factor $\frac{1}{4\pi}$ in Eq. (2.14) is the normalization factor for the angular part of the wavefunction.
9. Eq. (2.14) was derived independently by J. S. Bell. Private communication to one of us (J.P.) in 1979.
10. We have assumed $U(0) = 0$; otherwise replace E by $E - U(0)$ and $U\left(\pm \frac{\hbar}{\sqrt{2mE}}\right)$ by $U\left(\pm \frac{\hbar}{\sqrt{2m(E - U(0))}}\right) - U(0)$ in Eq. (2.21). Notice that a JWKB estimate

of the correction can be obtained from the knowledge of $\frac{dE}{dn}$ by the

$$\text{inversion formula } r(V) = \frac{2\hbar}{(2m)^{1/2}} \int_0^V \frac{dE}{(V-E)^{1/2}} \left(\frac{dE}{dn} \right)^{-1}.$$

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