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The JWKB Method in Central-Field Problems. Planar Radial Wave Equation and Resolution of Kramers' Dilemma[†]

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It is well-known that applications of the JWKB method to central-field problems in three dimensions require half-integral quantization of the angular momentum for their success. Thus, the square of the angular momentum must be represented by the term $(\ell + {}^1/_2)^2\hbar^2$ rather than $\ell(\ell + 1)\hbar^2$. This was first shown by Kramers in 1926 and has subsequently been discussed by several authors including, in particular, Langer (1937). While Kramers based his discussion on the ordinary radial variable r, Langer switched to the variable x defined by $r = e^x$. In this new representation of the central-field problem, the expression $(\ell + {}^1/_2)^2\hbar^2$ emerges naturally. The ad hoc character of the Langer transformation has, however, often been emphasized. In the present communication, we choose a different entry to the problem. We keep the variable r and focus on physically equivalent forms of the radial Schrödinger equation in this variable. This leads to a smoother emergence of the $(\ell + {}^1/_2)^2\hbar^2$ term. Our analysis is carried out for a general dimension D. For a given D, there are D physically equivalent radial equations, corresponding to the subdimensions $d = 1, 2, ..., D$. We show that it is only the $d = 2$ equation that can be satisfactorily treated by the JWKB approximation. In the past, the focus was always on the $d = 1$ equation, and this was the reason behind the problems encountered by Kramers and Langer. As to the $d = 2$ equation, we finally show that this equation also is the most convenient starting point for determining the exact solutions of a central-field problem for general values of D and angular-momentum quantum number L.

1. Introduction

An important version of semiclassical quantum mechanics is the so-called Jeffreys−Wentzel−Kramers−Brillouin method (JWKB or WKB method). In the present paper we discuss an old dilemma which complicates the application of this method to central-field problems. It has been with us since 1926, and has attracted much interest in the intervening years, but the dilemma has so far not been fully resolved.

To state the dilemma, consider the time-independent Schrödinger equation for a particle moving in a central field $V(r)$

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r}) + V(r)\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{1}$$

where $\mathbf{r} = (x, y, z)$ is the radius vector of the particle, μ is its mass, and E is its energy. The potential function $V(r)$ may be singular at the origin, but we assume that $|V(r)|$ diverges less strongly than $1/r^2$. The eigenfunctions of the Schrödinger equation may be written in the well-known form

$$\psi(\mathbf{r}) = R(r)Y_{\ell m}(\theta,\phi) \tag{2}$$

where (θ,ϕ) are the spherical polar coordinates of the particle, $Y_{\ell m}(\theta,\phi)$ is a normalized spherical harmonic, and ℓ and m are the usual angular-momentum quantum numbers. Besides $R(r)$, it is customary to introduce the radial function $P(r)$, as given by the definition

$$P(r) = rR(r) \tag{3}$$

The radial function $R(r)$ is determined by the radial Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\left(\frac{d^2R(r)}{dr^2} + \frac{2}{r}\frac{dR(r)}{dr}\right) + V(r)R(r) + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2}R(r) = ER(r) \tag{4}$$

while $P(r)$ satisfies the equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2P(r)}{dr^2} + V(r)P(r) + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2}P(r) = EP(r) \tag{5}$$

The differential equation for $P(r)$ has the same form as the Schrödinger equation for a one-dimensional particle moving in the effective potential

$$V_{\rm eff}(r) = V(r) + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2} \tag{6}$$

It is therefore tempting to try to solve it by applying the JWKB method to it. By this method,[1−4] one first finds analytical solutions that are approximately valid away from the so-called

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classical turning points, that is, the points at which the function

$$Q^2(r) = \frac{2\mu}{\hbar^2}[E - V_{\text{eff}}(r)] \tag{7}$$

becomes zero and changes sign. These solutions are then matched at the two sides of a turning point under the application of connection formulas[3,5−8] and perhaps continued through the turning-point region as Airy functions.[3,5] For bound states, where two or more turning points must be considered simultaneously, this is only possible at certain energies which, accordingly, become the approximate bound-state energies.

An investigation of eq 5 along these lines was first made by Kramers,[3] with $V(r)$ being an attractive Coulomb-like potential. He found, however, that such a procedure led to an unacceptable behavior of $P(r)$ for small values of r. And for $\ell = 0$ it could not be applied at all because expression 6 only defines a single turning point in this case. Kramers showed, however, that if one adds a term $\hbar^2/8\mu r^2$ to $V(r)$ or, equivalently, modifies the centrifugal term by writing $(\ell + {}^1/_2)^2$ instead of $\ell(\ell + 1)$, to get the modified effective potential

$$V_{\text{eff}}^{\text{mod}}(r) = V(r) + \frac{\left(\ell + \frac{1}{2}\right)^2 \hbar^2}{2\mu r^2} \tag{8}$$

then the difficulties associated with the JWKB method disappeared. With this modified potential, the method was found to give very satisfactory results, both for attractive and repulsive potentials.[3,9,10] It is now well-known that it even gives the correct bound-state energy eigenvalues for the harmonic potential and the attractive Coulomb potential (see section 6).

The classical central-field problem is defined by the effective potential

$$V_{\text{cl}}(r) = V(r) + \frac{l^2}{2\mu r^2} \tag{9}$$

where l is the classical angular momentum. Expression 8 may therefore be said to originate from expression 9 by half-integral quantization of the classical angular momentum.[3]

The fact that one must choose between the two expressions 6 and 8, and make an ad hoc choice rather than a rational one to get acceptable results, is what we refer to as *Kramers' dilemma* in the present paper. It is the resolution of this dilemma that is the theme of our article. The article is organized as follows. In section 2 we describe some earlier work on the resolution of Kramers' dilemma in ordinary three-dimensional space and add a qualitative presentation of our own entrance to the problem. Our quantitative analysis is carried out in a general D-dimensional space and is deferred to the following sections. Thus, a discussion of the general D-dimensional central-field problem is given in section 3, with emphasis put on the fact that the radial Schrödinger equation may be written in D physically equivalent ways, corresponding to the respective subdimensions $d = 1, 2, ..., D$. In section 4 we investigate the possibility of applying the JWKB approximation to each of the D radial equations in turn and conclude that a satisfactory result only is attainable for $d = 2$. We then collect the quantization formulas based on the $d = 2$ equation in section 5. In section 6 we specialize to the isotropic harmonic oscillator and the hydrogen atom for which the JWKB energies, as already mentioned, agree with the exact ones. We make the observation that the $d = 2$ radial equation also is the most convenient starting point for an exact treatment of a D-dimensional radial problem and illustrate this with the harmonic oscillator and the hydrogen atom as examples. In section 7 we comment on the fact that the Kramers correction is independent of D. Section 8 contains our conclusion.

2. Resolving Kramers' Dilemma

2.1. Langer's Transformation. We begin by noting that the domain of the independent variable r in the Schrödinger eq 5 is from 0 to ∞. In a genuine one-dimensional problem the domain would be from $-\infty$ to ∞. In an important paper, Langer[5] pointed to this difference as the source of the problem of applying the JWKB method to eq 5. While concentrating on the Coulomb case

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} \tag{10}$$

he therefore transformed eq 5 into a new equation by the substitution

$$r = e^x, \quad P = e^{x/2}u \tag{11}$$

The domain of the independent variable, x, is now from $-\infty$ to ∞, the differential equation for $u(x)$ taking the form

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \frac{2\mu}{\hbar^2}\left(Ee^{2x} + \frac{Ze^2}{4\pi\epsilon_0}e^x\right)u(x) - \left(\ell + \frac{1}{2}\right)^2 u(x) = 0 \tag{12}$$

In this differential equation, the angular-momentum quantum number ℓ appears in the combination $(\ell + {}^1/_2)^2$ rather than $\ell(\ell + 1)$. As Langer showed, the application of the JWKB method to eq 12 is unproblematic. It leads to a quantization condition that, expressed in the original r-coordinate, is defined by the modified effective potential (eq 8). Hence, it produces the correct energies for the Coulomb problem.

The Langer transformation is, however, not unique.[11−13] Other transformations of the form $r = f(x)$ may be constructed and lead to different modified effective potentials and hence to less satisfactory energies. How then does one choose one transformation over another? A simple qualified answer to this question has been given by Adams and Miller.[14] They suggested that the transformation, and hence the modified potential, be so chosen that the correct quantum-mechanical result, either for the scattering phase shift or for the energy eigenvalues, is obtained if the original potential is set to zero. They applied this condition both for semi-infinite intervals such as $0 \leq r < \infty$ and for finite intervals $a \leq r \leq b$ and showed, in particular, that it made the Langer transformation unique.

2.2. The Planar Radial Wave Equation. In the present paper, we take a new look at Kramers' dilemma. It is based on the conjecture that it is not the domain of the independent variable r that causes the problem, but solely the fact that the differential eq 5 is singular at the origin. In accordance with this viewpoint, we do not dismiss r as a proper independent variable. Instead, we merely consider alternative, but physically equivalent forms of the differential equation itself and try to apply the JWKB description to each of these equations separately. It turns out that only one of the physically equivalent equations can be satisfactorily attacked by the JWKB method. This conclusion, then, resolves Kramers' dilemma in an unforced way.

To be specific, we note that for a normalized wave function of form 2, we have that

$$\int_0^\infty R^2(r)r^2\,\mathrm{d}r = \int_0^\infty P^2(r)\,\mathrm{d}r = 1 \tag{13}$$

Hence, $R^2(r)$ may be referred to as a spatial probability density (with the "volume element" defined as $r^2\,dr$). On the other hand, $P^2(r)$ is a radial probability density. But we may also introduce a new function,[15] $T(r)$, which determines a planar probability density, $T^2(r)$, in the sense that

$$\int_0^\infty T^2(r) r\,\mathrm{d}r = 1 \tag{14}$$

The function $T(r)$ is defined as

$$T(r) = \sqrt{r}R(r) \tag{15}$$

It satisfies the differential equation

$$-\frac{\hbar^2}{2\mu}\left(\frac{\mathrm{d}^2T(r)}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}T(r)}{\mathrm{d}r}\right) + V(r)T(r) + \frac{\left(\ell + \frac{1}{2}\right)^2\hbar^2}{2\mu r^2}T(r) = ET(r) \tag{16}$$

which we shall refer to as the planar radial wave equation. We note that it also contains ℓ in the same way as expression 8 does, namely, in the combination $(\ell + {}^1/_2)^2$.

Let us temporarily write the three equations, eq 4, eq 16, and eq 5, as

$$\hat{H}^{(3)}R(r) = ER(r) \tag{17}$$

$$\hat{H}^{(2)}T(r) = ET(r) \tag{18}$$

$$\hat{H}^{(1)}P(r) = EP(r) \tag{19}$$

respectively. We have then that

$$\hat{H}^{(2)} = r^{1/2}\hat{H}^{(3)}r^{-1/2} \tag{20}$$

and

$$\begin{aligned}\hat{H}^{(1)} &= r^{1/2}\hat{H}^{(2)}r^{-1/2} \\ &= r\hat{H}^{(3)}r^{-1}\end{aligned} \tag{21}$$

These relations specify the sense in which the three physically equivalent equations, eq 17, eq 18, and eq 19, are mathematically equivalent. Obviously, the origin plays a complicated singular role because of the factors $r^{-1/2}$ and r^{-1}.

From the outset, there is no reason eq 19 should be more fundamental than eqs 17 and 18 as a candidate for an application of the JWKB method. Admittedly, the equation is the only one that does not contain a first-order term in d/dr, but actually, a first-order term presents no difficulties, as already emphasized by Wentzel.[2] Hence, a complete JWKB analysis of the radial problem should investigate the possible application of the JWKB method to each of the three equations separately. Due to the singular status given to the origin by relations 20 and 21, there is no guarantee that each equation is equally favorable in this respect. This is the philosophy behind the present work.

In this spirit, we have also applied the JWKB approximation to eq 4. We have found similar problems as Kramers noted for eq 5. However, the application of the JWKB approximation to eq 16 turns out to be unproblematic.

Kramers' dilemma is thus fully resolved by noting that it is eq 16 which is the proper starting point for the application of the JWKB approximation. The optimal procedure is therefore to concentrate on $T(r)$ and subsequently determine $R(r)$ and $P(r)$ from the relations

$$R(r) = T(r)/\sqrt{r} \tag{22}$$

$$P(r) = \sqrt{r}T(r) \tag{23}$$

instead of looking for them as JWKB solutions to eqs 4 and 5.

Our approach also throws new light on the success behind Langer's method. His analysis may, in fact, be considered as nothing more than a somewhat complicated way of solving eq 16 by the JWKB method. For as eq 23 shows, the function $u(x)$ defined by eq 11 is exactly the function $T(r)$ expressed in the variable x instead of the variable r. Equations 12 and 16 are accordingly equivalent.

The importance of our conclusions is amplified by noting that they may be extended from three dimensions to any dimension. In the D-dimensional central-field problem, one may define D radial functions. Thus, we obtain D differential equations. But it turns out that among those, the JWKB approximation may only be applied to the planar equation. We prove these assertions in the following sections. The results of the present section follow from the general case by putting $D = 3$. Hence, we do not derive them independently here.

3. The Central-Field Problem in *D* Dimensions

The Schrödinger eq 1 is readily generalized to D dimensions ($D \geq 2$) by letting $\mathbf{r} = (x_1, x_2, ..., x_D)$ denote the position vector of a "particle" moving in D-dimensional position space,[16] where $(x_1, x_2, ..., x_D)$ are Cartesian coordinates. r is now the hyperradius as given by the relation $r^2 = x_1^2 + x_2^2 + ... + x_D^2$, and ∇^2 denotes the D-dimensional Laplacian.

The eigenfunctions of the Schrödinger equation may now be written

$$\psi(\mathbf{r}) = R^{(D)}(r)Y_{L\gamma}(\Omega) \tag{24}$$

Here, Ω is a collective notation for $D - 1$ angular coordinates, and $Y_{L\gamma}(\Omega)$ is a hyperspherical harmonic.[17-22] The hyperspherical harmonics are eigenfunctions of the grand angular-momentum operator

$$\hat{L}^2 = \frac{1}{2}\sum_{i=1}^{D}\sum_{j=1}^{D}\hat{\ell}_{ij}^2 \tag{25}$$

where

$$\hat{\ell}_{ij} = x_i\hat{p}_j - x_j\hat{p}_i, \quad i, j = 1, 2, ..., D \tag{26}$$

are the components of the angular-momentum tensor. The operators $\hat{p}_i$ are the components of the D-dimensional momentum operator.

The operator $\hat{L}^2$ has the eigenvalues

$$L(L + D - 2), \quad L = 0, 1, ... \tag{27}$$

with the degeneracy corresponding to the eigenvalue L being[21,22]

$$g(D, L) = \frac{(2L + D - 2)(L + D - 3)!}{L!(D - 2)!} \tag{28}$$

In a central-field problem, this is the number of hyperspherical harmonics associated with a given L-value. In eq 24 they are denoted by $Y_{L\gamma}(\Omega)$.

The Schrödinger equation for the radial function $R^{(D)}(r)$ of eq 24 is

$$\frac{d^2R^{(D)}(r)}{dr^2} + \frac{D-1}{r}\frac{dR^{(D)}(r)}{dr} - \frac{L(L+D-2)}{r^2}R^{(D)}(r) + \frac{2\mu}{\hbar^2}[E-V(r)]R^{(D)}(r) = 0 \quad (29)$$

For a normalized wave function, $\psi(\mathbf{r})$, we have that

$$\int_0^\infty [R^{(D)}(r)]^2 r^{D-1}\, dr = 1 \quad (30)$$

Hence, $[R^{(D)}(r)]^2$ is a probability density in D-dimensional space, the "volume element" being r^{D-1} dr.

The function $P^{(D)}(r)$ which determines the corresponding radial probability density as $[P^{(D)}(r)]^2$, such that

$$\int_0^\infty [P^{(D)}(r)]^2\, dr = 1 \quad (31)$$

is

$$P^{(D)}(r) = r^{(D-1)/2}\, R^{(D)}(r) \quad (32)$$

It satisfies the differential equation

$$\frac{d^2P^{(D)}(r)}{dr^2} - \left[\frac{L(L+D-2)}{r^2} + \frac{(D-1)(D-3)}{4r^2}\right]P^{(D)}(r) + \frac{2\mu}{\hbar^2}[E-V(r)]P^{(D)}(r) = 0 \quad (33)$$

Equations 9 and 33 are the generalizations to D dimensions of the corresponding eqs 4 and 5 in three dimensions. We note that the effective potential defined by eq 33 has the form

$$V_{\text{eff}}^{(D,1)}(r) = V(r) + \frac{L(L+D-2)\hbar^2}{2\mu r^2} + \frac{(D-1)(D-3)\hbar^2}{8\mu r^2} \quad (34)$$

The last term in the expression for $V_{\text{eff}}^{(D,1)}(r)$ is the *quantum fictitious potential* that we have discussed in earlier work.[23] We note that it disappears in three dimensions, in accordance with eq 5.

The functions $R^{(D)}(r)$ and $P^{(D)}(r)$ are just two members of a set of D radial functions, defined by the relation

$$R^{(D,d)}(r) = r^{(D-d)/2}\, R^{(D)}(r), \quad d = 1, 2, ..., D \quad (35)$$

Obviously, $R^{(D,1)}(r) = P(r)$ and $R^{(D,D)}(r) = R^{(D)}(r)$. For a normalized wave function of the form 24 we have that

$$\int_0^\infty [R^{(D,d)}(r)]^2 r^{d-1}\, dr = 1 \quad (36)$$

Hence, $[R^{(D,d)}(r)]^2$ is a probability density in a d-dimensional subspace.

The Schrödinger equation determining the radial function $R^{(D,d)}(r)$ is found to be

$$\frac{d^2R^{(D,d)}(r)}{dr^2} + \frac{d-1}{r}\frac{dR^{(D,d)}(r)}{dr} - \left[\frac{L(L+D-2)}{r^2} + \frac{(D-d)(D+d-4)}{4r^2}\right]R^{(D,d)}(r) + \frac{2\mu}{\hbar^2}[E-V(r)]R^{(D,d)}(r) = 0 \quad (37)$$

or

$$\frac{d^2R^{(D,d)}(r)}{dr^2} + \frac{d-1}{r}\frac{dR^{(D,d)}(r)}{dr} - \frac{\mathscr{L}(\mathscr{L}+d-2)}{r^2}R^{(D,d)}(r) + \frac{2\mu}{\hbar^2}[E-V(r)]R^{(D,d)}(r) = 0 \quad (38)$$

where

$$\mathscr{L} = L + \frac{D-d}{2} \quad (39)$$

In the following, we shall consider the possible application of the JWKB method to eq 38.

4. The Radial JWKB Problem in *D* Dimensions

We begin by writing eq 38 in the form

$$\frac{d^2R^{(D,d)}(r)}{dr^2} + \frac{d-1}{r}\frac{dR^{(D,d)}(r)}{dr} + Q^2(r)R^{(D,d)}(r) = 0 \quad (40)$$

with

$$Q(r) = \frac{1}{\hbar}\left\{2\mu[E-V(r)] - \frac{\mathscr{L}(\mathscr{L}+d-2)\hbar^2}{r^2}\right\}^{1/2} \quad (41)$$

We then seek solutions of eq 40 of the form

$$\varphi(r) = A(r)e^{i\sigma(r)} \quad (42)$$

For the sake of simplicity, we have suppressed the (D, d)-dependence of the functions $Q(r)$, $\varphi(r)$, $A(r)$, and $\sigma(r)$. We take $A(r)$ and $\sigma(r)$ to be even and odd functions of $\hbar$, respectively. Since eq 40 is invariant under the substitution $\hbar \to -\hbar$, this implies that $A(r)e^{-i\sigma(r)}$ is a solution of this equation when $A(r)e^{i\sigma(r)}$ is. Hence $R^{(D,d)}(r)$ may be written

$$R^{(D,d)}(r) = A(r)\{c_1e^{i\sigma(r)} + c_2e^{-i\sigma(r)}\} \quad (43)$$

where c_1 and c_2 are complex constants. Our problem is to determine the approximate form of $A(r)$ and $\sigma(r)$.

To this end, we substitute expression 42 into eq 40 to get

$$\frac{d^2A}{dr^2} + \frac{d-1}{r}\frac{dA}{dr} - A\left(\frac{d\sigma}{dr}\right)^2 + Q^2A + i\left[A\frac{d^2\sigma}{dr^2} + \frac{d-1}{r}A\frac{d\sigma}{dr} + 2\frac{dA}{dr}\frac{d\sigma}{dr}\right] = 0 \quad (44)$$

Because A is an even function of $\hbar$, while σ is an odd function, this equation falls apart in two separate equations, namely,

$$\frac{d^2A}{dr^2} + \frac{d-1}{r}\frac{dA}{dr} - A\left(\frac{d\sigma}{dr}\right)^2 + Q^2A = 0 \quad (45)$$

and

$$A\frac{\mathrm{d}^2\sigma}{\mathrm{d}r^2} + \frac{d-1}{r}A\frac{\mathrm{d}\sigma}{\mathrm{d}r} + 2\frac{\mathrm{d}A}{\mathrm{d}r}\frac{\mathrm{d}\sigma}{\mathrm{d}r} = 0 \tag{46}$$

The second of these equations has the solution

$$A(r) = \frac{C}{r^{(d-1)/2}}\frac{1}{(\sigma'(r))^{1/2}} \tag{47}$$

where C is an arbitrary constant and the prime denotes differentiation with respect to r.

We now divide eq 45 from the left by $A(r)$ to get

$$\frac{1}{A}\frac{\mathrm{d}^2A}{\mathrm{d}r^2} + \frac{d-1}{r}\frac{1}{A}\frac{\mathrm{d}A}{\mathrm{d}r} - \left(\frac{\mathrm{d}\sigma}{\mathrm{d}r}\right)^2 + Q^2 = 0 \tag{48}$$

and then substitute the form of $A(r)$ into this equation. After some cumbersome reductions this leads to the equation

$$(\sigma')^2 - Q^2 + \frac{(d-1)(d-3)}{4r^2} + \frac{1}{2}\frac{\sigma'''}{\sigma'} - \frac{3}{4}\left(\frac{\sigma''}{\sigma'}\right)^2 = 0 \tag{49}$$

To proceed, we now put

$$\sigma(r) = \int^r q(r)\,\mathrm{d}r \tag{50}$$

and substitute this expression into eq 49. This gives

$$q(r)^2 - Q(r)^2 + \frac{1}{4}\frac{(d-1)(d-3)}{r^2} + \frac{1}{2}\frac{q''(r)}{q(r)} - \frac{3}{4}\left(\frac{q'(r)}{q(r)}\right)^2 = 0 \tag{51}$$

We shall not pursue the problem of determining the general form $q(r)$ from eq 51. We are interested in determining if $q(r) = Q(r)$ is already a reasonable approximate solution. For expression 43 for $R^{(D,d)}(r)$, together with eq 47, would then give

$$R^{(D,d)}(r) = \frac{1}{r^{(d-1)/2}}\frac{1}{Q(r)^{1/2}}\{c_1\mathrm{e}^{\mathrm{i}\int^r Q(r)\mathrm{d}r} + c_2\mathrm{e}^{-\mathrm{i}\int^r Q(r)\mathrm{d}r}\} \tag{52}$$

which is the JWKB expression for $R^{(D,d)}(r)$.

Thus, we must direct our attention toward the function

$$\tau(r) = \frac{1}{4}\frac{(d-1)(d-3)}{r^2} + \frac{1}{2}\frac{Q''(r)}{Q(r)} - \frac{3}{4}\left(\frac{Q'(r)}{Q(r)}\right)^2 \tag{53}$$

which must be small for eq 52 to be approximately valid. Obviously, $\tau(r)$ is ill behaved at the zeros of the function $Q(r)$, but eq 52 is only sought as a solution away from these zeros anyway. The serious problem is that, in general, $\tau(r)$ must also be suspected to blow up for values of r close to the origin. This was, in fact, the behavior noted by Kramers[3] and Langer[5] for the three-dimensional hydrogen atom, with $d = 1$. In their case, the first term on the right-hand side of eq 53 is absent, and $\tau(r)$ becomes identical with Langer's auxiliary function $\omega_0(r)$, apart from a change of sign. It was the undesired behavior of $\omega_0(r)$ that led Langer to introduce transformation 11 which bears his name. In our more general analysis, we are free to choose d different from 1, and we shall now see how to take advantage of this freedom.

We begin by assuming that the term $\mathscr{L}(\mathscr{L} + d - 2)\hbar^2/r^2$ in expression 41 for $Q(r)$ is nonzero. As always, we also assume that $|V(r)|$ diverges less strongly than $1/r^2$ at the origin. We then have, for sufficiently small values of r, that

$$Q(r) \approx \frac{a}{r} \tag{54}$$

where a is a complex constant. With this expression for $Q(r)$, we find that

$$\frac{1}{2}\frac{Q''(r)}{Q(r)} - \frac{3}{4}\left(\frac{Q'(r)}{Q(r)}\right)^2 \approx \frac{1}{4r^2} \tag{55}$$

and eq 53 becomes

$$\tau(r) \approx \frac{1}{4}\frac{(d-1)(d-3)}{r^2} + \frac{1}{4r^2} \tag{56}$$

Obviously, the condition for $\tau(r)$ to become approximately zero close to the origin, is that $(d-1)(d-3) = -1$. But the only value of d for which this happens is $d = 2$.

We have thus arrived at the important conclusion that the only circumstance under which the JWKB description may be expected to give reasonable results is when it is applied to the radial eq 38 with $d = 2$. But can it be applied for any D? The condition is that eq 54 hold, that is, the quantity $\mathscr{L}(\mathscr{L} + d - 2)$ must be nonzero. With the definition 39 of $\mathscr{L}$, we have that

$$\mathscr{L}(\mathscr{L} + d - 2) \overset{d=2}{=\!=} \mathscr{L}^2 = \left(L + \frac{D}{2} - 1\right)^2 \tag{57}$$

This expression is actually nonzero, apart from the particular case where $D = 2$ and $L = 0$. Hence, the JWKB description should, in fact, be a reasonable description for any D and any L, except for the special case $(D, L) = (2, 0)$.[24]

In light of this conclusion, let us now introduce a special notation when $d = 2$ and, in analogy with the terminology of section 2, denote the radial function $R^{(D,2)}(r)$ by $T^{(D)}(r)$. We have then, in accordance with eq 35

$$T^{(D)}(r) = r^{(D-2)/2}R^{(D)}(r) \tag{58}$$

and

$$\int_0^\infty [T^{(D)}(r)]^2 r\,\mathrm{d}r = 1 \tag{59}$$

$[T^{(D)}(r)]^2$ is a planar probability density.

According to eqs 38 and 57 the radial equation for $T^{(D)}(r)$ is

$$\frac{\mathrm{d}^2T^{(D)}(r)}{\mathrm{d}r^2} + \frac{1}{r}\frac{\mathrm{d}T^{(D)}(r)}{\mathrm{d}r} - \frac{\left(L + \frac{D}{2} - 1\right)^2}{r^2}T^{(D)}(r) + \frac{2\mu}{\hbar^2}[E - V(r)]T^{(D)}(r) = 0 \tag{60}$$

The effective potential defined by this equation is

$$V_{\mathrm{eff}}^{(D,2)}(r) = V(r) + \frac{\left(L + \frac{D}{2} - 1\right)^2\hbar^2}{2\mu r^2} \tag{61}$$

The function $Q(r)$ of eq 41 therefore takes the form

$$Q^{(D,2)}(r) = \frac{1}{\hbar}\left\{2\mu[E - V(r)] - \frac{\left(L + \frac{D}{2} - 1\right)^2\hbar^2}{r^2}\right\}^{1/2} \tag{62}$$

and the JWKB solution 52 away from the zeros of $Q^{(D,2)}(r)$

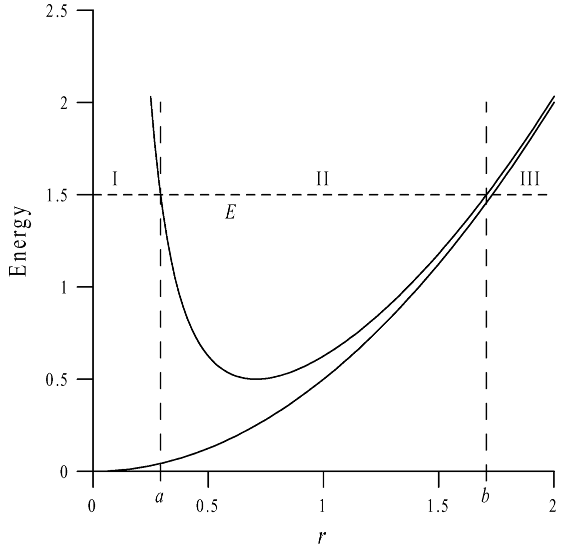

Figure 1. JWKB description of the isotropic harmonic oscillator in three dimensions ($D = 3$), $L = 0$ states. The lower curve shows the potential energy $V(r) = {}^1\!/_2\mu\omega^2 r^2$, the upper curve shows the effective potential defined by eq 61, which in this case ($D = 3$, $L = 0$) reads $V_{\text{eff}}^{(3,2)}(r) = V(r) + \hbar^2/8\mu r^2$. The variable r is measured in units of the characteristic length $\sqrt{\hbar/\mu\omega}$; energies are measured in units of $\hbar\omega$; a and b are the modified classical turning points corresponding to the energy E.

becomes

$$T^{(D)}(r) = \frac{1}{\sqrt{r}}\frac{1}{Q^{(D,2)}(r)^{1/2}}\{c_1 \mathrm{e}^{\mathrm{i}\int^r Q(D,2)(r)\mathrm{d}r} + c_2 \mathrm{e}^{-\mathrm{i}\int^r Q(D,2)(r)\mathrm{d}r}\} \quad (63)$$

These expressions give the general solution of the radial JWKB problem in D dimensions. The results for the three-dimensional case discussed in sections 1 and 2 follow, of course, from these expressions by putting $D = 3$. Thus, eq 16 results from eq 60 in this way.

As to the values of the coefficients c_1 and c_2, they stay constant within a region of r free from zeros of the function $Q^{(D,2)}(r)$ but change in a discontinuous way when one passes a zero of $Q^{(D,2)}(r)$. The pattern is the usual one known from the JWKB discussion of motion in a single dimension. In the following section, we list the bound-state results for an attractive potential, where the effective potential $V_{\text{eff}}^{(D,2)}(r)$ of eq 61 defines a single potential well.

5. JWKB Quantization

As an illustration, Figure 1 shows the effective-potential well associated with the $L = 0$ states of an isotropic harmonic oscillator in three dimensions ($D = 3$). The qualitative form of the well is shared with other attractive potentials and other D- and L-values, and the expressions below refer to such general potentials. a and b are the modified classical turning points corresponding to the energy E. They are defined by the zeros of the function $Q^{(D,2)}(r)$ of eq 62. The regions I, II, and III refer to the domains $0 < r < a$, $a < r < b$, and $r > b$, respectively.

For a bound state, the JWKB wave function 63 takes the following form in the various regions, where indices I and III refer to the regions I and III, while indices a and b refer to the left and right parts, respectively, of region II:

$$T_I^{(D)}(r) = \frac{c}{2\sqrt{r}}\frac{1}{|Q^{(D,2)}(r)|^{1/2}}\exp(-\int_r^a |Q^{(D,2)}(r)|\,\mathrm{d}r) \quad (64)$$

$$T_{III}^{(D)}(r) = \frac{c'}{2\sqrt{r}}\frac{1}{|Q^{(D,2)}(r)|^{1/2}}\exp(-\int_b^r |Q^{(D,2)}(r)|\,\mathrm{d}r) \quad (65)$$

$$T_a^{(D)}(r) = \frac{c}{\sqrt{r}}\frac{1}{Q^{(D,2)}(r)^{1/2}}\cos(\int_a^r Q^{(D,2)}(r)\,\mathrm{d}r - \pi/4) \quad (66)$$

$$T_b^{(D)}(r) = \frac{c'}{\sqrt{r}}\frac{1}{Q^{(D,2)}(r)^{1/2}}\cos(\int_r^b Q^{(D,2)}(r)\,\mathrm{d}r - \pi/4) \quad (67)$$

with the requirement that $T_a^{(D)}(r) = T_b^{(D)}(r)$. We have drawn on the well-known connection formulas for one-dimensional JWKB problems.[3,5−8,25,26]

The condition $T_a^{(D)}(r) = T_b^{(D)}(r)$ gives the quantization requirement

$$\int_a^b Q^{(D,2)}(r)\,\mathrm{d}r = \left(s + \frac{1}{2}\right)\pi, \quad s = 0, 1, 2, ... \quad (68)$$

with $c' = c$ for s even, and $c' = -c$ for s odd. This relation determines the possible bound-state energies. It is, of course, the standard quantization condition of one-dimensional JWKB theory, with the effective potential 61 playing the role of the one-dimensional potential.

Having determined an allowed energy from relation 68, the JWKB approximation to the corresponding radial function $T^{(D)}(r)$ is given by expressions 64−67. The whole set of D radial functions corresponding to the chosen energy may then be obtained via eq 35. In particular, the radial function $P^{(D)}(r)$ of eq 32 is obtained by multiplying expressions 64−67 by $\sqrt{r}$.

6. The Isotropic Harmonic Oscillator and the Hydrogen Atom in *D* Dimensions

6.1. JWKB Energies. With the application of appropriate techniques[27] for evaluating the integral on the left-hand side of eq 68, it is readily shown that the quantization condition represented by that equation reproduces the exact energies, as given below, for the isotropic harmonic oscillator and the hydrogen atom in any dimension. This is even true for the case $(D, L) = (2, 0)$, if the origin is taken as the left turning point. The combination $(D, L) = (2, 0)$ was excluded from the general analysis because the factor $(L + D/2 - 1)$ in eq 57 becomes zero in this case. To understand that it may nevertheless be included, we note that our whole analysis holds for any positive, nonzero value of L, even if L is not an integer. The validity for $(D, L) = (2, 0)$ may therefore be considered to follow as a limiting case during the transition $(2, L) \rightarrow (2, 0)$.

That the JWKB method gives the correct energy eigenvalues for the harmonic oscillator and the hydrogen atom in any dimension is, to a large extent, well-known. For $D = 3$, the reason for the success of the JWKB method in this respect has been discussed by several authors, most conclusively by Rosenzweig and Krieger.[28] Their conclusions may be readily extended to cover all values of D.

6.2. Exact Solutions From the Planar Radial Wave Equation. The exact analytical solutions for the harmonic oscillator and the hydrogen atom in D dimensions have been carefully studied in the literature.[20,29] The point of departure for determining the solutions has usually been eq 29 for the radial function $R^{(D)}(r)$ or eq 33 for the radial function $P^{(D)}(r)$. Here we want to point out, that among the D radial equations given by expression 38, eq 60 for $T^{(D)}(r)$ has an especially simple form because, according to eq 57, the factor $\mathscr{L}(\mathscr{L} + d - 2)$ reduces to the square $(L + D/2 - 1)^2$. This implies, in turn, that not only does the equation for $T^{(D)}(r)$ hold a preferred position as far as the JWKB approximation goes, it is also a more convenient starting point for obtaining analytical solutions of the Schrödinger equation, when such solutions exist. This holds for a general potential $V(r)$. In the following we demonstrate it for the isotropic harmonic oscillator and the hydrogen atom in arbitrary dimensions.

According to eq 60, the function $T^{(D)}(r)$ only depends upon the dimension D and the angular momentum L through the parameter

$$\alpha = L + \frac{D}{2} - 1 \qquad (69)$$

We may hence rewrite eq 60 as

$$\frac{d^2T_\alpha(r)}{dr^2} + \frac{1}{r}\frac{dT_\alpha(r)}{dr} - \frac{\alpha^2}{r^2}T_\alpha(r) + \frac{2\mu}{\hbar^2}[E - V(r)]T_\alpha(r) = 0 \qquad (70)$$

The fact that this differential equation only contains the orbital angular momentum L and the dimension D in the combination $\alpha = L + D/2 - 1$ implies an isomorphism in the sense that $D \rightarrow D + 2$ is equivalent to $L \rightarrow L + 1$. This isomorphism, which holds for any central-field potential, is well-known,[30] but it is usually derived in a somewhat less direct way from the differential equation for $R^{(D)}(r)$, or the differential equation for $P^{(D)}(r)$.

For the harmonic potential

$$V(r) = \frac{1}{2}\mu\omega^2 r^2 \qquad (71)$$

eq 70 may be solved analytically by the well-known polynomial method.[31] Applying this method, one finds the bound-state energies to be

$$E(\alpha, s) = (\alpha + 2s + 1)\hbar\omega, \quad s = 0, 1, 2, ... \qquad (72)$$

The corresponding eigenfunctions are

$$T_{\alpha,\, s}(r) = \mathcal{N}(\alpha, s)\xi^{\alpha}M(-s, \alpha + 1, \xi^2)e^{-\xi^2/2} \qquad (73)$$

where

$$\xi = \sqrt{\frac{\mu\omega}{\hbar}}r \qquad (74)$$

and $M(-s, \alpha + 1, \xi^2)$ is the confluent hypergeometric, or Kummer's, function,[32] and $\mathcal{N}(\alpha, s)$ is a normalization constant. s is referred to as the radial quantum number.

For the Coulomb potential 10 the bound-state energies are similarly found to be

$$E(\alpha, s) = -\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2 \frac{\mu}{2\hbar^2\left(\alpha + s + \frac{1}{2}\right)^2}, \quad s = 0, 1, 2, ... \qquad (75)$$

where s is again the radial quantum number. The so-called principal quantum number N is

$$N = \alpha + s + \frac{1}{2} \qquad (76)$$

The eigenfunctions for the Coulomb problem are

$$T_{\alpha,s}(r) = \mathcal{N}'(\alpha, s)\rho^{\alpha}e^{-\rho/2}M(-s, 2\alpha + 1, \rho) \qquad (77)$$

where

$$\rho = \frac{2Z}{Na_0}r \qquad (78)$$

with $a_0 = 4\pi\epsilon_0\hbar^2/\mu e^2$, and $\mathcal{N}'(\alpha, s)$ is a normalization constant.

Let us note that the principal quantum number N of eq 76 is integral for D odd and half integral for D even. The reverse is the case for the factor $\alpha + 2s + 1$ contained in the energy expression 72 for the harmonic oscillator. This alternation between integral and half-integral values was an interesting observation in early wave mechanics, primarily for the transition $(D = 2) \rightarrow (D = 3)$. It was, in particular, emphasized by Sommerfeld[33] and van Vleck.[34]

7. Comment

As we have shown, a successful application of the JWKB method to the central-field problem in D dimensions requires that one takes the planar eq 60 as the preferred equation, rather than the one-dimensional eq 33. We may define a general Kramers correction as the difference between the effective potentials defined by eqs 61 and 34. We find easily

$$V_{\text{eff}}^{(D,2)}(r) - V_{\text{eff}}^{(D,1)}(r) = \frac{\hbar^2}{8\mu r^2} \qquad (79)$$

Thus, the Kramers correction is independent of D. This reflects the fact that the differential operator in the equation determining $R^{(D,d)}(r)$ only depends upon d, and not upon D, as shown in eq 38.

That the Kramers correction is the same for all D, implies that the Langer transformation 11 may be invoked for any D. This possibility has, in fact, already been recognized by Morehead.[35]

8. Conclusions

The D-dimensional central-field problem defines D physically equivalent radial Schrödinger equations, corresponding to the subdimensions $d = 1, 2, ..., D$. These equations are all singular at the origin. In the present paper, we have shown that this causes them to be nonequivalent as far as the JWKB approximation is concerned. In fact, we have shown that only the $d = 2$ equation can be directly attacked by the JWKB approximation. In the past, focus was always put on the $d = 1$ equation. This led to difficulties that could only be overcome in an indirect way. Thus, Kramers had to add an ad hoc term to the central-field potential in order to get satisfactory results, while Langer made an ad hoc transformation of the independent variable r.

A direct application of the JWKB approximation to the $d = 2$ radial equation leads to the exact energy expressions for the hydrogen atom and the harmonic oscillator. That Kramers and Langer also got the exact expressions is understood by noting that the Kramers correction turns the $d = 1$ effective potential into the $d = 2$ effective potential, while Langer's differential equation can be interpreted as an indirect representation of our $d = 2$ equation.

As to determining the exact solutions of a central-field problem, the $d = 1$ and the $d = D$ equations have been the preferred equations in the past. We have shown, however, that the $d = 2$ equation is, in fact, a more convenient equation to use also in this case. This is because this equation has the same formal appearance for all D-values and for all values of the angular-momentum quantum number L, the significant parameter being $\alpha = L + D/2 - 1$.

In closing, we remark that the preferred role played by the $d = 2$ radial equation in the quantum-mechanical context has a parallel in classical mechanics. For in the classical-mechanical central-field problem the motion is always two-dimensional, no matter what the value of D. It takes place in a plane through the origin.

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