A perturbation technique which is superior to the weak-coupling WKB method

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We formulate a perturbation theory for the Schrödinger equation which we believe makes the weak-coupling WKB method in many practical cases obsolete. In particular we show that the entire solution consists of various pieces which are of two distinct types: one type in terms of parabolic cylinder functions (valid near an extremum of the potential), and another type in terms of certain exponential functions (valid in regions away from an extremum). Both types are similarly constructed and can be matched in regions of common validity. Below the turning point of an appropriately constructed function the argument of the wave function is real, and one and the same eigenvalue expansion is obtained together with both types of solutions. Above such a point the argument is complex, and the wave function is formulated in terms of an auxiliary parameter determined from the secular equation. Finally it is shown that the systematics of our approach also permits the generation of the exponential type of solution by the second-quantization procedure in analogy to the well-known method used for the harmonic oscillator. In the subsequent paper the large-order behavior of our solutions is derived.

I. INTRODUCTION

The WKB method has for a long time been a useful tool for estimating the wave functions or eigenvalues of almost any problem in quantum mechanics, and there are standard texts[1,2] on the subject. It is also well known that approximations to eigenvalues can usually be found by expanding the potential in the neighborhood of the appropriate minimum. However, it is not so well known that the eigenvalue expansions derived by these different methods are the same and that the appropriate solutions are related. This connection cannot be seen in the traditional formulation of the WKB method. In the following we develop a technique which exhibits this connection in a transparent manner. In fact, we show that two similarly constructed pairs of solutions of the Schrödinger equation can be derived which belong to one and the same eigenvalue: one pair in terms of parabolic cylinder functions and the other pair in terms of a certain type of exponential functions. The first type of solution corresponds to the solution around an extremum of the potential, and the second type is WKB-like. The solutions can be matched in regions of common validity, and can be continued into the classically forbidden domain. Each of our solutions depends on a parameter q. In the discrete sector of the spectrum, q is an odd integer corresponding to the usual radial quantum number; in the continuous sector of the spectrum, q is a function of the energy and is determined as the solution of the secular equation. Each of our solutions is an expansion which is asymptotic in a certain parameter. Owing to the systematics of our procedure, it is also possible to formulate a second-quantization method for the derivation of the WKB-like discrete eigenfunctions in analogy to the familiar method used for the harmonic-oscillator functions.

The method we shall develop resulted from a detailed investigation of a large number of specific eigenvalue problems. It will therefore be developed in a very general form without recourse to specific examples, of which many can be found in the literature. Originally the motivation was to develop a systematic procedure for deriving complete asymptotic expansions which allow an investigation of the large-order behavior of the perturbation expansion and then, depending on this behavior, the application of Dingle's converging factors[2,3] for the extraction of exact or almost exact results. This program was started with a consideration of the Mathieu equation[4] (i.e., the Schrödinger equation for a periodic potential) and spheroidal[5] and ellipsoidal[6] wave equations. Later, appropriate procedures were developed for deriving asymptotic expansions for the solutions and eigenvalues of a large number of other equations, such as the wave equation for Yukawa,[7] Gauss,[8] power,[9,10] and logarithmic[11] potentials and the Bethe-Salpeter equation of the Wick-Cutkosky model.[12] The approach used for these latter examples is necessarily somewhat different from the method used for solving the simpler Mathieu equation, but in essence it is still the same. More recently, we have also applied the method to multidimensional[13,14] and multichannel[15] equations, and we expect it to be useful even in the limit of an infinite number of dimensions. The success in solving this large number of diverse examples may be taken as an indication of the usefulness of our approach. Of course, our treatment here is only concerned with the case of weak coupling which permits oscillatorlike expansions near a trough of the potential. The case of strong coupling is much more difficult to deal with and is presumably of secondary importance in field theory. The significance of this distinction has been discussed by Dashen *et al.*[16]

In concluding this introduction it may be useful to point out some of the advantages of our method over the usual WKB approach. Foremost among these is the unified treatment of solutions and eigenvalues over the entire domain of the independent variable. One and the same eigenvalue expansion is derived explicitly in association with different solutions valid in adjoining domains. The solutions can be matched in regions of common validity and the discrete solutions can be normalized. The solutions are obtained in a systematic way which makes the calculation of higher-order contributions particularly straightforward, whereas the calculation of higher-order WKB corrections is cumbersome. This difference can be seen particularly clearly by comparing our calculation of the Yukawa eigenvalues[7] with the corresponding WKB calculations carried out by Boukema.[17] Of course, one problem which remains the same is the continuation of the exponential type of solutions across Stokes singularities (corresponding to classical turning points). This point will therefore not be elaborated on in this paper.

II. A FIRST PAIR OF ASYMPTOTIC EIGENSOLUTIONS: QUANTUM FLUCTUATIONS AROUND A LOCAL MINIMUM OF THE POTENTIAL

As in classical mechanics, we are concerned with a completely arbitary form of the potential (which for simplicity we assume to be everywhere continuous), except that the boundary constraint in the discrete sector of the spectrum is the condition of square integrability of the wave function.

We consider the one-dimensional Schrödinger equation $H\psi = E\psi$ for the motion of a particle of mass μ in a potential $V(r)$. We write the radial equation

$$\frac{d^2\psi}{dr^2} + \frac{2\mu}{\hbar^2}[E - V(r)]\psi = 0. \tag{1}$$

In applications where this equation describes the relative motion of two particles, μ is the reduced mass and $V(r)$ contains the centrifugal term $l(l+1)\hbar^2/2\mu r^2$. We remove the latter from $V(r)$ and set

$$\alpha = 2\mu E/\hbar^2, \quad L^2 = (l+\tfrac{1}{2})^2.$$

We also set

$$r = e^z \quad (-\infty < z < \infty)$$

and (2)

$$\psi = e^{z/2}\phi \; .$$

The equation then assumes the basic form

$$\frac{d^2\phi}{dz^2} + [-L^2 + v(z)]\phi = 0 \; , \tag{3}$$

where

$$v(z) = \left\{\frac{2\mu}{\hbar^2} r^2 [E - V(r)]\right\}_{r=e^z} . \tag{4}$$

Thus $v(z)$ plays the role of the negative of a potential, and a local minimum of V corresponds to a local maximum of v. In the vicinity of this maximum, $v(z) - L^2$ can become positive and the solutions therefore oscillatory as required for the existence of eigenvalues. Thus, if $v^{(1)}(z) \equiv dv/dz$ and $v^{(i)}(z_0) < 0$ for $i > 1$ and $\alpha > 0$ we have

$$v(z) = v(z_0) + \sum_{i=2}^{\infty} \frac{(z-z_0)^i}{i!} v^{(i)}(z_0) \; . \tag{5}$$

In some cases it may be difficult to determine z_0 exactly by solving $v^{(1)}(z) = 0$. However, in these cases we can usually determine z_0 in the form of an expansion (which can be asymptotic or convergent). This can be seen as follows. Suppose

$$v^{(1)}(z) \equiv f(z) = f_0(z) + \delta g(z) \; ,$$

where $f_0(z)$ is the dominant part of $v^{(1)}(z)$ near $z = z_0$ such that its zeros $z_0^{(0)}$ are easily determinable; then δ is a parameter which can be taken to be small. It is now possible to calculate z_0 in the form

$$z_0 = z_0^{(0)} + \sum_{i=1}^{\infty} \delta^i p_i \; .$$

The coefficients p_i follow from the equation

$$0 = f_0\left(z_0^{(0)} + \sum_{i=1}^{\infty}\delta^i p_i\right) + \delta g\left(z_0^{(0)} + \sum_{i=1}^{\infty}\delta^i p_i\right) \; ,$$

which after expansion around $z_0^{(0)}$ yields

$$p_1 = -\left(\frac{g}{f_0^{(1)}}\right)_{z_0^{(0)}} \; ,$$

$$p_2 = \left[\frac{g g^{(1)}}{(f_0^{(1)})^2} - \frac{g^2 f_0^{(2)}}{2(f_0^{(1)})^3}\right]_{z_0^{(0)}} \; ,$$

and so on.

We now set

$$h = [-2v^{(2)}(z_0)]^{1/4} \tag{6}$$

and change the independent variable in (3) to

$$\omega = h(z - z_0) \; . \tag{7}$$

The equation then becomes

$$\frac{d^2\phi}{d\omega^2}+\left[\frac{-L^2+v(z_0)}{h^2}-\frac{\omega^2}{4}\right]\phi=\sum_{i=3}^{\infty}\left[\frac{v^{(i)}(z_0)}{2v^{(2)}(z_0)}\right]\frac{\omega^i}{i!h^{i-2}}\phi. \tag{8}$$

For large values of h the right-hand side of Eq. (8) can—to a first approximation—be neglected. The corresponding behavior of the eigenvalues $[-L^2+v(z_0)]/h^2$ can then be determined by comparing the equation with the equation of parabolic cylinder functions. The solutions are normalizable only if $[-L^2+v(z_0)]/h^2=\frac{1}{2}q$, where q is an odd integer, i.e., $2n+1$, $n=0,1,2,\ldots$ [provided the wave function is required to vanish at infinity; otherwise it is only approximately an odd integer[18] (i.e., $q=2n+1+O(1/a)$) if ψ is required to vanish at $r=a<\infty$]. For the complete solution we set

$$\frac{1}{h^2}[-L^2+v(z_0)]=\tfrac{1}{2}q+\Delta. \tag{9}$$

The quantity Δ in (9) vanishes in the limit $h\to\infty$ and remains to be determined. We proceed as follows. Substituting (9) into (8) we have an equation which can be written

$$\mathfrak{D}_q\phi=2\Delta\phi-\sum_{i=3}^{\infty}\frac{v^{(i)}(z_0)}{v^{(2)}(z_0)}\frac{\omega^i}{i!h^{i-2}}\phi, \tag{10}$$

where

$$\mathfrak{D}_q\equiv-2\frac{d^2}{d\omega^2}+\tfrac{1}{2}\omega^2-q. \tag{11}$$

Equation (10) is now in a form suitable for the application of a perturbation method. To a first approximation, $\phi=\phi^{(0)}$ is simply a parabolic cylinder function $D_{(q-1)/2}(\omega)$, i.e.,

$$\phi^{(0)}=\phi_q=D_{(q-1)/2}(\omega),\quad \mathfrak{D}_q\phi_q=0. \tag{12}$$

We have

$$D_{(q-1)/2}(\omega)=2^{(q-3)/4}e^{-\omega^2/4}\Psi\left(\frac{3-q}{4},\frac{3}{2};\frac{\omega^2}{2}\right), \tag{13}$$

where Ψ is a confluent hypergeometric function. The function ϕ_q is well-known to obey the recurrence formula

$$\omega\phi_q=(q,q+2)\phi_{q+2}+(q,q-2)\phi_{q-2}, \tag{14}$$

where

$$(q,q+2)=1,\quad (q,q-2)=\tfrac{1}{2}(q-1).$$

For higher powers we have

$$\omega^i\phi_q=\sum_{j=2i,2i-4,\ldots}^{-2i}S_i(q,j)\phi_{q+j}, \tag{15}$$

and a recurrence relation can be written down for the coefficients S_i, i.e.,

$$S_i(q,j)=S_{i-1}(q,j+2)(q+j+2,q+j)+S_{i-1}(q,j-2)(q+j-2,q+j).$$

The first approximation $\phi=\phi^{(0)}$ then leaves uncompensated terms amounting to

$$R_q^{(0)}=\left[2\Delta-\sum_{i=3}^{\infty}\frac{v^{(i)}(z_0)}{v^{(2)}(z_0)}\frac{\omega^i}{i!h^{i-2}}\right]\phi_q(\omega)=2\Delta\phi_q-\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}\sum_{j=2i,2i-4,\ldots}^{-2i}\tilde{S}_i(q,j)\phi_{q+j}(\omega), \tag{16}$$

where we have set

$$\tilde{S}_i(q,j)=\frac{v^{(i)}(z_0)}{v^{(2)}(z_0)}\frac{1}{i!}S_i(q,j). \tag{17}$$

We rewrite (16) in the form

$$R_q^{(0)}=\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}\sum_{j=2i,2i-4,\ldots}^{-2i}[q,q+j]_{i-2}\phi_{q+j}(\omega), \tag{18}$$

where for $i\geq 3$, $-2i\leq j\leq 2i$,

$$[q,q+j]_{i-2}=-\tilde{S}_i(q,j), \tag{19a}$$

with the exception that

$$[q,q]_1=2\Delta h-\tilde{S}_3(q,0). \tag{19b}$$

Since $\mathfrak{D}_{q+j}=\mathfrak{D}_q-j$, $\mathfrak{D}_q\phi_{q+j}=j\phi_{q+j}$, a term $\mu\phi_{q+j}$ in $R_q^{(0)}$ can be removed by adding to $\phi^{(0)}$ the contribution $\mu\phi_{q+j}/j$, except, of course, when $j=0$. Thus the next order contribution of ϕ becomes

$$\phi^{(1)}=\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}\sum_{\substack{j=2i,2i-4,\ldots\\ j\neq 0}}^{-2i}\frac{[q,q+j]_{i-2}}{j}\phi_{q+j}(\omega). \tag{20}$$

In its turn this contribution leaves uncompensated

$$R_q^{(1)}=\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}\sum_{\substack{j=2i,2i-4,\ldots\\ j\neq 0}}^{-2i}\frac{[q,q+j]_{i-2}}{j}R_{q+j}^{(0)} \tag{21}$$

and yields the next contribution of ϕ:

$$\phi^{(2)}=\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}\sum_{\substack{j=2i,2i-4,\ldots\\ j\neq 0}}^{-2i}\frac{[q,q+j]_{i-2}}{j}\sum_{i'=3}^{\infty}\frac{1}{h^{i'-2}}\sum_{j'=2i',2i'-4}^{-2i'}\frac{[q+j,q+j+j']_{i'-2}}{j+j'}\phi_{q+j+j'}. \tag{22}$$

Proceeding in this way we obtain the solution

$$\phi=\phi^{(0)}+\phi^{(1)}+\phi^{(2)}+\cdots,$$

which is an asymptotic expansion in descending powers of h valid for

$$z-z_0=O\left(\frac{1}{h^{\alpha}}\right),\quad \alpha>0 \tag{23}$$

i.e., around the minimum of the potential at $z=z_0$ (for the determination of α see Ref. 10). However, the sum of the contributions $\phi^{(0)}$, $\phi^{(1)}$, ... is a solution only if the sum of the terms containing ϕ_q in $R_q^{(0)}$, $R_q^{(1)}$, ... (left unaccounted for so far) is set equal to zero. Thus

$$0=\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}[q,q]_{i-2}+\sum_{i=3}^{\infty}\frac{1}{h^{i-2}}\sum_{\substack{j=2i,2i-4,\ldots\\ j\neq 0}}^{-2i}\frac{[q,q+j]_{i-2}}{j}\times\sum_{i'=3}^{\infty}\frac{1}{h^{i'-2}}[q+j,q]_{i-2}+\cdots$$

or

$$0=\frac{1}{h}[q,q]_1+\frac{1}{h^2}\left[[q,q]_2+\sum_{\substack{j=6,2,\ldots\\ j\neq 0}}^{-6}\frac{[q,q+j]_1}{j}[q+j,q]_1\right]+O\left(\frac{1}{h^3}\right). \tag{24}$$

This is the equation from which Δ and hence the eigenvalues are determined. We find

$$\Delta=\frac{1}{2h^2}\left[\frac{(q^2+1)}{2^4}\frac{v^{(4)}(z_0)}{v^{(2)}(z_0)}-\frac{(15q^2+7)}{2^4 3^2}\left(\frac{v^{(3)}(z_0)}{v^{(2)}(z_0)}\right)^2\right]+O\left(\frac{1}{h^4}\right) \tag{25a}$$

and hence

$$-(l+\tfrac{1}{2})^2+v(z_0)=\tfrac{1}{2}qh^2+\frac{1}{2}\left[\frac{(q^2+1)}{2^4}\frac{v^{(4)}(z_0)}{v^{(2)}(z_0)}-\frac{(15q^2+7)}{2^4 3^2}\left(\frac{v^{(3)}(z_0)}{v^{(2)}(z_0)}\right)^2\right]+O\left(\frac{1}{h^2}\right). \tag{25b}$$

We have thus obtained one large-h asymptotic expansion of the eigenfunctions of the Schrödinger equation (valid in the region around $z=z_0$ or $\ln r=z_0$). A second linearly independent solution in the same domain is obtained by changing the signs of q and h^2 throughout or by replacing ω^2 by $-\omega^2$. The corresponding eigenvalues, of course, are unaffected by this interchange. It should be observed that the oscillatorlike solutions derived here are not (as they stand) identical with the usual textbook Rayleigh-Schrödinger expansions. Except for the first term, each term contains contributions of higher order than its own leading contribution. Thus only after further expansion will our expansion become identical with the Rayleigh-Schrödinger expansion.

Another important point should be observed with regard to the eigenvalue expansion (25b). We can rewrite this expansion in the form

$$(l+\tfrac{1}{2})^2=v(z_0)\exp\left[-\frac{1}{v(z_0)}\left(\frac{a}{h^2}+\frac{b}{(h^2)^2}+\cdots\right)\right]=v(z_0)-\frac{a}{h^2}+\frac{1}{h^4}\left(\frac{a_1^{\,2}}{2v(z_0)}-b_1\right)+\cdots, \tag{25c}$$

where the coefficients $a, b, \ldots$ can be determined by comparison with (25b). The form (25c) demonstrates very clearly the nonanalyticity of the eigenvalue at $h^2=0$. In field-theory models with coupling constant g^2 this corresponds to the nonanalyticity of an eigenenergy $E\sim e^{-A/g^2}$ at $g^2=0$. The expansion therefore corresponds to the so-called "nonperturbative" expansion (meaning perturbation theory in terms of g^2). See, for instance, Dashen *et al.*[16]

Finally, we reformulate our solutions in terms of Fock-space creation and annihilation operators. Of course, for the simple harmonic oscillator this formulation is well known. Here, however, we are interested in its extension to a case involving an arbitrary number of anharmonic contributions, and particularly in its relation to the corresponding formulation of the WKB-like solutions to be discussed later.

Thus, using the variables introduced above, we have

$$\left[\frac{d}{d\omega},\omega\right]=1. \tag{26}$$

Defining creation and annihilation operators $a^{\dagger}$, a by

$$a^{\dagger}=-i\frac{d}{d\omega}+\frac{i}{2}\omega,\qquad a=-i\frac{d}{d\omega}-\frac{i}{2}\omega, \tag{27}$$

we have

$$[a,a^{\dagger}]=1. \tag{28}$$

It is easily verified that

$$\mathfrak{D}_q\equiv\mathcal{H}-q,\quad \text{where } \mathcal{H}=2a^{\dagger}a+1. \tag{29}$$

The vacuum state $|0\rangle$ or ground-state wave function $\langle\omega|0\rangle$ is defined by

$$a|0\rangle=0, \text{ i.e., } a(\omega)\langle\omega|0\rangle=0\ . \tag{30}$$

Inserting a of (27) we find

$$\langle\omega|0\rangle=e^{-\omega^2/4}\propto\phi_1\ , \tag{31}$$

apart from a normalization constant [ϕ_1 being ϕ_q of (12) for $q=1$ or $n=0$]. The radial excitations ϕ_3, ϕ_5, . . . are now obtained in the usual way by the action of creation operators on the vacuum, i.e.,

$$\langle\omega|a^\dagger|0\rangle=\phi_{q=3}(\omega)\equiv\phi_{n=1}(\omega)\ ,$$

$$\langle\omega|a^\dagger a^\dagger|0\rangle=\phi_{q=5}(\omega)\equiv\phi_{n=2}(\omega)\ ,$$

and so on. Hence (inserting $-i$ for convenience)

$$(\mathcal{K}-q)\langle\omega|(-ia^\dagger)^{(q-1)/2}|0\rangle=0$$

and (32)

$$\langle\omega|(-ia^\dagger)^{(q-1)/2}|0\rangle=\phi_q(\omega)\ .$$

Again we treat the anharmonic terms of (10) perturbatively. This requires a recurrence relation. The relation corresponding to (14) is

$$i(a-a^\dagger)(-ia^\dagger)^{(q-1)/2}|0\rangle =(-ia^\dagger)^{(q+1)/2}|0\rangle+\tfrac{1}{2}(q-1)(-ia^\dagger)^{(q-3)/2}|0\rangle\ , \tag{33}$$

i.e.,

$$\omega\phi_q=(q,q+2)\phi_{q+2}+(q,q-2)\phi_{q-2}\ ,$$

where we have used (28), and the coefficients are the same as in (14).

III. A SECOND PAIR OF ASYMPTOTIC EIGENSOLUTIONS: THE WKB-LIKE SOLUTIONS

We now derive a second pair of large-h asymptotic expansions for the eigenfunctions of the wave equation. This pair is valid in regions of large $|z-z_0|$, i.e., away from z_0, where the expansions obtained above are no longer applicable. The corresponding eigenvalue expansion, however, will be seen to be identical with (25) above.

Our starting point is Eq. (3), in which we insert for L^2 the expression (9) in terms of the quantity Δ which is again to be determined by iteration. In the usual formulation of the WKB method, this substitution corresponds to assuming that deviations of the particle from its classically allowed path are of $O(1/h)$. We then have the equation

$$\frac{d^2\phi}{dz^2}+[v(z)-v(z_0)+\tfrac{1}{2}qh^2+\Delta h^2]\phi=0\ . \tag{34}$$

It is convenient to make the substitution

$$y=z-z_0=\frac{\omega}{h}\ . \tag{35}$$

Then Eq. (34) can be written

$$\frac{d^2\phi(y)}{dy^2}-\frac{h^4}{4}w(y)\phi(y)+(\tfrac{1}{2}qh^2+\Delta h^2)\phi(y)=0\ , \tag{36}$$

where

$$\frac{h^4}{4}w(y)=v(z_0)-v(z)\ . \tag{37}$$

With (5) we have equivalently as the expression defining the function $w(y)$

$$\frac{h^4}{4}w(y)=-\sum_{i=2}^{\infty}\frac{y^i}{i!}v^{(i)}(z_0) \tag{38}$$

and (6) shows that the first term of this expansion is of $O(h^4)$. We therefore remove this term by the following substitution:

$$\phi(y)=\chi(y)\exp\left\{\pm\frac{h^2}{2}\int^y[w(y)]^{1/2}dy\right\}. \tag{39}$$

The exponential factor corresponds only roughly to the exponential factor in the usual WKB procedure. We do not specify a path because this has already been taken care of by incorporating the behavior (9) of the eigenvalues on the assumption that h is large. Thus, substituting (39) into (36) we find that $\chi(y)$ satisfies

$$\frac{d^2\chi}{dy^2}\pm h^2w^{1/2}(y)\frac{d\chi}{dy}\pm\frac{h^2}{4}\frac{w'(y)}{w^{1/2}(y)}\chi+(\tfrac{1}{2}qh^2+\Delta h^2)\chi=0\ . \tag{40}$$

From now on we consider only the equation for the upper signs. The equation for the lower signs leads to another solution which can be obtained from the solution we shall derive by changing the signs of q and h^2 throughout. Thus, choosing the upper signs in (40), we can rewrite the equation in the form

$$\mathfrak{D}_q\chi=\frac{2}{h^2}\left(\frac{d^2\chi}{dy^2}+\Delta h^2\chi\right)\ , \tag{41}$$

where

$$\mathfrak{D}_q=-2w^{1/2}\frac{d}{dy}-\frac{1}{2}\frac{\omega'}{\omega^{1/2}}-q$$

and (42)

$$2w^{1/2}d/dy=w'd/dw^{1/2}\ .$$

By construction Δh^2 is at most of $O(0)$ in h^2, and $w^{1/2}=O(h^2)$. Hence for $h^2\to\infty$, i.e., to a first approximation, the right-hand side of (41) can be neglected and we can write for the solution to that order

$$\chi^{(0)} = \chi_q ,$$

where χ_q is the solution of

$$\mathfrak{D}_q \chi_q = 0 ,$$

i.e.,

$$\chi_q = \frac{C}{w^{1/4}} \exp\left(-\frac{q}{2}\int^y \frac{dy}{w^{1/2}}\right) , \tag{43}$$

where C is an overall multiplicative constant which we ignore in the following except in the context of normalization. It should be observed that in view of (37) and (38) the function $\chi(q)$ is singular at $z = z_0$ or $y = 0$ (this is here the Stokes singularity), and the domain of validity of the solution therefore excludes a region around this point.

Proceeding as in the derivation of our first solution, we evaluate $d^2\chi_q/dy^2$ and obtain

$$\frac{d^2\chi_q}{dy^2} + \Delta h^2 \chi_q = \left(\Delta h^2 + \frac{5}{16}\frac{w'^2}{w^2} + \frac{qw'}{2w^{3/2}} + \frac{q^2}{4w} - \frac{w''}{4w}\right)\chi_q . \tag{44}$$

Looking at the solution (43) we observe the following relations:

$$\frac{\chi_{q+j}}{\chi_q} = \left(\frac{\chi_{q+1}}{\chi_q}\right)^j , \quad \frac{\chi_{q+j}}{\chi_q} = \frac{\chi_q}{\chi_{q-j}} . \tag{45}$$

Further, since

$$\mathfrak{D}_{q+j} = \mathfrak{D}_q - j$$

and (46)

$$\mathfrak{D}_q \chi_{q+j} = j\chi_{q+j} ,$$

it is desirable to reexpress (44) as a sum over various χ_{q+j} because then the perturbation procedure parallels that of the first solution and becomes particularly simple. Since $\chi_q = y^{-(q+1)/2}[1 + O(1/h)]$ for $h \to \infty$, this type of expansion implies simply a reshuffling of terms on the right-hand side of (44) in terms of a suitable set of functions. In order to derive this expansion we have to use χ_q and express y in terms of χ_q. It is not difficult to convince oneself that the series reversion which this step implies is possible only if $\omega(y)$ is expanded around a point $y = y_0$ for which both

$$\omega(y_0) = 0 \text{ and } \omega'(y_0) = 0 .$$

Looking at (37) we see that $y_0 = 0$, i.e., $z = z_0$. Then

$$\omega(y) = \sum_{i=2}^{\infty} \frac{y^i}{i!}\omega^{(i)}(0) ,$$

where for $i = 2, 3, \ldots$

$$w^{(i)}(0) = \frac{2v^{(i)}(z_0)}{v^{(2)}(z_0)} .$$

This, of course, is simply the expression defining $w(y)$, i.e., (38). We then have for the integral in (43) (apart from an additive constant)

$$\frac{1}{2}\int^y \frac{dy}{w^{1/2}} = \tfrac{1}{2}\ln y + \sum_{i=1}^{\infty} \gamma_i y^i , \tag{47}$$

where γ_i are easily calculable coefficients. Substituting (47) into the relation

$$\frac{\chi_{q-1}}{\chi_q} = \exp\left(\frac{1}{2}\int^y \frac{dy}{w^{1/2}}\right)$$

and reversing the resulting series, we obtain (after squaring)

$$y = \sum_{i=0}^{\infty} d_{2i+1}\frac{\chi_{q-(2i+1)}}{\chi_q} , \tag{48}$$

with coefficients d_{2i+1}, where

$$d_1 = 1, \quad d_3 = \frac{1}{6}\frac{v^{(3)}(z_0)}{v^{(2)}(z_0)}, \ldots .$$

Inserting (48) into $w(y)$ and inverting the series we obtain

$$\frac{1}{w(y)} = \sum_{i=2,1,0,\ldots}^{-\infty} \delta_{2i}\frac{\chi_{q+2i}}{\chi_q} \tag{49}$$

with coefficients δ_{2i}. In a similar way we find

$$\frac{w'^2}{w^2} = \sum_{i=2,1,0,\ldots}^{-\infty} \tau_{2i}\frac{\chi_{q+2i}}{\chi_q} \tag{50}$$

with coefficients τ_{2i},

$$\frac{w''}{w} = \sum_{i=2,1,0,\ldots}^{-\infty} \epsilon_{2i}\frac{\chi_{q+2i}}{\chi_q} \tag{51}$$

with coefficients ϵ_{2i}, and

$$\frac{w'}{w^{3/2}} = \sum_{i=2,1,0,\ldots}^{-\infty} \kappa_{2i}\frac{\chi_{q+2i}}{\chi_q} \tag{52}$$

with coefficients κ_{2i}. These expansions can now be substituted in (44). Then

$$\frac{d^2\chi_q}{dy^2} + \Delta h^2\chi_q = \sum_{j=2,1,0,\ldots}^{-\infty} (q, q+2j)\chi_{q+2j} , \tag{53}$$

where for $j \neq 0$

$$(q, q+2j) = \tfrac{5}{16}\tau_{2i} + \frac{q}{2}\kappa_{2i} + \frac{q^2}{4}\delta_{2i} - \tfrac{1}{4}\epsilon_{2i} \tag{54}$$

and for $j = 0$

$$(q, q) = \Delta h^2 + \tfrac{5}{16}\tau_0 + \frac{q}{2}\kappa_0 + \frac{q^2}{4}\delta_0 - \tfrac{1}{4}\epsilon_0 . \tag{55}$$

Thus the first approximation $\chi^{(0)} = \chi_q$ leaves uncompensated on the right-hand side of (41) a sum of terms amounting to

$$R_q^{(0)}=\frac{2}{h^2}\sum_{j=2,1,0,\ldots}^{-\infty}(q,q+2j)\chi_{q+2j}\,. \tag{56}$$

Using (46) we see that these terms can be taken care of by adding to $\chi^{(0)}$ the next-order contribution

$$\chi^{(1)}=\frac{2}{h^2}\sum_{\substack{j=2,1,\ldots\\ j\neq 0}}^{-\infty}\frac{(q,q+2j)}{2j}\chi_{q+2j}\,, \tag{57}$$

excluding, of course, the term in χ_q. The coefficient of χ_q in (56) set equal to zero, i.e.,

$$(q,q)=0\,,$$

yields an expression for Δ to the same order of approximation and is identical with the expression obtained previously for our first solution, as we have demonstrated explicitly for several examples.[8-11]

The complete solution is obtained in our standard fashion as in Sec. II, leading to the sum

$$\chi=\chi^{(0)}+\chi^{(1)}+\chi^{(2)}+\cdots \tag{58}$$

in descending power of h^2. The corresponding equation for Δ and thus for the eigenvalues is

$$0=(q,q)+\frac{2}{h^2}\sum_{\substack{j=2,1,\ldots\\ j\neq 0}}^{-\infty}\frac{(q,q+2j)}{2j}(q+2j,q)+\cdots\,. \tag{59}$$

Solving this equation for Δ (note that the terms on the right contain Δ), one obtains an expansion which is termwise identical with the expansion derived from (24), i.e., by means of a completely different method. For explicit verification up to a nontrivial order see Refs. 8, 9, and 11 and the Appendix of Ref. 10.

Successive contributions $\chi^{(0)}$, $\chi^{(1)}$, ... of χ form a rapidly decreasing sequence provided that

$$\frac{2}{h^2}\frac{\chi_{q\pm 2}}{\chi_q}<1\,,$$

i.e.,

$$\exp\left(\mp\int^y\frac{dy}{w^{1/2}}\right)<\tfrac{1}{2}h^2\,.$$

This relation allows arbitrarily large values of y (since $h^2\to\infty$) but excludes the region around $y=0$ or $z=z_0$ in view of the logarithmic term in (47). The latter region is, of course, precisely the region in which our previous expansion is valid, i.e., the region around a local minimum of the potential. However, the solution χ has a further restriction which we did not encounter in the case of the first solution. From (43) we see that the solutions χ possess singularities at the points where $w(y)=0$. Singularities of this type are well known from WKB solutions, where they represent classical turning points. The solutions χ can therefore be defined only in sectors between successive singularities of this type, and the complete solution requires the matching of these branches. It is well known that the proper comparison functions for the matching in these regions are Airy functions, as was shown long ago by Langer.[19] This is, however, a very intricate problem (see, e.g., the critical evaluation by Dingle[2]) and requires a separate detailed investigation. In any case it should be noted that the two branches to be matched depend on the parameters (i.e., q,h) associated with different extrema.

Finally we observe that since (as pointed out above) a linearly independent solution is obtained by changing throughout the signs of q and h^2, the joint "eigenvalue equation" (which is, in general, simply an equation determining the auxiliary parameter q) must also be invariant under this change of signs (as is, in fact, verified by explicit calculation). Of course, the choice of the exponentially damped (square integrable) solution makes q (exactly or approximately, depending on the explicit form of the boundary conditions[17]) an odd integer.

Next, we develop the Fock-space formulation for these solutions. We define the following operators for $j\neq 0$:

$$\alpha_{q+j}=\frac{1}{j}\exp\left(\frac{j}{2}\int\frac{dy}{w^{1/2}}\right)\mathfrak{D}_q\,,\qquad \alpha^*_{q+j}=\frac{1}{j}\mathfrak{D}_q\exp\left(-\frac{j}{2}\int\frac{dy}{w^{1/2}}\right). \tag{60}$$

It is readily verified that these operators satisfy the relations ($j\neq 0$)

$$[\mathfrak{D}_q,\alpha_{q+j}]=-j\alpha_{q+j}\,,\qquad [\mathfrak{D}_q,\alpha^*_{q+j}]=+j\alpha^*_{q+j}\,. \tag{61}$$

We see that α^* seems to act as a creation operator and α as an annihilation operator. In order to check this, we look at the commutators of α and α^* among themselves. Using the relation

$$\left[\mathfrak{D}_q,\exp\left(-\frac{j}{2}\int\frac{dy}{w^{1/2}}\right)\right]=j\exp\left(-\frac{j}{2}\int\frac{dy}{w^{1/2}}\right)=\alpha^*_{q+j}+\alpha_{q-j}\,, \tag{62}$$

one finds

$$[\alpha_{q+i},\alpha_{q+j}]=\left(\frac{i^2-j^2}{ij}\right)\alpha_{q+i+j}\,,\qquad [\alpha^*_{q+i},\alpha^*_{q+j}]=-\left(\frac{i^2-j^2}{ij}\right)\alpha^*_{q+i+j} \tag{63}$$

and

$$[\alpha_{q+i},\alpha^*_{q+j}]=\frac{j-i}{i}\alpha^*_{q+j-i}+\frac{i-j}{j}\alpha_{q+i-j}+\frac{\chi_{q+j-i}}{\chi_q}\,. \tag{64}$$

For $i=j$ these relations correspond to (28), i.e.,

$$[\alpha_{q+i},\alpha_{q+i}]=0,\quad [\alpha^*_{q+i},\alpha^*_{q+i}]=0,\quad [\alpha_{q+i},\alpha^*_{q+i}]=1. \tag{65}$$

We now let $|0\}$ be the vacuum state defined by

$$\alpha_{q+i}|0\}=0,$$

i.e., (66)

$$\mathfrak{D}_q(y|0\}=0.$$

Then

$$(y|0\}=\chi_q \tag{67}$$

in our earlier notation, apart from a normalization constant. Using (62) we obtain

$$\begin{aligned}\left(y\left|\frac{1}{j!}(\alpha^*_{q+1})^j\right|0\right\}&=\exp\left(\frac{-j}{2}\int\frac{dy}{w^{1/2}}\right)\chi_q\\&=\alpha^*_{q+j}|0\},\\&=\frac{1}{j}\mathfrak{D}_q\exp\left(-\frac{j}{2}\int\frac{dy}{w^{1/2}}\right)\chi_q,\\&=\frac{1}{j}\mathfrak{D}_q\chi_{q+j},\\&=\chi_{q+j}.\end{aligned} \tag{68}$$

We have thus shown that any function χ_{q+j} can be generated by the repeated action of the operator α^*_{q+1} on the vacuum $|0\}$. Finally, in order to complete the perturbation theory in terms of the operators (60), we have to reexpress powers of y in terms of these operators. From (62) we have

$$\begin{aligned}\alpha^*_{q-1}+\alpha_{q+1}&=-\exp\left(\tfrac{1}{2}\int\frac{dy}{w^{1/2}}\right)\\&=-y^{1/2}\exp\left(\sum_{i=1}^{\infty}\gamma_i y^i\right)\end{aligned} \tag{69}$$

on using (47). Expanding the exponential and reversing the series we obtain $y^{1/2}$ and hence y as a sum over powers of α^*_{q-1} and α_{q+1}. On the right-hand side of (44) we expand the coefficient of χ_q in powers of y and then reexpress the latter in terms of $\alpha^*_{q-1},\alpha_{q+1}$. Then, using (66) and (68) we again obtain $R_q^{(0)}$ as in (56).

IV. MATCHING OF THE SOLUTIONS

In the preceding sections we derived two pairs of linearly independent solutions of the wave equation which are valid in complementary domains of the independent variable. The solutions ϕ of Sec. II are (observe that in general these solutions are valid in different domains)

$$\phi_1(q,h^2;\omega)=A(q,h^2)\phi(q,h^2;\omega)$$

and (70)

$$\bar{\phi}_1(q,h^2;\omega)=\phi_1(-q,-h^2;\omega),$$

and the solutions of Sec. III are

$$\phi_2(q,h^2;y)=B(q,h^2)\exp\left\{\frac{h^2}{2}\int dy[w(y)]^{1/2}\right\}\chi(q,h^2;y)$$

and (71)

$$\bar{\phi}_2(q,h^2;y)=\phi_2(-q,-h^2;y),$$

where we have introduced normalization constants A, B, and the variables and parameters are defined as above. The constant A can be related to the constant B by going to a region of common validity of our solutions. Thus, inserting the large-h asymptotic expansion of $\phi_q(\omega)$ into ϕ_1, i.e.,

$$\phi_q(\omega)=e^{-\omega^2/4}\omega^{(q-1)/2}\left[1-\frac{(q-1)(q-3)}{8\omega^2}+\cdots\right] \tag{72}$$

[recall that $\omega=h(z-z_0)=hy$ and h is assumed to be large] we see that ϕ_1 behaves as

$$\phi_1(q,h^2;\omega)=A(q,h^2)e^{-h^2y^2/4}(hy)^{(q-1)/2}[1+O(1/h)]. \tag{73}$$

Next we insert (38) and (43) into (71). Then

$$\bar{\phi}_2(q,h^2;y)=\bar{B}(q,h^2)e^{-(h^2y^2)/4}y^{(q-1)/2}[1+O(1/h)], \tag{74}$$

where $\bar{B}(q,h^2)=B(-q,-h^2)$, etc. Since $\phi_1,\bar{\phi}_2$ must be the same in the domain where they overlap we have

$$\bar{B}(q,h^2)=A(q,h^2)h^{(q-1)/2}[1+O(1/h)]. \tag{75}$$

Clearly, it is easy to calculate the first few terms of the expansion on the right. The relation (75) thus establishes the continuation of the oscillatorlike solution of Sec. II to the WKB-like solution of Sec. III.

We have pointed out at the beginning that a minimum of the potential $V(r)$ of the Schrödinger equation corresponds to a maximum of the function $v(z)$ of our basic equation (3). The parameter h defined by (6) is therefore real if z_0 is the value of $z=\ln r$ corresponding to a minimum of $V(r)$, and it is complex if z_0 corresponds to a maximum (i.e., point of instability) of $V(r)$; in fact, in the latter case h^2 is pure imaginary. Thus, in the region between the minimum of $V(r)$ at $z=z_0$ and the nearest Stokes singularity at (say) $z=z_s$, we have a domain $d(z)$ in which the two types of solutions which we have derived merge into one another, the oscillatorlike solution being valid around z_0 and the WKB-like solution away from z_0. Moreover, both solutions are real and q is (at least approximately) an odd integer. In the region above the Stokes singularity [this is the point where $w(y)$ of (37) changes from positive to negative] but below the next extremum, i.e., maximum of $V(r)$, we again have two pairs of solutions as before, but this time they are complex and q is a complicated function of E obtained by solving the secular equation. Thus from (25b)

$$q=\frac{2}{h^2}[v(z_0)-(l+\tfrac{1}{2})^2]-2\Delta\left(q,\frac{1}{h^2}\right).$$

Solving this equation for $q=q(E)$ by iteration and inserting $q(E)$ for q in our previous solutions, we obtain the solutions valid in the domain above z_s. Clearly this procedure can be repeated for any number of wiggles of the potential. Of course, in the case of a periodic potential[4] (in this case the Schrödinger equation is the Mathieu equation) the solutions simply repeat themselves. The complex pieces of these solutions describe the tunneling of the quantum-mechanical particle from one trough of the potential to the next. The states associated with these troughs are weakly coupled (in symmetric cases one has a degeneracy) via the exponentially damped tunneling amplitude. We are therefore here concerned with the case of weak-coupling, i.e., weak inharmonic contributions, as pointed out at the beginning.[16]

V. CONCLUSIONS

In the preceding sections we have developed a method for deriving complete sets of asymptotic solutions of the Schrödinger wave equation in any part of the domain of the independent variable, and we have shown that the two sets of solutions can be matched in regions of common validity. We have also shown that a Fock-space formulation can be found in each case; for the oscillator-like solutions this formulation is well known; for the WKB-like solutions this is new. Another new aspect of the method is the explicit demonstration that oscillatorlike solutions and the WKB-like solutions are asymptotic expansions in one and the same parameter. Moreover, one and the same eigenvalue expansion is obtained in conjunction with either type of solution. We have demonstrated elsewhere[7] that in the case of scattering potentials, the solutions can even be used to construct the S matrix. In a separate paper we show that the eigenvalue expansions have the large-order behavior conjectured long ago by Dingle,[2,3] which has also been found for the corresponding expansions of the eigenvalues of the Mathieu and other equations.[4]

The general form of our solutions shows that the coefficient of a term of order $1/h^i$ can be written down from a consideration of all possible moves from q to $q+t$ in at most i steps. In the case of the corresponding coefficient of the eigenvalue equation, these steps go from q to q and may be associated with closed paths in a one-dimensional Euclidean lattice space. It is obvious that in the multidimensional generalization of our perturbation theory the coefficients of the eigenvalue equation are associated with closed paths in the appropriate multidimensional Euclidean lattice space.

In concluding it may be interesting to observe that it is also possible to derive solutions of the wave equation in rising powers of h. These expansions are either convergent or else asymptotic in a parameter ν related to the Floquet parameter of the Mathieu equation. The general features of these solutions will be similar to those of corresponding solutions of the Mathieu equation.[20,21] In particular, a relation between ν and the radial quantum number q can be calculated.[21,22]

Note added in proof: A procedure for matching our solutions across Stokes discontinuities due to classical turning points, i.e., where $f(z)\equiv L^2-v(z)$ of Eq. (3) changes sign, can be seen as follows. Classical WKB matching[2] extends (e.g.) the approximate solution

$$\frac{1}{f^{1/4}}\exp\left(\int^z f^{1/2}dz\right)$$

beyond the Stokes singularity. By rewriting f as

$$f=[v(z_0)-v(z)]\left[1+\frac{L^2-v(z_0)}{v(z_0)-v(z)}\right]$$

and expanding $f^{1/4}$, $f^{1/2}$ in the domain of z far away from z_0, the WKB solution and our appropriate WKB-like solution become proportional. The matching therefore proceeds along the usual lines. The classical turning point (apparently shifted to an extremum) is only hidden in our solutions.

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