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LANGER'S METHOD FOR WEAKLY BOUND STATES OF THE HELMHOLTZ EQUATION WITH SYMMETRIC PROFILES

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ABSTRACT

Use of the harmonic oscillator equation as the comparison equation in the application of Langer's method to bound states of the Helmholtz equation, $w'' + k_0^2 g(z)w(z) = 0$, with symmetric profiles $k_0^2 g(z)$ produces the W.K.B. eigenvalue condition. In the case of weakly bound states, this condition gives eigenvalue estimates of low accuracy. Use of the Helmholtz equation with the symmetric Epstein profile, $G(x) = \left[\hat{E} + U_o(\cosh \alpha x)^{-2}\right]$, as the comparison equation provides the basis for a convenient method to obtain eigenvalue estimates of substantially increased accuracy in the case of weakly bound states. In addition to the usual condition of equality of the phase integrals of the original and comparison equations between the turning points, the conditions $k_0^2 g(0) = G(0)$ and $k_0^2 g(\infty) = G(\infty)$ are imposed. An eigenvalue condition which is a simple generalization of the usual W.K.B. eigenvalue condition is obtained. Its application to selected diverse examples of the Helmholtz equation indicates that it has a broad range of utility.

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1. Introduction

We consider the one-dimensional Helmholtz equation,

$$w'' + k_0^2 g(z) w(z) = 0, \tag{1}$$

in the interval $-\infty < z < \infty$. The profile $k_0^2 g(z)$ is characterized by the symmetric curve of Fig. 1. It is positive at $z = 0$. It decreases monotonically away from $z = 0$ and approaches a finite negative limit as $|z| \to \infty$. Thus it has two turning points. The profile $k_0^2 g(z)$ depends on a parameter, which we do not denote explicitly. The functional dependence of the profile on the parameter is arbitrary. The Schrödinger equation is thus considered here a special case of the Helmholtz equation. For a discrete set of values of the parameter, the eigenvalues, the equation has solutions, the eigenfunctions or bound states, which approach zero as $|z| \to \infty$. We consider weakly bound states. Accordingly, we have the condition $k_0^2 g(0) \gtrsim -k_0^2 g(\infty)$. We are interested in obtaining estimates of eigenvalues which are more accurate than those provided by the usual W.K.B. eigenvalue condition. This condition, which can be obtained by Langer's method, using the Schrödinger equation for the harmonic oscillator as the comparison equation, gives eigenvalue estimates of low accuracy in the case of weakly bound states.

In Sec. 2 we derive Langer's transformation. In Sec. 3 we present the usual Langer's method treatment of the problem of bound states with two turning points, using the harmonic oscillator equation as the comparison equation. We examine in detail the reason why the resulting eigenvalue condition gives eigenvalue estimates of low accuracy in the case of weakly bound states. In Sec. 4 we present a parallel development, using the symmetric Epstein equation, an example of the Helmholtz equation in which the profile is $G(x) = \left[\tilde{E} + U_o(\cosh \alpha x)^{-2}\right]$, as the comparison equation.

Note that the parametric dependence of this equation is not completely determined, as it is the case of the harmonic oscillator equation, by the usual condition of equality of the phase integrals of the original and comparison equations between the turning points. We argue that the optimal disposition of the additional parametric dependence is achieved by imposing the additional conditions $k_0^2 g(0) = G(0)$ and $k_0^2 g(\infty) = G(\infty)$. This choice leads to an eigenvalue condition which is a simple generalization of the usual W.K.B. eigenvalue condition. It asserts the equality of the phase integral of the original equation between the turning points, not to $(n + 1/2)\pi$, as in the W.K.B. eigenvalue condition, but to an algebraic function of $k_0^2 g(0)$ and $k_0^2 g(\infty)$. In Sec. 5 we examine the utility of our eigenvalue condition by applying it to selected diverse examples of the Helmholtz equation. In order to provide a rigorous test, we examine ground states. We find that our eigenvalue condition yields eigenvalue estimates of substantially increased accuracy, relative to W.K.B. eigenvalue estimates, for the Helmholtz equation with a wide range of dependences of $k_0^2 g(z)$ on z and the eigenvalue.

2. Langer's Transformation

Following Langer,[1] we first express w(z) in the form

$$w(z) = u(z)\, v[x(z)] \tag{2}$$

where u(z), v(x), and x(z) are functions which are to be determined; v(x) is a new dependent variable and x(z) is a new independent variable. Introducing (2) into (1), we obtain the differential equation

$$ux'^2 \frac{d^2v}{dx^2} + (ux'' + 2u'x') \frac{dv}{dx} + (u'' + k_0^2 gu)v(x) = 0. \tag{3}$$

Equating to zero the coefficient of dv/dx, we obtain

$$ux'' + 2u'x' = 0 \tag{4}$$

which, upon integration, yields

$$u(z) = Nx'^{-1/2}, \tag{5}$$

where N is an undetermined normalization constant. Dividing (3) by ux'^2, we obtain the equation

$$\frac{d^2v}{dx^2} + \left(\frac{k_0^2 g}{x'^2} + \frac{u''}{ux'^2} \right) v(x) = 0. \tag{6}$$

The term u''/ux'^2 in (6) presents a serious obstacle to further progress in obtaining convenient approximate solutions of (1). The lowest order approximation is obtained by neglecting this unwanted term. In Appendix A we investigate the conditions under which neglect of the unwanted term is justified.

We equate the quantity $k_0^2 g(z)/x'^2$ to G(x), the profile function in the equation

$$\frac{d^2v}{dx^2} + G(x)\, v(x) = 0, \tag{7}$$

which is referred to as the comparison equation. It satisfies the following requirements. First, it must be similar to the original equation, (1). This is an imprecise requirement, but it is central to our program. In general, the comparison equation is required to have the same structure of turning points and singularities as the original equation. The symmetric Epstein equation clearly satisfies this requirement in the present case. The harmonic oscillator equation satisfies this requirement for strongly bound states. The divergence between the profiles of the original and comparison equations at large values of the independent variables has a negligible effect on the analysis. For weakly bound states, on the other hand, the divergence is significant. Accordingly, for such states the harmonic oscillator equation

does not satisfy the requirement that it be similar to the original equation. The second requirement is that the comparison equation must be analytically solvable. The third requirement is that the phase integral of the comparison equation must be integrable in closed form. The second and third requirements are satisfied by both comparison equations.

The transformation of independent variables, which is expressed as the functional relation $x = x(z)$, is determined from the relation between $k_0^2 g(z)/x'^2$ and $G(x)$ which we have imposed. We write it as a differential equation:

$$G(x)x'^2 = k_0^2 g(z). \tag{8}$$

Extracting the square root of this equation and integrating, we obtain the functional relation $x = x(z)$ implicitly as the equality of two definite integrals,

$$\int_{x_o}^{x} [G(\xi)]^{1/2} d\xi = \int_{z_o}^{z} [k_0^2 g(s)]^{1/2} ds, \tag{9}$$

integrating from corresponding reference points x_o and z_o. For the problem at hand it is convenient to choose $x_o = 0$ and $z_o = 0$ as the reference points. The transformation of independent variables must provide that the turning points of the original and comparison equations correspond to each other. Thus we require that

$$\int_{x_-}^{x_+} [G(\xi)]^{1/2} d\xi = \int_{z_-}^{z_+} [k_0^2 g(s)]^{1/2} ds, \tag{10}$$

where $z_\pm$ and $x_\pm$ are the right- and left-hand turning points of the original and transformed equations, respectively.

3. Harmonic Oscillator Comparison Equation

The standard treatment of the problem of two turning points[2,3] is based on the use of the harmonic oscillator equation, in which

$$G(x) = \tilde{E} - U_o x^2, \tag{11}$$

as the comparison equation. The eigenvalues of this equation are given by[4]

$$\tilde{E}_n = U_o^{1/2} (1 + 2n) \quad (n = 0,1,2,\ldots). \tag{12}$$

In this case the condition stated in (10) becomes

$$\int_{z_-}^{z_+} \left[k_0^2 g(s)\right]^{1/2} ds = \int_{x_-}^{x_+} \left[U_o^{1/2}(1 + 2n) - U_o x^2\right]^{1/2} dx. \tag{13}$$

The value of the integral on the right-hand side of (13) is $(n + 1/2)\pi$. Thus we obtain the eigenvalue condition

$$\int_{z_-}^{z_+} \left[k_0^2 g(s)\right]^{1/2} ds = (n + 1/2)\pi. \tag{14}$$

This is the same as the W.K.B. eigenvalue condition.[5] Note that the parametric dependence of the comparison equation in this case is completely determined by the requirement that the phase integrals of the original and comparison equations between the turning points be equal to each other.

We can now see in detail the reason why the eigenvalue condition (14) gives eigenvalue estimates of low accuracy in the case of weakly bound states. The phase integrals of $k_0^2 g(z)$ and $G(x)$ contain substantial contributions from ranges of the independent variables in which the behavior of the two profiles deviate significantly from each other. In the case of strongly bound states, on the other hand, ranges of the independent variables in which the behavior of $k_0^2 g(z)$ and $G(x)$ deviate significantly from each other lie outside the range of integration.

4. Symmetric Epstein Comparison Equation

A class of examples of the Helmholtz equation which are analytically solvable in terms of solutions of the hypergeometric equation was applied to ionospheric radio waves by Epstein[6] and to quantum mechanics by Eckart.[7] The symmetric Epstein equation has the profile

$$G(x) = \left[\hat{E} + U_o(\cosh \alpha x)^{-2}\right]. \tag{15}$$

For weakly bound states, this equation is similar to the original equation. The harmonic oscillator equation is not. The eigenvalue condition for the symmetric Epstein equation is[8]

$$\hat{E} = -\frac{1}{4}\alpha^2 \left[-(1 + 2n) + (1 + 4U_o\alpha^{-2})^{1/2}\right]^2, \tag{16}$$

where n takes non-negative integral values starting from zero. There is a finite number of levels, determined by the condition

$$2n < (1 + 4U_o{}^{-2})^{1/2} - 1. \tag{17}$$

The phase integral between the turning points of the comparison equation is

$$\int_{x_-}^{x_+} \left[\hat{E} + U_o\ (\cosh \alpha x)^{-2}\right]^{1/2} dx = \pi\alpha^{-1} \left[U_o{}^{1/2} - (-\hat{E})^{1/2}\right]. \tag{18}$$

In contrast to the parametric dependence of the harmonic oscillator equation, that of the symmetric Epstein equation is not completely determined by the condition of equality of the phase integrals of the original and comparison equations between the turning points. Thus we must impose additional conditions in order to obtain an eigenvalue condition. The phase integral condition is unique. The choice of additional conditions is more arbitrary. In making it, we are guided by considerations of simplicity and plausibility. We choose

to impose the conditions that U_o and $\tilde{E}$ be equal to the corresponding quantities of the original equation, i.e.,

$$U_o = k_0^2 g(0) - k_0^2 g(\infty) \equiv \Delta(k_0^2 g) \tag{19}$$

and

$$\tilde{E} = G(\infty) = k_0^2 g(\infty). \tag{20}$$

We eliminate the remaining quantity in (18), namely α, by means of (16), making use of (19) and (20) to express it in terms of $\Delta(k_0^2 g)$ and $k_0^2 g(\infty)$. Note that there is no simple and plausible way to choose α. Thus the conditions that we have imposed in order to obtain an eigenvalue condition are the appropriate ones. The following expressions for α as a function of U_o and $\tilde{E}$ are obtained from (16) for $n = 0$ and $n \neq 0$, respectively:

$$\alpha_o = (-\tilde{E}_o)^{-1/2} \left[U_o - (-\tilde{E}_o)\right] \tag{21}$$

$$\alpha_{n \neq 0} = \frac{2(1 + 2n)(-\tilde{E}_n)^{1/2}}{\left[(1 + 2n)^2 - 1\right]} \times \left[\left\{1 + \frac{\left[U_o - (-\tilde{E}_n)\right]\left[(1 + 2n)^2 - 1\right]}{(1 + 2n)^2 (-\tilde{E}_n)}\right\}^{1/2} - 1\right] \tag{22}$$

The eigenvalue condition is thus given by the relation

$$\int_{z_-}^{z_+} \left[k_0^2 g(s)\right]^{1/2} ds = \pi \left\{\alpha_n \left[\Delta(k_0^2 g), k_0^2 g(\infty)\right]\right\}^{-1} \left\{\left[\Delta(k_0^2 g)\right]^{1/2} - \left[-k_0^2 g(\infty)\right]^{1/2}\right\}. \tag{23}$$

This condition is a simple generalization of the W.K.B. eigenvalue condition, (14). In the case of the ground state, $n = 0$, the eigenvalue condition has a particularly simple form, namely

$$\int_{z_-}^{z_+} \left[k_0^2 g(s)\right]^{1/2} ds = \pi \left\{ \frac{\left[-k_0^2 g(\infty)\right]^{1/2}}{\left[\Delta(k_0^2 g)\right]^{1/2} + \left[-k_0^2 g(\infty)\right]^{1/2}} \right\} . \qquad (24)$$

In the case of strongly bound ground states, $\left\{ \left[-k_0^2 g(\infty)\right] / \Delta(k_0^2 g) \right\} \to 1$ and the quantity in curly brackets in (24) approaches 1/2, in agreement with the W.K.B. eigenvalue condition. In the case of strongly bound higher states, the right-hand side of the eigenvalue condition (23) approaches $(n + 1/2)\pi$, in agreement with the W.K.B. eigenvalue condition.

5. Numerical Examples

In order to examine the utility of the eigenvalue condition which we have obtained, we apply it to selected diverse examples of the Helmholtz equation. In order to provide a rigorous test, we examine ground states. Since the scale lengths of higher states are smaller relative to that of the profile, we expect that the eigenvalue estimates for them will be more accurate. The results which we obtain indicate that our eigenvalue condition yields eigenvalue estimates which are of substantially increased accuracy, relative to W.K.B. eigenvalue estimates, for the Helmholtz equation with a wide range of dependences of $k_0^2 g(z)$ on z and the eigenvalue.

The first equation which we consider is the Schrödinger equation with a gaussian potential:

$$k_0^2 g(z) = E + V_o \exp(-z^2). \qquad (25)$$

The second equation is the Schrödinger equation with a potential whose magnitude is the square of a Lorentzian:

$$k_0^2 g(z) = E + V_o (1 + z^2)^{-2} . \qquad (26)$$

These equations provide an indication of the applicability of our eigenvalue condition to equations in which the asymptotic behavior of $k_0^2 g(z)$ as $|z| \to \infty$ is different from that of G(x) as $|x| \to \infty$. Since the asymptotic behavior

of the difference $[G(x) - G(\infty)]$ is exponential, namely, as $x \to \infty$

$$[G(x) - \tilde{E}] \sim 4U_o \exp(-2\alpha x), \tag{27}$$

the equations considered provide an appropriate indication. In the case of the gaussian potential, the asymptotic behavior is

$$[k_0^2 g(z) - E] \sim V_o \exp(-z^2) . \tag{28}$$

In the case of the squared Lorentzian potential, the asymptotic behavior is algebraic:

$$[k_0^2 g(z) - E] \sim V_0 z^{-4} . \tag{29}$$

Note that parameters multiplying the independent variables in the potentials of these equations can be scaled away in the eigenvalue condition, so that the particular equations considered do not embody restrictions on their generality with respect to such parameters.

The other equations which we consider are examples of the Helmholtz equation in which

$$k_0^2 g(z) = E + V_o \exp(s\sqrt{-E} - z^2) \qquad (s = \pm 1) \tag{30 a,b}$$

$$k_0^2 g(z) = E + V_o \exp[-(1 - s\sqrt{-E})z^2] \qquad (s = \pm 1) \tag{31 a,b}$$

Note that the dependence of $k_0^2 g(z)$ on z of (30) and (31) is the same as that of (25). Considered together, these four equations provide an indication of the applicability of our eigenvalue condition to equations with a wide range of dependences of $k_0^2 g(z)$ on the eigenvalue. We consider $E = k_0^2 g(\infty)$ to be the effective eigenvalue. In (30), $[k_0^2 g(0) - k_0^2 g(\infty)]$ increases (decreases) with increasing (-E) for $s = 1$ ($s = -1$). In (31), the width of $[k_0^2 g(z) - k_0^2 g(\infty)]$ increases (decreases) with increasing (-E) for $s = 1$ ($s = -1$).

In (30) and (31), we choose $[k_0^2 g(z) - k_0^2 g(\infty)]$ to be functions of $\sqrt{-E}$, instead of $-E$. Thereby we produce stronger variations of $[k_0^2 g(z) - k_0^2 g(\infty)]$ with respect to $-E$ for small values of $-E$, which will occur in the numerical examples, and more severe tests of our eigenvalue condition.

In order to provide a simple and uniform basis for evaluating the accuracy of the estimates provided by our eigenvalue condition, in each case we choose the value of V_o for which the ground state eigenvalue estimate given by the W.K.B. eigenvalue condition is zero. For the examples of $k_0^2 g(z)$ chosen, there is in each case a bound ground state corresponding to this value of V_o. Thus the relative error produced by the W.K.B. eigenvalue condition in each case is equal to -1. The choice of a squared Lorentzian instead of a Lorentzian has been made in (26) in order to ensure the existence of the phase integral for $E = 0$.

The numerical integration of the phase integrals presents a particular difficulty. In the neighborhood of a turning point at $z = z_t$, the dominant behavior of the integrand is proportional to $(z - z_t)^{1/2}$. The first derivative of the integrand increases in magnitude without limit as $z \to z_t$. A convenient technique for the numerical evaluation of the phase integrals involves the introduction of a simple transformation of the variable of integration which removes the singularity in the derivative of the integrand. For the class of integrands considered here on the interval $0 \leq z \leq z_+$, a suitable transformation is

$$z(t) = z_+ \left[\frac{1}{2}(3t - t^3)\right] \qquad (0 \leq t \leq 1). \tag{32}$$

With the introduction of this transformation, the phase integrals between the turning points can be expressed in the form

$$I = 3z_+ \int_0^1 \left\{k_0^2 g[z(t)]\right\}^{1/2} (1 - t^2)dt. \tag{33}$$

In the neighborhood of t = 1, the dominant behavior of $(k_0^2 g)^{1/2}$ is given by

$$\left\{ k_0^2 g[z(t)] \right\}^{1/2} \approx \left[-\frac{3}{2} z_+ k_0^2 g'(z_+) \right]^{1/2} (1 - t). \qquad (34)$$

Use of the transformation (32) results in a dramatic improvement in the accuracy of the numerical integration of the phase integrals.

The numerical integration of the differential equations to determine the exact eigenvalues is performed using a fourth-order Runge-Kutta approximation.

The numerical results are shown in Table 1. For each differential equation, the value of V_o, the exact value of $-E$, $-E_e$, the approximate value of $-E$ obtained from our eigenvalue condition, $-E_a$, and the relative error of $-E$, $[\Delta(-E)/(-E)] = [(-E_a)/(-E_e) - 1]$, are presented in succeeding columns. Recall that the relative error produced by the W.K.B. eigenvalue condition is -1 because the values of V_o have been selected to give zero W.K.B. ground state eigenvalue.

The relative error produced by our eigenvalue condition is very small in each case. The sign of the relative error is the same for all equations except the equation with the squared Lorentzian potential. Presumably, this behavior is a consequence of the fact that in all the other equations $[k_0^2 g(z) - k_0^2 g(\infty)]$ is a gaussian in z. Considered together, the six equations suggest that our eigenvalue condition yields eigenvalue estimates of substantially increased accuracy, relative to W.K.B. eigenvalue estimates, for the Helmholtz equation with a wide range of dependences of $k_0^2 g(z)$ on z and the eigenvalue.

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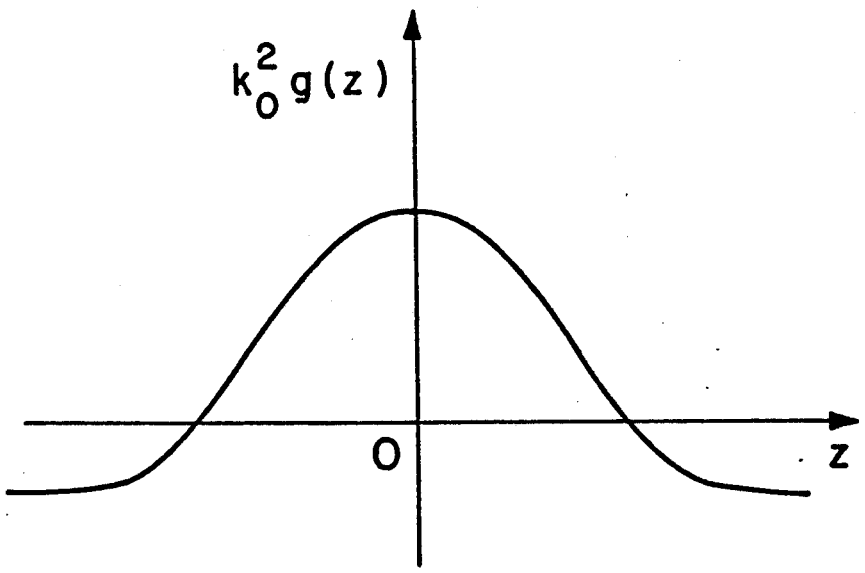

Fig. 1. Characteristic curve of $k_0^2 g(z)$ arising from symmetric profiles which correspond to weakly bound eigenstates.

(a) Equation	(b) V_o	(c) $-E_e$	(d) $-E_a$	(e) $[\Delta(-E)/(-E)]$
(25)	$(1/8)\pi$	.0801003	.0815364	.0179280
(26)	1/4	.0289241	.0285590	-.0126252
(30a)	$(1/8)\pi$	.152063	.157108	.0331721
(30b)	$(1/8)\pi$	.0539366	.0545201	.0108161
(31a)	$(1/8)\pi$	.0680584	.0688818	.0120983
(31b)	$(1/8)\pi$	.102742	.105456	.0264201

Table 1. Numerical results. Entries in (a) designate equations in the text. Corresponding to each equation, (b) gives the value of V_o, (c) the exact value of -E, (d) the approximate value of -E given by our eigenvalue condition, and (e) the relative error, $[(-E_a)/(-E_e)-1]$. For each equation, the value of V_o is chosen so that the W.K.B. eigenvalue condition gives a ground state at E = 0. Thus, the relative error produced by the W.K.B. eigenvalue condition in each case is equal to -1.

Appendix A: Negligibility of Unwanted Term

In Sec. 2 we neglected the unwanted term in (6), u''/ux'^2, in order to permit the development of the lowest order approximation to the solution of (1). Here we examine the unwanted term in detail and attempt to understand the conditions under which its neglect can be justified.

The explicit form of u(z) is

$$u(z) = N \left\{\frac{G[x(z)]}{k_0^2 g(z)}\right\}^{1/4} . \tag{A1}$$

The explicit statement of the condition for the negligibility of the unwanted term is

$$\left|\frac{u''}{uk_0^2 g(z)}\right| \ll 1. \tag{A2}$$

The condition which is typically invoked to justify the satisfaction of the inequality (A2) is that the ratio of the scale length on which the solution of (1) varies to the scale length on which the profile varies is small compared to unity or is less than or approximately equal to unity, depending on the situation considered. We shall find that the ratio can be permitted to exceed unity in some cases.

The role played by this ratio in determining the negligibility of the unwanted term is particularly clear in the case of the W.K.B. approximation, which can be obtained from Langer's transformation by using a comparison equation in which G(x) is a constant. In that case u(x) is the W.K.B. swelling factor and

$$\frac{u''}{u[k_0^2 g(z)]} = \frac{5}{16}\frac{[k_0^2 g'(z)]^2}{[k_0^2 g(z)]^3} - \frac{1}{4}\frac{[k_0^2 g''(z)]}{[k_0^2 g(z)]^2} . \tag{A3}$$

If the scale length of $g(z)$ is κ_0^{-1}, so that $|g'(z)| \simeq \kappa_0 |g(z)|$ and $|g''(z)| \simeq \kappa_0^2 |g(z)|$, the condition (A2) implies that $\kappa_0^2 << k_0^2$. If $g(z)$ is of order unity, k_0^{-1} is the scale length of the solution of (1).

If $G(x)$is not a constant, the situation is considerably more complicated and explicit results can be obtained only in particular circumstances. For example, in a study of the penetration of symmetric barriers using a comparison equation in which

$$G(x) = x^2 + \eta \ , \tag{A4}$$

where η is a constant, Baños[3] includes a detailed consideration of the unwanted term associated with an original equation which is a symmetric Epstein equation with profile

$$k_0^2 g(z) = k_0^2 \tanh^2(z/2\lambda), \tag{A5}$$

in which case $\eta = 0$. He develops a two-term expansion in powers of x^2 for the unwanted term:

$$u''/ux'^2 = \alpha - \beta x^2 + \cdots, \tag{A6}$$

with coefficients

$$\alpha = (1/16\pi)(\lambda_0/\lambda), \ \beta = (3/128\pi^2)(\lambda_0/\lambda)^2, \tag{A7}$$

where $\lambda_0 = 2\pi/k_0$. Examining the coefficients of the expansion, he concludes that a necessary and sufficient criterion for the applicability of Langer's method in this case is $\lambda/\lambda_0 \geq 1$.

It is impossible to perform a similar analysis in the case considered here. We are dealing with an eigenvalue problem and we use a more complicated comparison equation. Furthermore, the condition $k_0^2 g(0)=0$, which makes an explicit calculation possible in that case, is a very special one which is not available to us. We can, however, develop a fairly specific intuitive

understanding of the situation by considering (A1). Note that u is proportional to the one-fourth power of the ratio of profiles and hence that u varies weakly with deviations of the ratio from its value of unity at $z = 0$ and in the limit as $|z| \to \infty$. For states which are sufficiently weakly bound, the scale length of the state may exceed that of the profile. If the profile of the comparison equation is sufficiently similar to that of the original equation, the eigenvalue condition may nevertheless give an eigenvalue estimate of high accuracy. Unfortunately, it is a practical impossibility to ascertain this on an a priori basis.