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Quantisation and density of eigenvalues from the Schrödinger equation for bounded systems

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Abstract. A general formulation of the eigenvalue condition is pointed out for a one-dimensional stationary part of a separable Schrödinger equation with finite bounds, i.e. where the wavefunction vanishes at two arbitrary values of the independent variable. The procedure is general and applies equally to other eigenvalue problems of second-order, homogeneous differential equations. Where appropriate a continuous density of eigenvalues can be defined and evaluated without first solving the eigenvalue problem. Illustrative examples are provided, including gravitational and harmonic oscillator potentials.

1. Introduction

It is well known that the quantisation of the one-dimensional, stationary Schrödinger equation with coordinate z and energy E

$$-(\hbar^2/2m) d^2\psi(z)/dz^2 + (V(z) - E)\psi(z) = 0 \quad (1)$$

can be formulated as a boundary value problem for the wavefunction $\psi(z)$ for a particle of mass m moving in a potential $V(z)$.

There are other forms of the stationary Schrödinger equation, such as the radial equation for the three-dimensional problem in a spherically symmetric potential, and other equations in physics and elsewhere, such as the equation of the classical vibrating string, which lead to similar eigenvalue problems (Courant and Hilbert 1953). For definiteness we shall consider only (1), as the results may be easily generalised.

We shall consider boundary conditions defined at two distinct points A and B

$$\psi(A) = \psi(B) = 0. \quad (2)$$

Only for certain values of the energy E may (1) have solutions which satisfy (2). Finding the energies E_n , where n is an integer quantum number, and the associated eigenfunctions $\psi_n(z)$ constitutes the problem of quantisation. It is, of course, known how to proceed with this in numerous cases, but in general the problems become more complicated if the interval (A, B) is finite and $V(z)$ is not zero inside (A, B) . In the present paper we shall not attempt rigorous proofs of the statements made. Rather, we shall rely on the obvious existence of relevant cases which follow the proposed general principle to be stated in § 2. Although we find it hard to believe that a method of the present character can be really new, it does not appear to be mentioned in the more common references on quantum mechanics or differential

equations in physics. As some problems involving finite bounds appear to be more easily tractable within the present method than with those previously applied (see for example Auluck and Kothari (1945), Hull and Julius (1956), Dean (1966), Vawter (1968) and references therein), it may be reasonable to call attention to it.

2. General formulation

Let us assume that the second-order, linear, homogeneous differential equation in question depends on the variable x and one or more parameters, among which, for simplicity, we distinguish only one, denoted λ . It may be the energy E , for example. Let us also assume that a fundamental set of two linearly independent solutions $u_1(x, \lambda)$ and $u_2(x, \lambda)$ has been found, such that the general solution is

$$u(x, \lambda) = c_1 u_1(x, \lambda) + c_2 u_2(x, \lambda), \quad (3)$$

where c_1 and c_2 are two constants. Given this, we assume boundary conditions

$$u(a, \lambda) = u(b, \lambda) = 0 \quad (4)$$

at two points $a \neq b$. Equations (3) and (4) imply that c_1 and c_2 satisfy the equations

$$c_1 u_1(a, \lambda) + c_2 u_2(a, \lambda) = 0, \quad c_1 u_1(b, \lambda) + c_2 u_2(b, \lambda) = 0. \quad (5)$$

This problem is not in general well posed, and equations (5) may not have non-trivial solutions for c_1 and c_2 unless the determinant vanishes:

$$u_2(a, \lambda)/u_1(a, \lambda) = u_2(b, \lambda)/u_1(b, \lambda). \quad (6)$$

This will in general only be true for a discrete set of values of λ , which we may denote λ_n . In this case the condition (6) imposes the quantisation of λ .

When u_1 and u_2 are linearly independent the ratios in (6) are not constant but functions of the arguments of u_1 and u_2 . We consider now the cases in which u_1 and u_2 as functions of x have a number of simple zeros. In particular, there may be no zeros. The zeros of u_2 and u_1 may be assumed to separate each other, which can be seen in the following way, unless in one of them there is precisely one zero, which case should not be difficult to analyse explicitly, should it occur. The mutual separation of the zeros follows, when there are two or more zeros of both functions, if we can exclude the possibility that one of the functions (u_2) has two (or more) zeros between two consecutive zeros of the other (u_1). There remains then only the possibility that each function has precisely one zero between two consecutive zeros of the other. Between two zeros α and β any solution of the differential equation, say u_1 , is also a solution of the eigenvalue problem corresponding to bounds $a = \alpha$ and $b = \beta$, and the parameter λ is automatically an eigenvalue. If the zeros are consecutive the solution corresponds to the lowest eigenvalue. If there is another solution u_2 of the same equation, but with λ replaced by λ' , with two zeros at α' and β' such that

$$a = \alpha < \alpha' < \beta' < \beta = b$$

then it is known that for the equations of the Sturm–Liouville type, including the Schrödinger equation, this second solution must correspond to an eigenvalue λ' , which is larger than λ , if the interval (α', β') is smaller than (a, b) . The only way in which u_2 can be a solution of the same equation as u_1 , corresponding to the same eigenvalue $\lambda' = \lambda$, is by letting $\alpha = \alpha'$ and $\beta = \beta'$. In this case, the two solutions u_2 and u_1 are

proportional to each other, because the eigenvalues are non-degenerate. This contradicts that they are linearly independent solutions of the original problem. Hence there cannot be two zeros of u_2 between two consecutive zeros of u_1 . As more zeros of u_2 between two consecutive zeros of u_1 correspond to solutions which belong to larger eigenvalues than the lowest, the result follows also for more than two zeros.

The ratios in (6) will oscillate rapidly between $+\infty$ and $-\infty$, which implies that we may define a phase function $\theta(x, \lambda)$ by letting

$$\tan \theta(x, \lambda) = u_2(x, \lambda)/u_1(x, \lambda), \tag{7}$$

and that $\theta(x, \lambda)$ will be a continuous function of x and λ . Thus, at the zeros of u_1 we will have $\theta = \pi/2 + p\pi$, and at the zeros of u_2 , $\theta = p\pi$, for a number of integers p , which denumerate the zeros of u_1 and u_2 , of which there are often infinitely many. In the simplest cases $\theta(x, \lambda)$ is a monotonic function of x , decreasing or increasing depending on the choice of u_1 and u_2 . For simplicity we henceforth assume this property of $\theta(x, \lambda)$. Therefore, for the equations which satisfy the criteria, the condition of quantisation (6) may be expressed in the form

$$\theta(b, \lambda_n) - \theta(a, \lambda_n) = \pm n\pi \tag{8}$$

where, if $b > a$, and θ is increasing (decreasing) with x , we should choose the positive (negative) sign and

$$n = 1, 2, 3, \dots \tag{9}$$

This is a formal statement from which the eigenvalues λ_n can be deduced if the phase function θ is known.

Some properties of equation (8) seem to be of interest. Firstly, the function θ is expressible in terms of standard functions in numerous cases, so its calculation does not depend on quadrature. Secondly, the phase function may be assumed sufficiently well behaved that the solution of (8) can be performed, if not analytically, then by rapidly converging methods, which can achieve arbitrarily high accuracy. It should in general, for a given n , only be a question of finding the value of λ corresponding to the intersection of two curves provided by $\theta(b, \lambda)$ and $\theta(a, \lambda) \pm n\pi$, unless it can be shown that no solution exists. In a large number of problems the assured existence of an infinite range of non-degenerate eigenvalues asserts that this problem has one and only one solution. If the interval (a, b) is finite this holds for the Schrödinger equation, for example, while if the interval is infinite there may occur a continuous range of eigenvalues, as well as a discrete one in which there may be limit points. The present method offers the opportunity in such cases to regard the interval as arbitrarily large, but finite, in which case the eigenvalues may be close but discrete.

If we consider the possibility of describing the set of eigenvalues λ_n in terms of a continuum density $\rho(\lambda)$, then we find that the number of eigenvalues, starting for simplicity at $\lambda_1 = 0$, up to a given value λ is

$$N(\lambda) = \pm \pi^{-1}(\theta(b, \lambda) - \theta(a, \lambda)). \tag{10}$$

Therefore, the density is, for $\lambda \geq 0$,

$$\rho(\lambda) = dN(\lambda)/d\lambda = \pm \pi^{-1}(\theta'(b, \lambda) - \theta'(a, \lambda)), \tag{11}$$

where

$$\theta'(x, \lambda) = \partial\theta(x, \lambda)/\partial\lambda. \tag{12}$$

Consider the simplest example of a freely propagating particle or a standing wave, determined by the equation

$$d^2u/dx^2 + \lambda u = 0. \quad (13)$$

The set of linearly independent solutions is

$$u_1(x, \lambda) = \cos\sqrt{\lambda}x, \quad u_2(x, \lambda) = \sin\sqrt{\lambda}x, \quad (14)$$

with the phase function

$$\theta(x, \lambda) = \sqrt{\lambda}x. \quad (15)$$

The quantisation rule (8) gives

$$\sqrt{\lambda_n}(b-a) = n\pi.$$

Hence

$$\lambda_n = [n\pi/(b-a)]^2. \quad (16)$$

The continuous density of eigenvalues becomes

$$\rho(\lambda) = [(b-a)/2\pi](1/\sqrt{\lambda}). \quad (17)$$

This example also shows the separation of zeros and monotonicity of $\theta(x, \lambda)$. It is, for finite potentials in the interval (a, b) , also the general asymptotic limit for large n of the Schrödinger equation. For non-vanishing potentials, however, the classical limit will be a better approximation (cf § 3 and 4).

If the boundary conditions are specified at one or two singular points in some problems of physical relevance (cf for example the radial equation in spherically symmetric potentials), it may be appropriate to require rather that $u(x, \lambda)$ should remain finite. Other prescriptions regarding the behaviour of u may also be considered. In such cases it seems that defining a new function

$$v(x, \lambda) = f(x)u(x, \lambda) \quad (18)$$

may be possible, such that the boundary values of $v(x, \lambda)$ have the form (4), while v now satisfies another second-order equation. As the present method does not require that a and b are regular points, there is no need for this transformation to remove the singular points from the original equation, or to avoid creating new ones in the equation for v . It only has to alter the boundary conditions. If, according to (18), $v_1 = fu_1$ and $v_2 = fu_2$ then the Wronskians are related by

$$W(v_1, v_2) = f(x)^2 W(u_1, u_2) \quad (19)$$

which implies that when u_1 and u_2 are linearly independent so are v_1 and v_2 . Therefore the phase function is not changed by the transformation (18), and the quantisation condition (8) holds for the entire class of problems, which can be cast into the form (4) by means of a transformation (18). The radial Schrödinger equation for a spherical box of radius R , inside which the potential vanishes, with the boundary conditions (Messiah 1965)

$$\lim_{r \rightarrow 0} r\psi(r) = 0 \quad \text{and} \quad \psi(R) = 0 \quad (20)$$

provides an example of this, where $r = 0$ is a singular point.

If one of u_1 and u_2 is singular at a boundary, and for that reason immediately excluded by having its coefficient c_1 or c_2 equal to zero, then the problem reduces to the familiar

$$u_1(b, \lambda) = 0 \tag{21}$$

if u_2 is singular at a and $u_1(a, \lambda) = 0$. In such cases the present method offers no advantage. For the radial equation it can be shown explicitly that the quantisation by the phase function reduces to the familiar $j_l(kR) = 0$, where l is the angular momentum, corresponding to (21). In this example (21) holds because the indicial exponents for v_1 and v_2 are $\alpha_1 = l + 1$ and $\alpha_2 = -l$ (or l and $-l - 1$ for the spherical Bessel functions j_l and y_l), but in general opposite signs of these exponents do not occur as a rule.

In cases when the solutions u_1 and u_2 may not be standard functions, it is possible to apply the quantisation by (8) when the phase function is obtained in the following way, which is standard. Let $R(x, \lambda)$ define an amplitude function, such that

$$u_1 = R \cos \theta, \quad u_2 = R \sin \theta. \tag{22}$$

Note that R and θ are not the conventionally defined amplitude and phase of the wavefunction itself, and therefore have a different significance from these quantities in methods such as the wkb (Messiah 1965). Here the (unnormalised) eigenfunctions are

$$u(x, \lambda_n) = R(x, \lambda_n) \sin[\theta(x, \lambda_n) - \theta(a, \lambda_n)], \tag{23}$$

or forms equivalent to this, subject to the condition (8). This follows immediately from (5). Then, for example, for an equation of the form

$$d^2u/dx^2 + p(x) du/dx + q(x, \lambda)u = 0, \tag{24}$$

with Wronskian

$$W(x) = \exp\left(-\int^x dt p(t)\right), \tag{25}$$

we have that R and θ satisfy the nonlinear equations

$$\frac{d^2R}{dx^2} - \frac{W(x)^2}{R^3} + p(x) \frac{dR}{dx} + q(x, \lambda)R = 0, \quad \frac{d\theta}{dx} = \frac{W}{R^2}, \tag{26}$$

and the phase function is given by

$$\theta(x, \lambda) = \int^x dy W(y)/R(y, \lambda)^2. \tag{27}$$

The amplitude function R has no zeros, because the zeros of u_1 and u_2 separate each other. Despite the need to use quadrature, this may provide a convenient expression of the quantisation condition

$$\int_a^b dx \frac{W(x)}{R(x, \lambda_n)^2} = n\pi, \tag{28}$$

where the positive sign is used, since for the choice $R > 0$, θ is increasing. This equation is exact. In the classical limit of the Schrödinger equation

$$h \rightarrow 0 \text{ and } n \rightarrow \infty, \quad \text{but } nh = \text{finite},$$

this leads to the Bohr–Sommerfeld quantisation rule, which for $p(x) = 0$ is

$$2 \int_a^b dx [2m(E_n - V(x))]^{1/2} = nh, \quad (29)$$

which is obtained directly from (26) by disregarding the second derivative, which is small compared with the other terms in the limit $\hbar \rightarrow 0$. It would also seem possible that a superperturbation theory (Blankenbecler 1966, Madan 1968) could be constructed from the present formulation, as the amplitude function is free from zeros by construction. We shall not pursue this approach, however.

3. Gravitation

A uniform gravitational field acting in the direction of negative z gives a potential energy

$$V(z) = mgz \quad (30)$$

where g is the gravitational acceleration. Then

$$-(\hbar^2/2m) d^2\psi/dz^2 + (mgz - E)\psi = 0. \quad (31)$$

Introducing the length scale l , defined by

$$l^3 = \hbar^2/2m^2g, \quad (32)$$

and the variable x , defined by

$$z = l(x + E/mgl) = l(x + \lambda), \quad (33)$$

the Schrödinger equation is then the Airy equation

$$d^2u/dx^2 - xu = 0, \quad (34)$$

and its linearly independent solutions are the Airy functions

$$u_1 = \text{Ai}(x), \quad u_2 = \text{Bi}(x), \quad (35)$$

where the dependence on the parameter λ is implicitly given by (33). The phase function is

$$\theta = \bar{\theta}(-x) \equiv \tan^{-1}[\text{Bi}(x)/\text{Ai}(x)], \quad (36)$$

which is a known function (Abramowitz and Stegun 1965). Considering bounds

$$A \leq z \leq B,$$

then

$$a \equiv A/l - \lambda \leq x \leq B/l - \lambda \equiv b. \quad (37)$$

Without loss of generality we may set $A = 0$. $\bar{\theta}$ is a decreasing function of its argument, hence θ is increasing when x increases and we should use the positive sign in (8). Then the quantisation gives

$$\bar{\theta}(\lambda_n - B/l) - \bar{\theta}(\lambda_n) = n\pi. \quad (38)$$

Consider first the semi-infinite case $B \rightarrow +\infty$. Using

$$\bar{\theta}(-x) \sim \tan^{-1}[2 \exp(\frac{4}{3}x^{3/2})] \rightarrow \frac{1}{2}\pi$$

for $x \rightarrow \infty$, we have

$$\frac{1}{2}\pi - \bar{\theta}(\lambda_n) = n\pi. \tag{39}$$

This shows that λ_n is given by

$$\text{Ai}(-\lambda_n) = 0,$$

as is well known. This result corresponds to the case (21) due to the singularity in Bi at $x \rightarrow \infty$. The present method handles the singularity without difficulty. Here, however, the singularity is absent whenever b is finite, and the complete solution is given by (38). When λ_n is large, using

$$\bar{\theta}(x) \sim \frac{1}{4}\pi - \frac{2}{3}x^{3/2}$$

for $x \rightarrow \infty$, we have the well known result

$$\lambda_n = E_n/mgl \sim [\frac{3}{2}\pi(n - \frac{1}{4})]^{2/3}. \tag{40}$$

Large values of λ may be regarded as corresponding to the classical limit of letting $\hbar \rightarrow 0$ in (32) simultaneously with letting the quantum number n become large in such a way that E_n remains finite. The relative magnitude of the correction to the leading term in the phase function is of the order x^{-3} , and the approximation is good even for rather small values of λ . The density of eigenvalues becomes

$$\rho(\lambda) = \pi^{-1}[\bar{\theta}'(\lambda - B/l) - \bar{\theta}'(\lambda)], \tag{41}$$

which in the leading order gives

$$\rho(\lambda) \sim \pi^{-1}\sqrt{\lambda}. \tag{42}$$

This approximation is accurate enough to be regarded as exact as far as a continuous density $\rho(\lambda)$ is reasonable, even for small λ .

When an upper bound is introduced the problem becomes somewhat more involved, and it is perhaps only in such cases that the present method may really be advantageous. It is evident that $\bar{\theta}$ is essentially constant if its argument is negative, i.e. if

$$B/l > \lambda_n,$$

which therefore corresponds to the limit just considered. When λ_n becomes larger than B/l , however, the variation in $\bar{\theta}(\lambda_n - B/l)$ will cause a significant change in the eigenvalue spectrum. The nature of this, which is given exactly by the relations (38) and (41), is perhaps best evaluated in the classical limit, where $\bar{\theta}$ has the value $\pi/2$ until $\lambda_n = B/l$, and then for larger λ_n the value given by the leading asymptotic term. This will produce a discontinuity, which is of course not really there, but for the density, which is the relevant quantity in this limit, it produces a good representation of the actual function. It is notable here that we do not have to calculate first a complicated discrete spectrum of eigenvalues, but may take the desired limit directly in the expression (41). We get

$$\rho(\lambda) \sim \begin{cases} \pi^{-1}\sqrt{\lambda} & \text{for } \lambda \leq B/l, \\ \pi^{-1}[\sqrt{\lambda} - (\lambda - B/l)^{1/2}] & \text{for } \lambda \geq B/l. \end{cases} \tag{43}$$

In particular, if $\lambda \gg B/l$ we have

$$\rho(\lambda) \sim (B/l2\pi)(1/\sqrt{\lambda}), \tag{44}$$

which is just the case of a particle in a box of extension $(0, B)$ and zero potential, and agrees with (17). The relative magnitude of the correction to (44) is of the order λ^{-1} . A better approximation is

$$\rho(\lambda) \sim (B/12\pi)(\lambda - B/2l)^{-1/2}, \quad (45)$$

where the correction is only of the order λ^{-2} . Thus, in the box, the energy is shifted upwards by

$$(B/2l)mgl = \frac{1}{2}mgB, \quad (46)$$

which is the average gravitational energy in the motion within the range $0 \leq z \leq B$, when this motion has become the plane wave of uniform density. This happens when the vertical motion becomes very energetic and the particle is reflected elastically at both the upper and lower bounds, rather than being redshifted when climbing the gravitational field until its wavelength reaches zero near the classical turning point before the upper bound is reached, as corresponds to the motion for values of λ less than B/l . Considerations of this nature, of course, apply to any finite potential.

The result corresponding to the classical limit can also be obtained by the Bohr-Sommerfeld quantisation rule. For $\lambda \geq B/l$ the classical turning point is at $z = B$, and

$$\int_0^B dz [2m(E - mgz)]^{1/2} = n\pi\hbar,$$

which gives

$$\frac{2}{3}[\lambda^{3/2} - (\lambda - B/l)^{3/2}] = n\pi, \quad (47)$$

and thereby the result (43). It does not, however, provide any estimate of the non-classical corrections. The WKB method may do this, while exact results may be obtained from the present method, at least in principle.

4. Oscillator

The Schrödinger equation for the harmonic oscillator is

$$-(\hbar^2/2m) d^2\psi/dz^2 + (\frac{1}{2}m\omega^2 z^2 - E)\psi = 0. \quad (48)$$

Introducing the length scale l defined by

$$l^2 = \hbar/2m\omega \quad (49)$$

and the variable x defined by

$$z = lx, \quad (50)$$

the Schrödinger equation becomes

$$d^2u/dx^2 - (\frac{1}{4}x^2 - \lambda)u = 0 \quad (51)$$

where

$$\lambda = E/\hbar\omega. \quad (52)$$

The parabolic cylinder functions provide two linearly independent solutions

$$u_1(x, \lambda) = U(-\lambda, x), \quad u_2(x, \lambda) = \Gamma(\frac{1}{2} + \lambda)V(-\lambda, x). \quad (53)$$

The phase function is given by

$$\theta(x, \lambda) = \bar{\chi}(-\lambda, x) \equiv \tan^{-1}[\Gamma(\frac{1}{2} + \lambda) V(-\lambda, x) / U(-\lambda, x)], \tag{54}$$

where $\bar{\chi}$ is a known function. The quantisation condition is

$$\bar{\chi}(-\lambda_n, b) - \bar{\chi}(-\lambda_n, a) = n\pi, \tag{55}$$

choosing the plus sign for the increasing function $\bar{\chi}$ of x . Here

$$b = B/l, \quad a = A/l. \tag{56}$$

This represents, formally, the complete solution to this quantisation problem. To the extent that $\bar{\chi}$ is computable with arbitrary accuracy it may also represent the practically most direct solution, as discussed in § 2.

For negative values of x we may use the relations

$$\begin{aligned} U(-\lambda, -x) &= (\cos \pi\lambda)u_2 + (\sin \pi\lambda)u_1, \\ \Gamma(\frac{1}{2} + \lambda)V(-\lambda, -x) &= (\cos \pi\lambda)u_1 - (\sin \pi\lambda)u_2, \end{aligned} \tag{57}$$

which imply

$$\tan \bar{\chi}(-\lambda, -x) = \cot[\bar{\chi}(-\lambda, x) + \pi\lambda]$$

or

$$\bar{\chi}(-\lambda, -x) = \frac{1}{2}\pi - \pi\lambda - \bar{\chi}(-\lambda, x). \tag{58}$$

Consider first the case of $A = 0$ and $B \rightarrow \infty$, which corresponds to a reflecting barrier at the centre. For $x = 0$

$$\bar{\chi}(-\lambda, 0) = \pi(\frac{1}{4} - \frac{1}{2}\lambda), \tag{59}$$

while for $x \rightarrow +\infty$

$$\bar{\chi}(-\lambda, x) \rightarrow \frac{1}{2}\pi. \tag{60}$$

Thus the quantisation gives

$$\lambda_n = (2n - 1) + \frac{1}{2}. \tag{61}$$

These are the odd quantum numbers corresponding to wavefunctions of odd parity, which vanish at $x = 0$. The density of eigenvalues is

$$\rho(\lambda) = -\pi^{-1} \bar{\chi}'(-\lambda, 0) = \frac{1}{2} \quad \text{for } \lambda \geq 0. \tag{62}$$

For the case of $A \rightarrow -\infty$ and $B \rightarrow +\infty$, using (58) in (55), we get

$$\lambda_n = (n - 1) + \frac{1}{2}, \tag{63}$$

as usual. The density now becomes

$$\rho(\lambda) = 1 \quad \text{for } \lambda \geq 0. \tag{64}$$

As it is generally true that there are no eigenvalues corresponding to energies smaller than the potential minimum, we shall not discuss the case of $\lambda \leq 0$ explicitly. However, as there are no oscillations of the solutions of the differential equation in this range, the phase function will not vary enough with x to provide a solution of the equation (55). For $n \geq 1$ the phase must change by at least π , and this requires zeros of u_1 and u_2 , which do not occur for $\lambda \leq 0$.

As in the previous section l is a quantum length, which becomes small in the classical limit. If λ_n is simultaneously large, for $0 \leq x < \infty$ we have (Abramowitz and Stegun 1965)

$$\bar{\chi}(-\lambda, x) \sim \tan^{-1}[\text{Bi}(t)/\text{Ai}(t)] = \bar{\theta}(-t), \tag{65}$$

where, defining

$$\xi = x/2\sqrt{\lambda}, \tag{66}$$

we have for $\xi \leq 1$

$$t = -\left\{\frac{3}{2}\lambda [\cos^{-1} \xi - \xi(1 - \xi^2)^{1/2}]\right\}^{2/3}, \tag{67}$$

and for $\xi \geq 1$

$$t = \left\{\frac{3}{2}\lambda [\xi(\xi^2 - 1)^{1/2} - \cosh^{-1} \xi]\right\}^{2/3}. \tag{68}$$

Using the leading asymptotic forms, which for finite ξ becomes justified by the large factor λ in (67) and (68),

$$\bar{\theta}(-t) \sim \frac{1}{4}\pi - \frac{2}{3}(-t)^{3/2} \quad \text{for } t < 0, \tag{69}$$

$$\bar{\theta}(-t) \sim \pi/2 \quad \text{for } t > 0, \tag{70}$$

the phase function becomes

$$\bar{\chi}(-\lambda, x) \sim \frac{1}{4}\pi - \lambda [\cos^{-1} \xi - \xi(1 - \xi^2)^{1/2}] \quad \text{for } 0 \leq \xi \leq 1, \tag{71}$$

$$\bar{\chi}(-\lambda, x) \sim \pi/2 \quad \text{for } \xi \geq 1, \tag{72}$$

valid for $x \geq 0$. The corresponding expressions for $x \leq 0$ can be obtained from (58). Defining

$$\xi_a = a/2\sqrt{\lambda}, \tag{73}$$

$$\xi_b = b/2\sqrt{\lambda}, \tag{74}$$

we find for the particular case of $b > 0$ and $a = -b < 0$ that the quantisation condition becomes

$$n\pi = 2\bar{\chi}(-\lambda_n, b) + \pi\lambda_n - \frac{1}{2}\pi. \tag{75}$$

For $\xi_b \geq 1$ this gives again the result (63), since the classical limit causes the transitional region to shrink to zero near $\xi_b = 1$. For $\xi_b \leq 1$

$$n = (2/\pi)\lambda_n [\sin^{-1} \xi_b + \xi_b(1 - \xi_b^2)^{1/2}], \tag{76}$$

where ξ_b depends on λ_n according to (74). This again is equivalent to the result obtained by the Bohr-Sommerfeld rule. For very large quantum numbers $\xi_b \rightarrow 0$, and expanding the right-hand side of (76) gives

$$\lambda_n = (n\pi/2b)^2 \tag{77}$$

corresponding to free motion in a box of length $b - a = 2b$. In this limit the density of eigenvalues becomes

$$\rho(\lambda) = (2/\pi)\bar{\chi}'(-\lambda, b) + 1. \tag{78}$$

Thus, for $\xi_b \geq 1$ again simply

$$\rho(\lambda) = 1 \quad \text{for } 0 \leq \lambda \leq \frac{1}{4}b^2, \tag{79}$$

and for $\xi_b \leq 1$

$$\rho(\lambda) = (2/\pi) \sin^{-1}(b/2\sqrt{\lambda}) \quad \text{for } \frac{1}{4}b^2 \leq \lambda. \quad (80)$$

For large λ this gives

$$\rho(\lambda) \approx (2b/2\pi)(1/\sqrt{\lambda}) \quad (81)$$

as for the free motion in the box, while $\rho(\lambda) \rightarrow 1$ for $\lambda \rightarrow \frac{1}{4}b^2$. The discontinuity in the first derivative of $\rho(\lambda)$ is, as in § 3, due to the classical limit. The point where it occurs corresponds to

$$E = \frac{1}{2}m\omega^2 B^2 = V(B) \quad (82)$$

where the potential is discontinuous if we regard the boundary conditions as caused by an infinitely large positive potential energy outside the interval (A, B) .

The relative size of the correction to (81) is of order λ^{-1} . This correction may be reduced to being of order λ^{-2} by taking

$$\rho(\lambda) \approx (2b/2\pi)(\lambda - b^2/12)^{-1/2}. \quad (83)$$

The quantity subtracted represents the average potential energy for a plane wave motion of uniform density inside the interval $(A, B) = (-B, B)$.

5. Conclusions

For a general class of homogeneous, linear, second-order differential equations we have discussed the eigenvalue conditions corresponding to solutions which are subject to boundary conditions at two different points, where they must vanish. This eigenvalue problem may be expressed in the simple form

$$\theta(b, \lambda_n) - \theta(a, \lambda_n) = n\pi, \quad (84)$$

where θ is a phase function related to two linearly independent solutions of the differential equation. If the equation is standard and these solutions are known standard functions, as is often the case, then the phase function may be regarded as equally available. The nature of the problem is such that solving the equation (84) in such cases should be comparatively straightforward, perhaps sufficiently straightforward that we may regard (84) as an exact solution. In the present paper, however, we have not attempted to demonstrate this explicitly. On the other hand, it has been shown analytically that the condition (84) is equivalent to a number of standard results of the quantisation of the Schrödinger equation, including the cases of a particle moving within finite bounds in a gravitational and a harmonic oscillator potential. In these cases we have shown that (84) provides the correct results in the classical limit, which results can be also, and more directly, obtained by the Bohr–Sommerfeld quantisation method. The method based on (84) allows also the consideration of the corrections to this limit, in an analytical way so far as asymptotic expansions are available for the independent solutions or the phase function directly. It is therefore conceivable that (84) may also be of use in analytical work.

The form of the eigenvalue condition is such that if the construction of a continuous density of eigenvalues is relevant, then it can be obtained directly, without first having

to calculate eigenvalues. This density is given by

$$\rho(\lambda) = \pi^{-1}[\theta'(b, \lambda) - \theta'(a, \lambda)] \quad (85)$$

in terms of the derivative of the phase function with respect to λ . In the same way as (84), if the phase function is available, this result does not depend on such procedures as quadrature. It is also of interest to note that if (85) provides the density of eigenvalues λ for a problem in which the one-dimensional equation considered here results from the separation of variables in an equation of three dimensions, then it may be relevant to form a convolution of $\rho(\lambda)$ with the corresponding densities arising in the other dimensions in order to obtain the density of the sum of the eigenvalues. As the density of eigenvalues for a two-dimensional problem is asymptotically constant, and for free motion in the two dimensions according to the Schrödinger equation is constant for all λ , the convolution of such a constant density with (85) may in some such cases reduce simply to the integral, and the total density becomes

$$\rho_3(\lambda) = \pi^{-1}[\theta(b, \lambda) - \theta(a, \lambda)]\rho_2, \quad (86)$$

where ρ_2 is the density for the two-dimensional part, and (a, b) is the range of the motion in the third dimension. Hence, in a one-dimensional potential in three-dimensional problems the density of the total eigenvalue, which may be the total energy, may be obtained directly from the phase function without differentiation.

References

- Abramowitz M and Stegun I A 1965 *Handbook of mathematical functions* (New York: Dover)
 Auluck F C and Kothari D S 1945 *Proc. Camb. Phil. Soc.* **41** 175
 Blankenbecler R 1966 *Phys. Rev.* **152** 1471
 Courant R and Hilbert D 1953 *Methods of mathematical physics* vol 1-3 (New York: Interscience)
 Dean P 1966 *Proc. Camb. Phil. Soc.* **62** 277
 Hull T E and Julius R S 1956 *Can. J. Phys.* **34** 914
 Madan R N 1968 *Phys. Rev.* **173** 1615
 Messiah A 1965 *Quantum Mechanics* vol 1-2 (Amsterdam: North-Holland)
 Vawter R 1968 *Phys. Rev.* **174** 749