An alternative to JWKB theory

1980 J. Phys. A: Math. Gen. 13 L231

(http://iopscience.iop.org/0305-4470/13/7/002)

J. Phys. A: Math. Gen. **13** (1980) L231–L234. Printed in Great Britain

LETTER TO THE EDITOR

An alternative to JWKB theory

J Killingbeck

Physics Department, University of Hull, Hull HU6 7RX, UK

Received 28 March 1980

Abstract. A method of numerical integration is presented which leads to a Bohr–Sommerfeld type formula yielding exact eigenvalues of the Schrödinger equation. Tests on simple potentials give much better results than those of the usual JWKB methods.

It is well known that the usual first-order JWKB theory yields a Bohr–Sommerfeld type of quantisation formula for bound-state energies, and gives poor results for the energies of low-lying bound states. We can display the quantisation condition in the canonical form

$$\int_B^A F(E, x)\,\mathrm{d}x = \pi(n+1+r) \tag{1}$$

for a problem involving one coordinate x, with E the energy, n an integer and r some remainder term. We take the Schrödinger equation to be

$$-\mathrm{D}^2\psi + V\psi = E\psi. \tag{2}$$

The traditional approach is to set the limits in A and B equal to the classical turning-point coordinates (for simple potentials such as x^{2N} with $N \geq 1$) and to set $r = 0$. First-order JWKB theory sets F equal to $[E - V(x)]^{1/2}$. Titchmarsh (1961) has shown that with this choice of A, B and F the equation (1) can be made exact with an appropriate choice of r. For large n, r turns out to be of order n^{-1}, which explains the success of the method for large n. Hioe *et al* (1976) have applied Titchmarsh's result in a study of anharmonic oscillator problems. However, to improve the accuracy of equation (1) it is still the overwhelming tradition to keep A, B and r fixed at their first-order JWKB values (with $r = 0$) and to introduce higher-order correction terms into the integrand F. Works by Dagens (1969), Dunham (1932), Fröman (1978), Berry and Mount (1972), Kesarwani and Varshni (1980) and many others have explored this approach. Newman and Thorson (1972) have developed what is essentially a numerical method for iteratively computing the higher-order corrections; their quantisation condition involves two 'connection angles' which arise from boundary conditions at the turning points.

It has long seemed peculiar to the present author that a calculation restricted to the classical region should be expected to give precise results about the energy eigenvalues; the characteristic property of the quantum mechanical problem is that the particle can spread outside the classical region, while it is not obvious that the JWKB approach can 'see' into the forbidden region. For example, if $V(x)$ has a 'wiggle' at $x > A$ which would allow quantum mechanical tunnelling, how do we allow for this? Recent work by

Colwell *et al* (1978) and Augustin and Rabitz (1979) seems to indicate that 'tunnelling corrections' to JWKB theory are indeed sometimes needed. Krieger *et al* (1967) have conjectured that even for potentials of x^{2N} type the result of higher and higher order JWKB approximations may only approach the correct eigenvalue in the manner of an asymptotic series. There do not seem at the moment to exist any numerical results of sufficient accuracy to check this idea.

A clue to an alternative approach can be found in two short notes by Young (1931, 1932). In his work on the concept of local momentum Young described a method which seems to have been largely neglected in the subsequent development of the theory. Dunham (1932) commented that Young's approach is difficult to apply numerically, while the few modern authors who have referred to Young's work have not analysed it in detail. In this short note we wish to point out that, with slight modifications, Young's approach leads to a method which is tractable using modern calculators. We treat the bound-state problem; Young (1932) also mentioned some results for potential scattering theory. Our view differs from Young's in that we use real wavefunctions rather than complex ones, and we study the differential equation for A, equation (6) below, rather than his more complicated equation for P. We consider a finite even-parity potential (e.g. $x^2+\lambda x^4$) in equation (2), and look for an even-parity solution of the form

$$\psi = A(x)\cos\left(\int_0^x P(y)\,\mathrm{d}y\right). \tag{3}$$

Substituting (3) into (2) and treating the sine and cosine equations separately leads to the equations

$$PA^2 = 1 \tag{4}$$

$$P^{1/2}\mathrm{D}^2(P^{-1/2}) = P^2 + (V-E) \tag{5}$$

$$\mathrm{D}^2A = A^{-3} + A(V-E). \tag{6}$$

Young (1931) commented that from (5) it can be established that P, which he called the local momentum, can never become negative. From (3) we see that the condition that ψ shall tend to zero at $\pm\infty$ is simply equation (1) with $r=0$ and $A=\infty$, $B=-\infty$ (the intuitively 'sensible' limits for this quantum mechanical problem), while $F=A^{-2}$, where A satisfies the differential equation (6). This equation, which was not given by Young, is the one needed for our numerical method. From equation (2) it follows that near $x=0$ we have

$$\psi(x) = 1 - \tfrac{1}{2}x^2[E-V(0)] + \ldots \tag{7}$$

if we arbitrarily set $\psi(0)=1$. By making the appropriate expansion in (3) we find that (7) is obeyed if we set $A(0)=1$ and $\mathrm{D}A(0)=0$ in (6). (The same result holds for odd-parity solutions, which are obtained by using a sine function in (3).) Equation (6) can easily be integrated numerically between 0 and ∞, the numerical integration of A^{-2} being performed simultaneously. Simply doubling then gives the results for the range $\pm\infty$. One simple way to integrate (6) is to use a finite-difference approach (Killingbeck 1977) based on the equations

$$A(x+h) = R(x)A(x) \tag{8}$$

$$R(x) + 1/R(x-h) = 2 + h^2[A^{-4} + (V-E)] \tag{9}$$

with the initial condition $R(0)\,R(-h) = 1$ (which ensures that $DA(0) = 0$). The integral of A^{-2} obtained using (8) and (9) and the midpoint rule differs from the exact ($h = 0$) value by a term of order h^2 for small h, and use of two h-values (0·01 and 0·02) gives a value accurate to about one part in 10^6. (Use of large h-values leads to an obvious error indication in that A becomes negative.) By using a more sophisticated integration method, and by using trial energies with smaller spacings, the results shown in tables 1 and 2 can be further improved, but the evidence is already quite striking. Our quoted energy values in the tables differ from the corresponding exact eigenvalues by about $\frac{1}{2}$ in the last quoted digit, and the first- and third-order versions of traditional JWKB theory are clearly nowhere near as accurate for the ground-state problems represented in table 2. For higher states the present calculation still involves a smooth positive A function; the nodes are produced by the cosine factor in equation (3). The infinite integration is no problem; A quickly becomes large enough to yield a converged value for the integral.

Table 1. Energy dependence of the phase integral ($V = x^6$).

E	1·144 8	1·144 9	9·073 0	9·073 1
I	1·570 794	1·570 869	4·712 314	4·712 403
ϵ†	1·144 803		9·073 084	

† Interpolated energies, using $\pi = 3{\cdot}141\ 5927$. Integrals taken between 0 and ∞.

Table 2. Some ground-state eigenvalue estimates.

Potential	W_1†	W_3†	This work
x^4	0·867 145	0·951 643	1·060 362
x^6	0·800 830	1·043 020	1·144 803
x^8	0·761 936	1·171 232	1·225 820
x^2+x^4	1·250 8‡		1·392 353

† First- and third-order JWKB results, from Krieger *et al* (1967).
‡ From Radmore (1980).

The present work is intended to point out the value of Young's ideas to workers in the field. There are obviously many questions yet to be explored, e.g. how must the method be modified to deal with Coulomb potentials?; how does it relate to the usual JWKB method which uses only the classical region?; is it possible to obtain asymptotic 'large n' formulae similar to those for JWKB theory?; can expectation values be calculated by direct integration? We hope that this note will stimulate work on such problems.

References

Augustin S D and Rabitz 1979 *J. Chem. Phys.* **71** 4956–68
Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315–97
Colwell S, Handy N and Miller W H 1978 *J. Chem. Phys.* **68** 745–9
Dagens L 1969 *J. Physique* **30** 593–7

Dunham J L 1932 *Phys. Rev.* **41** 713–20
Fröman N 1978 *Phys. Rev.* **17A** 493–504
Hioe F T, MacMillen D and Montroll E W 1976 *J. Math. Phys.* **17** 1320–37
Kesarwani R N and Varshni Y P 1980 *J. Math. Phys.* **21** 90–2
Killingbeck J 1977 *J. Phys. A: Math. Gen.* **10** L99–103
Krieger J B, Lewis M L and Rosenzweig C 1967 *J. Chem. Phys.* **47** 2942–5
Newman W I and Thorson W R 1972 *Phys. Rev. Lett.* **29** 1350–3
Radmore P M 1980 *J. Phys. A: Math. Gen.* **13** 173–9
Titchmarsh E C 1961 *Eigenfunction Expansions* vol 1 (Oxford: OUP)
Young L A 1931 *Phys. Rev.* **38** 1612–4
—— 1932 *Phys. Rev.* **39** 455–7