Eigenvalues of the Schrodinger equation with a Gaussian potential

1977 J. Phys. A: Math. Gen. 10 L229

(http://iopscience.iop.org/0305-4470/10/12/003)

J. Phys. A: Math. Gen., Vol. 10, No. 12, 1977. Printed in Great Britain. © 1977

LETTER TO THE EDITOR

Eigenvalues of the Schrödinger equation with a Gaussian potential

G Stephenson
Department of Mathematics, Imperial College, London, UK

Received 6 October 1977

Abstract. Eigenvalues of the three-dimensional Schrödinger equation with a radial Gaussian potential are obtained using the Liouville–Green uniform asymptotic method. The results are compared with those obtained by direct integration of the Schrödinger equation.

In some recent work (see Rowan and Stephenson 1976 and Rowan 1977) uniform asymptotic methods and the Liouville–Green technique have been used to obtain solutions of certain differential equations which arise in the theory of black holes. This technique is now applied to the calculation of the eigenvalues of the three-dimensional Schrödinger equation with an attractive radial Gaussian potential, a problem relevant to the theory of nucleon–nucleon scattering (see, for example, Buck 1977).

In a suitable non-dimensional form ($2m=\hbar=1$) the radial Schrödinger equation with $V=-A\,\mathrm{e}^{-r^2}$ may be written as

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2}+\left(E+A\,\mathrm{e}^{-r^2}-\frac{l(l+1)}{r^2}\right)\psi=0, \qquad (1)$$

where A is the depth of the Gaussian potential, $l=0, 1, 2, 3, \ldots$, and E is the energy. The boundary conditions are $\psi(0)=\psi(\infty)=0$.

We now make the transformations $r=r(\xi)$, $G=(\xi')^{1/2}\psi$ in (1), where $\xi'=\mathrm{d}\xi/\mathrm{d}r$, to obtain the equation

$$\frac{\mathrm{d}^2G}{\mathrm{d}\xi^2}=\left[\left(-E-A\,\mathrm{e}^{-r^2}+\frac{l(l+1)}{r^2}\right)\frac{1}{\xi'^2}+\frac{\xi'''}{2\xi'^3}-\frac{3}{4}\frac{\xi''^2}{\xi'^4}\right]G. \qquad (2)$$

For convenience in what follows we write

$$-E-A\,\mathrm{e}^{-r^2}+\frac{l(l+1)}{r^2}=f(r), \qquad \frac{\xi'''}{2\xi'^3}-\frac{3}{4}\frac{\xi''^2}{\xi'^4}=g(r). \qquad (3)$$

Now for certain values of E there will be two zeros of $f(r)$. Consequently if, by a suitable choice of ξ, $g(r)$ can be shown to be a small bounded slowly varying function which, under certain conditions, can be neglected in (2), then the resulting approximate form of (2) when $f(r)$ has two zeros will be an equation with two turning points. Accordingly we try to choose ξ in such a way as to take (2) (with $g(r)$ omitted) into the standard two-turning-point equation:

$$\mathrm{d}^2G/\mathrm{d}\xi^2=(\tfrac{1}{4}\xi^2-\lambda)G, \qquad (4)$$

where λ is a parameter. This is the Weber equation whose solutions are the parabolic cylinder functions. However, the obvious choice of $\xi'^2(\frac{1}{4}\xi^2-\lambda)=f(r)$ leads, after some lengthy calculations, to a form of $g(r)$ which is divergent at $r=0$. This singularity may be removed by a judicious re-grouping of terms so that part of the singularity in $f(r)$ at $r=0$ is used to cancel out the singularity in $g(r)$ at $r=0$. This can be done by writing (2) in the form

$$\frac{d^2G}{d\xi^2}=\left[\left(-E-A\,e^{-r^2}+\frac{(l+\frac{1}{2})^2}{r^2}\right)\frac{1}{\xi'^2}+g(r)-\frac{1}{4r^2\xi'^2}\right]G, \tag{5}$$

where ξ is now defined by the equation

$$\xi'^2(\tfrac{1}{4}\xi^2-\lambda)=-E-A\,e^{-r^2}+[(l+\tfrac{1}{2})^2/r^2]. \tag{6}$$

We note that the re-grouping of terms to produce (5) effectively replaces $l(l+1)$ by $(l+\frac{1}{2})^2$, which is the Langer correction (see Langer 1937). The origin of this correction lies therefore in the correct removal of the singularity in $g(r)$ at $r=0$.

Owing to the complexity of the relation between ξ and r the behaviour of the function $g(r)-1/4r^2\xi'^2$ is difficult to analyse analytically, but specific numerical calculations indicate that it is a bounded slowly varying function over the whole range $0\leqslant r<\infty$. In accordance with the Liouville–Green approximation this function will now be neglected in (5) in what follows.

Now from (6) we find by integration that

$$\frac{\xi}{2}\sqrt{\xi^2-4\lambda}-2\lambda\ln|\xi+\sqrt{\xi^2-4\lambda}|=2\int\left(\frac{(l+\frac{1}{2})^2}{r^2}-E-A\,e^{-r^2}\right)^{1/2}dr, \tag{7}$$

whence it follows that as $r\to 0$, $\xi\to-\infty$, and as $r\to\infty$, $\xi\to\infty$. Furthermore from (6) we see that at the turning points r_1 and r_2 (these being the zeros of $-E-A\,e^{-r^2}+(l+\frac{1}{2})^2/r^2$), $\xi=\pm 2\sqrt{\lambda}$. In the range between these two points where $r_1\leqslant r\leqslant r_2$, we have $\xi^2\leqslant 4\lambda$ and hence (6) integrates to give

$$\frac{\xi}{2}\sqrt{4\lambda-\xi^2}+2\lambda\sin^{-1}\left(\frac{\xi}{2\sqrt{\lambda}}\right)=2\int\left(E+A\,e^{-r^2}-\frac{(l+\frac{1}{2})^2}{r^2}\right)^{1/2}dr \tag{8}$$

from which we have

$$2\pi\lambda=2\int_{r_1}^{r_2}\left(E+A\,e^{-r^2}-\frac{(l+\frac{1}{2})^2}{r^2}\right)^{1/2}dr. \tag{9}$$

Now bounded polynomial solutions of the Weber equation (4) which satisfy the boundary conditions $G(-\infty)=G(\infty)=0$ (corresponding to $\psi(0)=\psi(\infty)=0$) exist only if

$$\lambda=n+\tfrac{1}{2}, \tag{10}$$

where n is zero or a positive integer.

Hence from (9) and (10) we finally have

$$\pi(n+\tfrac{1}{2})=\int_{r_1(E,\,l)}^{r_2(E,\,l)}\left(E+A\,e^{-r^2}-\frac{(l+\frac{1}{2})^2}{r^2}\right)^{1/2}dr, \tag{11}$$

where $r_1(E,l)$, $r_2(E,l)$ are the zeros of the expression under the square root sign. This result is precisely the Bohr–Sommerfeld quantisation formula with $l(l+1)$ replaced by $(l+\frac{1}{2})^2$.

Other work on two-turning-point problems has been discussed by Olver (1974) and Berry and Mount (1972) mainly using matched Airy function solutions at each turning point, a complication avoided by the present approach. Although in principle, as shown by Olver, upper bounds on the errors involved in all this uniform asymptotic work are known analytically, in practice these prove to be far too crude or impossible to obtain over the whole range analytically due to the complicated relationship between ξ and r. An estimation therefore of the error involved in neglecting the term $g(r)-1/4r^2\xi'^2$ in (5) is difficult to obtain, but numerical calculations in particular cases indicate that the neglected term is small in comparison to the terms retained in (5), the accuracy increasing with the magnitude of A.

The eignevalues for the case where the potential well has depth $A = 400$ have been computed using (11). These values are compared in table 1 with some unpublished results (in italics) obtained by Dr B Buck of the Department of Theoretical Physics, University of Oxford, by direct integration of the Schrödinger equation. Close agreement exists between these two sets of values for the range of (n, l) values considered.

Table 1.

n \ l	0	1	2	3	4	5	6	7	8	9
0	341·6	304·2	267·9	232·6	198·5	165·7	134·1	103·9	74·9	47·6
	341·9	*304·5*	*268·1*	*232·9*	*198·8*	*165·9*	*134·3*	*104·1*	*75·2*	*47·9*
1	269·4	235·2	202·2	170·4	139·9	110·7	83·0	56·9	32·6	10·2
	269·7	*235·5*	*202·4*	*170·6*	*140·1*	*111·0*	*83·3*	*57·2*	*32·8*	*10·5*
2	203·7	173·0	143·6	115·5	88·9	63·9	40·7	19·5	—	—
	204·0	*173·3*	*143·8*	*115·8*	*89·2*	*64·2*	*41·0*	*19·8*	—	—
3	145·1	118·1	92·6	68·7	46·6	26·5	8·8	—	—	—
	145·4	*118·4*	*92·9*	*69·0*	*46·9*	*26·8*	*9·1*	—	—	—
4	94·2	71·4	50·3	31·3	14·6	—	—	—	—	—
	94·5	*71·6*	*50·6*	*31·5*	*14·9*	—	—	—	—	—
5	51·9	33·9	18·2	—	—	—	—	—	—	—
	52·2	*34·2*	*18·5*	—	—	—	—	—	—	—
6	19·7	7·8	—	—	—	—	—	—	—	—
	20·0	*8·1*	—	—	—	—	—	—	—	—
7	1·1	—	—	—	—	—	—	—	—	—
	1·4	—	—	—	—	—	—	—	—	—

I am grateful to Robin Hughes of the Department of Physics, Imperial College, for carrying out the computation of the eigenvalues, and to Dr B Buck of the Department of Theoretical Physics, University of Oxford, for permission to publish his computations for comparison purposes.

I am also grateful to David Rowan for useful discussions, and to Professor R J Elliott for the hospitality shown to me during my stay in the Department of Theoretical Physics, University of Oxford, where this work was started.

References

Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315
Buck B 1977 *Nucl. Phys.* A **275** 246
Langer R F 1937 *Phys. Rev.* **51** 669
Olver F W J 1974 *Introduction to Asymptotics and Special Functions* (London: Academic Press)
Rowan D J 1977 *J. Phys. A: Math. Gen.* **10** 1105
Rowan D J and Stephenson G 1976 *J. Phys. A: Math. Gen.* **9** 1261, 1631