Single-particle rotational bands and the inverse bound-state problem

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Abstract. The empirical observation that the single-particle energies generated by solving the Schrödinger equation for a deep, bell-shaped potential form almost perfect rotational bands is examined within a semiclassical approximation. Formulae are deduced to reconstruct the potential $V(r)$ which gives rise to a bound-state energy spectrum of the form $E(v, \lambda) = f(\alpha v + \lambda) + \beta \lambda^2$ where α and β are arbitrary constants, $v - \frac{1}{2} = n$ is the number of internal nodes in the radial wavefunction and $\lambda - \frac{1}{2} = l$ is the angular momentum quantum number. We further find that the unspecified function f is, in fact, determined by α and β. A discussion is given of the conditions governing the possibility of making the inversion to obtain $V(r)$.

1. Introduction and background

In the course of calculations on a simple $\alpha + {}^{16}O$ model for states of ${}^{20}Ne$ it was discovered [1] that $\alpha - {}^{16}O$ potential shapes generated by folding the nuclear densities for varying distances between the centres of mass, i.e.

$$V(r) \propto \int^r \rho_1(r - s)\rho_2(s)\,\mathrm{d}s \tag{1.1}$$

gave rise to Schrödinger equation bound-state and resonance energies with a nearly perfect rotational spacing. Specifically, it was shown [1] that the five levels with a fixed value of $N = 2n + l = 8$, where l is the angular momentum and n is the number of nodes in the radial wavefunction for $0 < r < \infty$, i.e. the levels with $(n, l) = (4,0)$, $(3,2)$, $(2,4)$, $(1,6)$ and $(0,8)$, lie on a straight line when plotted against $l(l+1)$, and similarly for the five levels with $l = 1, 3, 5, 7$ and 9 belonging to $N = 2n + l = 9$. The above potential was generated by numerical folding of densities, but it was seen that its general shape was like that of a Gaussian potential (see figure 1); so it was felt to be of interest to investigate this phenomenon further using various analytic potentials with shapes similar to those given by folding procedures.

In the following we use units such that $2m = \hbar = 1$. Bound single-particle spectra calculated from the Schrödinger equation for the potentials

$$V(r) = -400\,\mathrm{sech}^2(r) \tag{1.2}$$

$$V(r) = -400\exp(-r^2) \tag{1.3}$$

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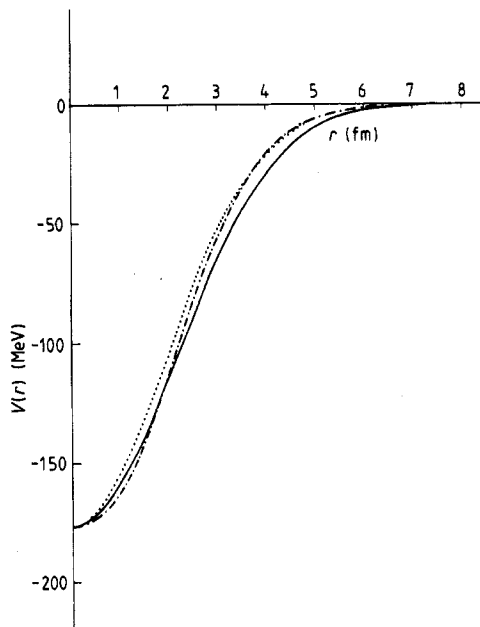
Figure 1. A comparison of three potentials for the ^{16}O + α system to emphasise the similarity of their shapes. The full curve represents the numerically evaluated folded potential of equation (1.1). The dotted curve is the Gaussian function $V_G(r) = -176\exp(-r^2/7.5)$. The chain curve is a second parametrisation proposed by Buck and Pilt [2], $V_C(r) = -V_0(1+\cosh(R_0/a_0))/[\cosh(r/a_0)+\cosh(R_0/a_0)]$, where $V_0 = 176$ MeV, $R_0 = 2.25$ fm and $a_0 = 0.8$ fm.

are shown in figures 2 and 3. Again we have plotted all levels with a fixed value of $N = 2n + l$ against $l(l+1)$, and we start with $N = 2$ as being the first real rotational band, since there is only one level each for the 'bands' with $N = 0$ and $N = 1$. It is rather startling to observe that for both potentials all the bound states fall into these nearly perfect rotational patterns, and indeed, the energy positions of the sharp resonance states in the continuum region also lie on such straight lines. It is even more surprising that the slopes of the bands for these potentials are all closely similar, i.e. the effective rotational moments of inertia are only weakly dependent on the band quantum number $N = 2n + l$.

A closer look at the numbers shows some slight departures from straight line fits, but fitting the best straight line to each band indicates that the level schemes for both potentials are represented very well (within fractions of a percent) by formulae of the type

$$E(n, l) = A(N) + B(N)[l(l+1)] \tag{1.4}$$

with $N = 2n + l$.

For the hyperbolic potential of type (1.2), but with arbitrary strength V, the quantity $A(N)$ is given accurately by the expression

$$A_H(N) = -[(V + \tfrac{1}{4})^{1/2} - (N + \tfrac{3}{2})]^2 \tag{1.5}$$

which is the exact result from the Schrödinger equation for the $l = 0$ levels (with N even), but also gives correct values when the N-odd bands are linearly extrapolated to
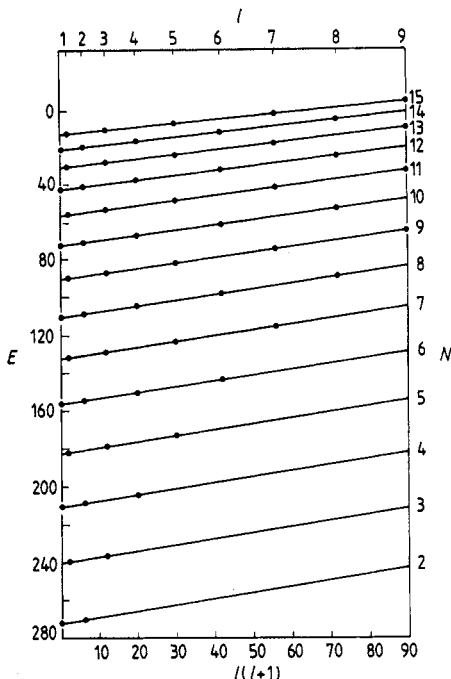
Figure 2. A plot of the energies of the bound states of the hyperbolic potential, $V_H(r) = -400 \ \mathrm{sech}^2(r)$, of equation (1.2) as a function of $l(l+1)$ for all levels with a fixed value of $N = 2n + l$. Note how the states with the same value of $N = 2n + l$ lie on almost perfect rotationally spaced bands.
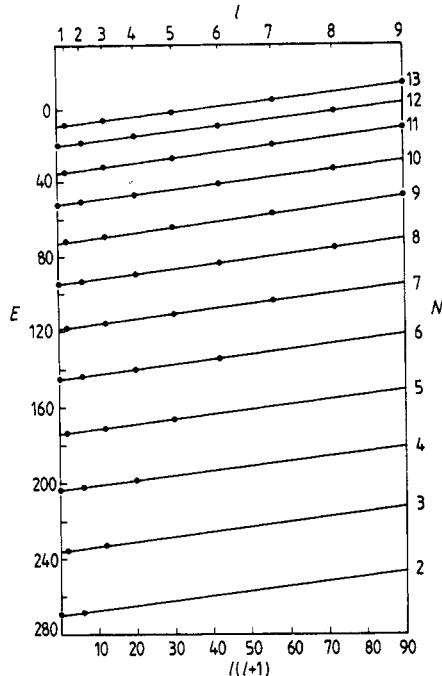
Figure 3. A plot of the energies of the bound states of the Gaussian potential, $V_G(r) = -400 \exp(-r^2)$, of equation (1.3) as a function of $l(l + 1)$ for all levels with a fixed value of $N = 2n + l$. Note how the states with the same value of $N = 2n + l$ lie on almost perfect rotationally spaced bands.

$l = 0$. The coefficient $B_H(N)$ coming from potential (2) has a weak linear dependence on N, i.e.

$$B_H(N) \simeq 0.332 - 0.005N \tag{1.6}$$

at least up to $N = 6$.

For the Gaussian potential equation (1.3), there does not seem to be any simple formula for $A_G(N)$, but there is an even weaker linear dependence of the B coefficient on N, i.e.

$$B_G(N) \simeq 0.252 + 0.002N \tag{1.7}$$

as far as $N = 10$ in this case. For $N > 10$, there are deviations of $B(N)$ from linearity in N for both potentials, but these higher levels still have almost perfect rotational spacings within the bands of fixed N. Other potentials with the same sort of smoothly changing shapes as illustrated in figure 1 also give rotational spectra similar to the results described above, but in general $A(N)$ does not have any simple representation.

It is the purpose of this paper to make a first attempt at explaining this behaviour. In particular, we note that many such potential shapes imply B coefficients of the form

$$B(N) = \beta + \gamma N \qquad \text{with} \quad \gamma \ll \beta \tag{1.8}$$

over an appreciable range of N.

2. The inverse problem

Consideration of these results led us to ask how potentials yielding spectra of the form given in equation (1.4) might be characterised. To simplify matters, we investigate what can be said about potentials implying spectra with band quantum numbers $N = 2n + l$ and with a constant rotational parameter $B(N) = \beta$, i.e. with spectra given by

$$E(n, l) = A(\alpha n + l) + \beta l(l + 1) \tag{2.1}$$

where $A(\alpha n + l)$ is an undetermined function. Our previous cases correspond to $\alpha = 2$ and $\beta \simeq \frac{1}{3}$ for the hyperbolic potential and $\beta \simeq \frac{1}{4}$ for the Gaussian. The modification of the global quantum number to $N = \alpha n + l$ enables us to include other interesting examples of band structure or degeneracy and some exactly soluble cases.

Some relevant work on this problem has been done by Rowley [3], using semi-classical methods (Bohr–Sommerfeld quantisation). He showed that the levels within a band of fixed $(2n + l)$ increase or decrease in energy with l depending on whether the potential lies above or below the oscillator potential which yields the same turning points in the Bohr–Sommerfeld integral. However, he was not able to say when a potential would give the striking rotational spacings proportional to $l(l + 1)$ within a band.

It turns out to be convenient in our work also to formulate the problem in terms of the Bohr–Sommerfeld quantisation formula (with the usual Langer replacement of $l(l + 1)$ by $(l + \frac{1}{2})^2$ in the local momentum expression). The energy eigenvalues are then given by the equation (see figure 4)

$$\int_{r_1}^{r_2} [E(n, l) - V(r) - (l + \tfrac{1}{2})^2/r^2]^{1/2} \mathrm{d}r = (n + \tfrac{1}{2})\pi \tag{2.2}$$

where we have assumed potentials such that there are two real turning points r_1 and r_2 where the integrand vanishes. The interval between r_1 and r_2 is the classically allowed region. The energy values $E(n, l)$ for integral n and l are of course only approximations to the correct Schrödinger equation eigenvalues, but for the smooth potentials of interest they are remarkably accurate. In fact, for the Gaussian potential of equation (1.3) the Bohr–Sommerfeld energies are all uniformly less than the exact energies by 0.3 units. These Bohr–Sommerfeld values have been computed by Stephenson [4] and he has given a table comparing these numbers with our exact Schrödinger equation eigenvalues. Hence, it is clear that using the Bohr–Sommerfeld integral (2.2) will not affect our conclusions about the spectra in this case and probably not much in similar cases.

The natural variables in equation (2.2) are

$$\nu = n + \tfrac{1}{2}$$
$$\lambda = l + \tfrac{1}{2}. \tag{2.3}$$

So, rewriting our formulae in terms of ν and λ, we want to investigate the properties of the potentials $V(r)$, which, when inserted in the integral equation

$$\int_{r_1}^{r_2} [E(\nu, \lambda) - V(r) - \lambda^2/r^2]^{1/2} \mathrm{d}r = \pi \nu \tag{2.4}$$
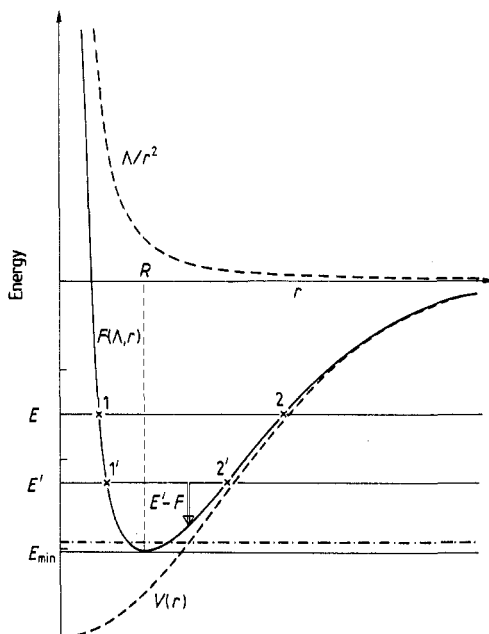
Figure 4. A plot of the effective potential $F(\Lambda, r) = V(r) + \Lambda/r^2$ as a function of the distance r. The minimum energy $E_{\min}$, a low energy associated with small v (chain line) and the classical turning points associated with the energies E and E' are highlighted.

yield a spectrum of the form

$$E(v, \lambda) = f(\alpha v + \lambda) + \beta \lambda^2 \tag{2.5}$$

where $f(\alpha v + \lambda)$ is an undetermined function, differing numerically from $A(\alpha n + l)$ by the constant $\beta/4$.

There are several advantages to using this semiclassical formulation.

(i) Energy spectra are almost the same as for an exact quantum mechanical calculation.

(ii) Only the part of the potential lying below a given $E(v, \lambda)$, and between the turning points, is relevant for determining $E(v, \lambda)$, so we do not need to worry about the tail behaviour of the potential (or wavefunction).

(iii) We can treat v and λ as continuously varying parameters so as to derive exact differential equations for the potential.

(iv) The equations we shall derive may also be extracted directly (though approximately) from the Schrödinger equation, as shown in appendix 1. Hence we have the choice of exact equations from an approximate theory, or approximate equations from an exact theory. We have chosen the first alternative.

The result we shall demonstrate is, at first sight, extremely surprising. That is, if there exists a potential $V(r)$ which gives a spectrum of the form of equation (2.5), then it is uniquely determined by the constants α and β, up to an arbitrary depth parameter and an arbitrary additive constant. It is not necessary to specify the function f *a priori* since it also is determined by the values of α and β. The basic reason for this result is that whatever $V(r)$ is assumed, consistent with two real turning points of the integrand in equation (2.4), the spectrum $E(v, \lambda)$ must obey two consistency conditions which

are independent of V. In other words, $E(v, \lambda)$ cannot be an arbitrary two-variable function and our assumption of a spectrum consisting of some function of a linear combination of v and λ plus a specified dependence on λ is sufficient to determine f and V almost completely. For the particular spectrum of equation (2.5), much simpler methods suffice and the consistency requirement reduces to a (non-linear) differential equation for f, from which we are able to derive the appropriate potential $V(r)$ in closed form. The complicated consistency conditions are given in appendix 2, but we shall not use these results in the rest of the paper. In general, we conjecture that they imply that $E(v, \lambda)$ need only be known along any line in the (v, λ) plane (in particular along the lines $(0, \lambda)$ or $(v, 0)$) for it to be determined everywhere up to the top of the barrier.

3. Derivation of basic equation

For the moment we set aside the assumed spectrum equation (2.5) and derive some simple equations from the Bohr–Sommerfeld formula, which we now write in the form

$$\int_{r_1}^{r_2} (E(v, \lambda) - F(\lambda, r))^{1/2} dr = \pi v \tag{3.1}$$

where

$$F(\lambda, r) = V(r) + \lambda^2/r^2. \tag{3.2}$$

We assume a potential such that the situation is as illustrated in figure 4. Bohr–Sommerfeld quantisation involves integrating the square root of the quantity $E(v, \lambda) - F(\lambda, r)$, indicated by the double arrow in figure 4, between the points where this quantity vanishes.

Consider now what happens if we set $v = 0$ in equation (3.1). It is clear from figure 4 that the turning points must coincide at $r_1 = r_2 = R$, say, and that at this point the integrand must vanish. The line corresponding to $E(0, \lambda)$ then just touches the minimum of the function $F(\lambda, r)$ which occurs also at $r = R$. Hence we deduce that

$$E(0, \lambda) = F(\lambda, R) = V(R) + \lambda^2/R^2 \tag{3.3}$$

and that

$$\left(\frac{\partial F(\lambda, r)}{\partial r}\right)_{r=R} = 0 = \left(\frac{\partial F(\lambda, R)}{\partial R}\right)_{\lambda \text{ fixed}} \tag{3.4}$$

from which it follows that

$$\lambda^2 = \frac{R^3}{2} \frac{dV(R)}{dR} \tag{3.5}$$

so that R is an implicit function of λ.

To illustrate the remarks at the end of § 2 we now show that in many cases it follows from equations (3.3) and (3.4) that V is determined by a knowledge of the spectrum along the line $v = 0$, i.e. from $E(0, \lambda)$ only. Since V is determined, then substituting it back in equation (3.1) gives $E(v, \lambda)$ everywhere.

Suppose we know $E(0, \lambda) = \varepsilon(\lambda)$, so that

$$\varepsilon(\lambda) = V(R) + \lambda^2/R^2 = F(\lambda, R). \tag{3.6}$$

Differentiating totally with respect to λ we easily find

$$\frac{\mathrm{d}\varepsilon(\lambda)}{\mathrm{d}\lambda} = \frac{2\lambda}{R^2} + \frac{\partial F(\lambda, R)}{\partial R}\frac{\mathrm{d}R}{\mathrm{d}\lambda}. \tag{3.7}$$

But, from equation (3.4), $\partial F(\lambda, R)/\partial R = 0$ and hence

$$R^2 = \frac{2\lambda}{\mathrm{d}\varepsilon/\mathrm{d}\lambda}. \tag{3.8}$$

Solving for λ we find $\lambda = \lambda(R)$ and on substituting back in equation (3.6) we obtain

$$V(R) = \varepsilon(\lambda(R)) - \frac{\lambda^2(R)}{R^2} \tag{3.9}$$

which partially determines the potential V, since changing λ implies changing R so that we obtain $V(R)$ for a range of values of R from a knowledge of $\varepsilon(\lambda)$.

Exactly soluble examples of this are the assumptions $\varepsilon(\lambda) = E(0, \lambda) = \lambda$ or $-1/\lambda^2$ from which we quickly find the potentials $V(r) = r^2/4$ and $-2/r$ respectively which yield the corresponding exact total spectra $E(v, \lambda) = 2v + \lambda$ or $-1/(v + \lambda)^2$. These cases are of course just the harmonic oscillator and the hydrogen atom respectively for which the Bohr–Sommerfeld integral can be evaluated analytically, giving results agreeing exactly with quantum mechanics.

In our problem the equations (3.3)–(3.5) are not sufficient by themselves to determine $V(r)$ since from the assumption of equation (3.5) we find only

$$E(0, \lambda) = \varepsilon(\lambda) = f(\lambda) + \beta\lambda^2 \tag{3.10}$$

which still contains the unknown function f. Thus we require another equation relating the spectrum to the potential. Fortunately, the required relation can be derived from the Bohr–Sommerfeld integral almost as easily as the preceding equations. We can explore the functions $F(\lambda, r)$ in the neighbourhood of the minimum point at $r = R$ by considering the Bohr–Sommerfeld integral for v increased from 0 to Δv where Δv is small enough that we can write, to sufficient approximation,

$$E(\Delta v, \lambda) \simeq E(0, \lambda) + \Delta v \left(\frac{\partial E}{\partial v}\right)_{v=0}. \tag{3.11}$$

This is represented by the chain line in figure 4 which cuts the curve $F(\lambda, r)$ near its minimum. Expanding this function in a Taylor series about $r = R$ and using equation (3.4) we find, to second order, that

$$F(\lambda, r) \simeq F(\lambda, R) + \frac{(r - R)^2}{2}\left(\frac{\partial^2 F(\lambda, r)}{\partial r^2}\right)_{r=R}. \tag{3.12}$$

Substituting equations (3.11) and (3.12) into (3.1) and using (3.3) gives

$$\int_{r_1}^{r_2}\left[\Delta v\left(\frac{\partial E}{\partial v}\right)_{v=0} - \frac{(r - R)^2}{2}\left(\frac{\partial^2 F}{\partial r^2}\right)_{r=R}\right]^{1/2}\mathrm{d}r = \pi(\Delta v) \tag{3.13}$$

where the turning points are given by

$$\tilde{r}_1, \tilde{r}_2 = R \mp 2 \left(\Delta v \frac{(\partial E/\partial v)}{(\partial^2 F/\partial r^2)} \right)^{1/2}. \tag{3.14}$$

This integral is elementary, Δv drops out, and equation (3.13) reduces to

$$\left(\frac{\partial E(v, \lambda)}{\partial v} \right)_{v=0} = \left[2 \left(\frac{\partial^2 F(\lambda, r)}{\partial r^2} \right)_{r=R} \right]^{1/2}. \tag{3.15}$$

It is an interesting fact that, given the spectrum (2.5), the non-linear equations (3.2)–(3.4) and (3.15) can be solved exactly for the potential V. Before demonstrating this we collect the equations and write them in a more convenient form. Hence if the minimum of $F(\lambda, r) = \lambda^2/r^2 + V(r)$ occurs at $r = R$ we have

$$E(0, \lambda) = \lambda^2/R^2 + V(R) \tag{3.16}$$

and, from the condition $(\partial F(\lambda, r)/\partial r)_{r=R} = 0$ we get

$$2\lambda^2 = R^3 \frac{\mathrm{d}V(R)}{\mathrm{d}R} = G(R) \tag{3.17}$$

which defines the function $G(R)$. Also, we easily find that

$$\left(\frac{\partial^2 F}{\partial r^2} \right)_{r=R} = \frac{6\lambda^2}{R^4} + \frac{\mathrm{d}^2 V(R)}{\mathrm{d}R^2} = \frac{3}{R} \frac{\mathrm{d}V(R)}{\mathrm{d}R} + \frac{\mathrm{d}^2 V(R)}{\mathrm{d}R^2}$$

$$= \frac{1}{R^3} \frac{\mathrm{d}}{\mathrm{d}R} \left(R^3 \frac{\mathrm{d}V}{\mathrm{d}R} \right) = \frac{1}{R^3} \frac{\mathrm{d}G}{\mathrm{d}R}.$$

and therefore

$$\left(\frac{\partial E(v, \lambda)}{\partial v} \right)_{v=0} = \left(\frac{2}{R^3} \frac{\mathrm{d}G(R)}{\mathrm{d}R} \right)^{1/2}. \tag{3.18}$$

Finally, it is straightforward to eliminate R and $V(R)$ from equations (3.16)–(3.18) so as to derive an equation involving $E(v, \lambda)$ only (i.e. a consistency condition on the spectrum for any V). This assumes its simplest form if we define $\Lambda = \lambda^2$, in which case $E(v, \lambda)$ must satisfy the relation

$$\frac{16}{(\partial E/\partial v)^2_{v=0, \lambda=0}} = \frac{\partial}{\partial \Lambda} \left(\frac{1}{(\partial E/\partial \Lambda)^2_{v=0}} \right). \tag{3.19}$$

4. Determination of the potential

We now apply equations (3.16)–(3.18) to the spectrum assumed in equation (2.5). This latter equation gives

$$E(0, \lambda) = f(\lambda) + \beta \lambda^2 \tag{4.1}$$

$$\left(\frac{\partial E(v, \lambda)}{\partial v} \right)_{v=0} = (\alpha f'(\alpha v + \lambda))_{v=0} = \alpha \frac{\mathrm{d}f(\lambda)}{\mathrm{d}\lambda}. \tag{4.2}$$

Substituting equation (4.1) in (3.16) and differentiating totally with respect to λ we obtain

$$\frac{\mathrm{d}f(\lambda)}{\mathrm{d}\lambda} + 2\beta\lambda = 2\frac{\lambda}{R^2}. \tag{4.3}$$

Also, from equations (3.18) and (4.2) we have

$$\alpha\frac{\mathrm{d}f(\lambda)}{\mathrm{d}\lambda} = \left(\frac{2}{R^3}\frac{\mathrm{d}G}{\mathrm{d}R}\right)^{1/2}. \tag{4.4}$$

Eliminating $\mathrm{d}f(\lambda)/\mathrm{d}\lambda$ yields

$$2\alpha\lambda\left(\frac{1}{R^2} - \beta\right) = \left(\frac{2}{R^3}\frac{\mathrm{d}G}{\mathrm{d}R}\right)^{1/2}$$

i.e.

$$2\alpha^2\lambda^2\left(\frac{1}{R^2} - \beta\right)^2 R^3 = \frac{\mathrm{d}G}{\mathrm{d}R}. \tag{4.5}$$

But, from equation (3.17), $2\lambda^2 = G$, so that equation (4.5) reduces to the ordinary differential equation

$$\frac{1}{G}\frac{\mathrm{d}G}{\mathrm{d}R} = \alpha^2 R^3\left(\frac{1}{R^2} - \beta\right)^2 \tag{4.6}$$

which may be integrated immediately to give

$$G(R) = AR^{\alpha^2}\exp[-\alpha^2\beta(R^2 - \beta R^4/4)]. \tag{4.7}$$

Also from equation (3.17) $G(R) = R^3\mathrm{d}V(R)/\mathrm{d}R$; hence

$$\frac{\mathrm{d}V(R)}{\mathrm{d}R} = AR^{\alpha^2-3}\exp[-\alpha^2\beta(R^2 - \beta R^4/4)]. \tag{4.8}$$

Integrating this formally, we have finally that

$$V(r) = A\int^r R^{\alpha^2-3}\exp[-\alpha^2\beta(R^2 - \beta R^4/4)]\mathrm{d}R + B \tag{4.9}$$

where A and B are arbitrary constants. In addition, the form of the function f in equation (2.5) is determined by substituting $(\partial E/\partial v)_{v=0}$ and $(\partial E/\partial\Lambda)_{v=0}$ into equation (3.19) but the resulting non-linear equation cannot in general be integrated in closed form. In spite of this, we can easily see that in the case that $\alpha = 2, \beta = \frac{1}{4}$, corresponding to the empirical Gaussian results shown earlier, the integrand in equation (4.9) reduces to $R\exp[-R^2 + R^4/16]$. For R appreciably less than 2 the term $R^4/16$ may be neglected, so that equation (4.9) implies that the required potential is Gaussian over part of its range. This is at least a partial justification of the striking properties of the Gaussian which were obtained numerically. The eventual effect of the $R^4/16$ term is to ensure that V continues to increase without limit; but this is of course required since we

have assumed that the spectrum $f(\alpha v + \lambda) + \beta \lambda^2$ holds everywhere and that there is no continuum.

There are also some interesting special cases for which the integration can be performed analytically. If the coefficient $\beta = 0$, so that $E(0, \lambda) = f(\lambda)$, we can obtain analytic predictions for the approximate (semiclassical) bound-state spectra of simple power-law and logarithmic potentials.

For the power-law spectra, we return to equation (4.9) and set $\beta = 0$, with $\alpha \neq 0$ or 2. Integration then clearly yields

$$V(r) = \frac{A r^{\alpha^2 - 2}}{\alpha^2 - 2} + B. \tag{4.10}$$

For convenience let us set $A = s = \alpha^2 - 2$ and $B = 0$ so that we are considering the spectrum associated with the potential $V(r) = r^s$. The simplest way to obtain the energy levels is to locate the minimum of $F(r) = \lambda^2/r^2 + r^s$ at $r = R$, so that

$$R = \left(\frac{2\lambda^2}{s} \right)^{1/(s+2)} \tag{4.11}$$

and then obtain $E(0, \lambda)$ by substitution into equation (3.16). Having thus found $E(0, \lambda) = f(\lambda)$, we can write $E(v, \lambda) = f(\alpha v + \lambda)$ for power-law potentials in the form

$$E(v, \lambda) = \frac{s+2}{2} \left(\frac{s}{2} \right)^{2/(s+2)} \left(\lambda + v\sqrt{s+2} \right)^{2s/(s+2)} \qquad s \neq -2, 0. \tag{4.12}$$

The two excluded cases $s = -2, 0$ (or equivalently $\alpha^2 = 0, 2$) correspond to the situation where E does not depend on v and to a logarithmic potential, respectively. If we set $\beta = 0$, $\alpha^2 = 2$ in equation (4.9) we readily find

$$V(r) = A \ln r + B. \tag{4.13}$$

Again, we set $A = 1$, $B = 0$ for convenience. We then locate the minimum of $F(\lambda, r)$ at $R = \sqrt{2}\lambda$ and find energy spectra associated with the logarithmic potential of the form

$$E(v, \lambda) = \tfrac{1}{2} + \ln[\sqrt{2}(\lambda + v\sqrt{2})]. \tag{4.14}$$

From the approximations inherent in our derivation it is clear that the energies predicted by equations (4.12) and (4.14) are expected to be most accurate for states of small v and large λ.

Thus we have proved, from the Bohr–Sommerfeld integral, that a spectrum of the form given in equation (2.5) can only be produced by the explicit potential of equation (4.9) and also that the unspecified function f is in fact determined by the constants α and β. However, this surprising result needs further discussion since it is easily misinterpreted. That a careful statement is needed is brought out by the observation, from numerical evaluation of the Bohr–Sommerfeld formula, that the potential of equation (4.9) does not, in general, exactly reproduce the spectrum given in equation (2.5). How can this be? The reason is that in general there is no potential which yields the specified spectrum and that such a formula can at best be only an approximate representation of an actual spectrum.

To see this, we first of all note that any spectrum generated by the Bohr–Sommerfeld expression must satisfy the consistency condition (3.19), and this suffices, for the particular spectrum (2.5), to derive the form of f. But, as mentioned earlier, a Bohr–Sommerfeld spectrum must satisfy *two* consistency conditions (see appendix 2), and this may well rule out completely a spectrum of some *a priori* specified form (e.g. that of equation (2.5)).

An alternative statement of our result is as follows. Suppose that, instead of equation (2.5), we specified that the spectrum had the form

$$E(v, \lambda) = f(\alpha v + \lambda) + \beta \lambda^2 + g(v, \lambda) \tag{4.15}$$

with $g(v, \lambda)$ having the properties

$$g(0, \lambda) = \left(\frac{\partial g(v, \lambda)}{\partial v} \right)_{v=0} = 0. \tag{4.16}$$

With these restrictions at $v = 0$ on $g(v, \lambda)$ and its first derivative, our previous analysis will go through exactly as before, since g will make no contribution to lowest order. We shall thus obtain exactly the same result for $f(\alpha v + \lambda)$. In this limit we are insensitive to $g(v, \lambda)$. It is actually possible, since we have two consistency conditions, to determine the forms of both $f(\alpha v + \lambda)$ and $g(v, \lambda)$ uniquely in terms of α and β in an exactly analogous manner.

Our earlier considerations involving only $f(\alpha v + \lambda)$ were so successful in closely reproducing the numerical spectra because we were essentially always working in the small-v limit, and so $g(v, \lambda)$ generally made only a small contribution to the energy. It is this contribution which is responsible for the small deviations of the spectra from perfect rotational spacing. We are justified in ignoring $g(v, \lambda)$ because we are effectively fixing λ and exploring the region of small v associated with that value of λ in our search for an expression for the energy. For this reason our approximations are at their best when v is close to zero, and steadily deteriorate as v increases. We emphasise, however, that a spectrum of the form given by equation (4.15), with the restrictions of (4.16), holding for all values of v and λ, can only arise from a potential of the form of equation (4.9).

5. Summary

We have considered the question of what type of potential $V(r)$ can generate bound-state energy spectra of the form $E(v, \lambda) = f(\alpha v + \lambda) + \beta \lambda^2$ where α and β are arbitrary constants, $v - \frac{1}{2} = n$ is the number of internal nodes in the radial wavefunction and $\lambda - \frac{1}{2} = l$ is the angular momentum quantum number. We have worked within the semiclassical approximation and deduced an expression for $V(r)$, which is given in equation (4.9). This potential can even be evaluated analytically in simple cases (as when $\beta = 0$).

The form of the unknown function f is entirely determined by the constants α and β, and this function must satisfy two consistency conditions (see appendix 2). *In general, a spectrum of the simple form specified cannot be exactly realised in practice.* It can, however, be very closely approximated with the formulae we have derived, which gives them some practical utility.

The most general form of spectrum determined by α and β would be $E(v, \lambda) = f(\alpha v + \lambda) + \beta \lambda^2 + g(v, \lambda)$, with the restrictions of equation (4.16) on the unknown function g. Further work is needed to determine $g(v, \lambda)$ and to understand its smallness in all the cases we have considered.

Acknowledgments

Appendix 1

In this appendix we derive the basic equations of § 3 directly from the Schrödinger equation. We suppose that we have a spectrum, specified by a set of parameters, and seek to deduce the potential U which produces the given spectrum as a function of those parameters.

We consider the radial Schrödinger equation for a state bound in a local, attractive potential $V(r) = U(r) - 1/(4r^2)$ such that there are only two classical turning points. For convenience we set $\hbar = 2m = 1$ and write

$$\frac{d^2\chi(r)}{dr^2} - \left(V(r) + \frac{\lambda^2}{r^2} - E\right)\chi(r) = 0 \tag{A1.1}$$

where E is the energy, $\lambda = l + \frac{1}{2}$ and χ is the radial wavefunction (multiplied by r). Our restrictions on $V(r)$ imply that the effective potential $F(\lambda, r)$, defined by

$$F(\lambda, r) = V(r) + \frac{\lambda^2}{r^2} \tag{A1.2}$$

has a single, local minimum at some point $r = R$. Bearing this in mind and differentiating with respect to r, we get (exactly as before in equation (3.5))

$$\frac{2\lambda^2}{R^3} = \frac{dV(R)}{dR}. \tag{A1.3}$$

Clearly, the lowest value that the energy can assume is $F(\lambda, R)$. Let us suppose that the energy depends on the two continuous parameters v and λ (defined in equation (2.3)) so that $E = E(v, \lambda)$. Now, let us associate $v = 0$ with the lowest value of the energy. Hence, we define

$$E(0, \lambda) = F(\lambda, R). \tag{A1.4}$$

For small values of $(r - R)$ we can make a Taylor expansion of $F(\lambda, r)$ about the point $r = R$ keeping λ fixed. Similarly, for small values of v we can make an analogous expansion of the energy about $v = 0$. To lowest order (cf equations (3.11) and (3.12)) this gives

$$F(\lambda, r) = F(\lambda, R) + \frac{(r - R)^2}{2}\left(\frac{\partial^2 F}{\partial r^2}\right)_{r=R} + \dots \tag{A1.5}$$

and

$$E(v, \lambda) = E(0, \lambda) + v \left(\frac{\partial E}{\partial v} \right)_{v=0} + \dots . \tag{A1.6}$$

If we now substitute equations (A1.5) and (A1.6) into equation (A1.1) we obtain

$$\frac{d^2 \chi}{dr^2} + \frac{(r-R)^2}{2} \left(\frac{\partial^2 F}{\partial r^2} \right)_{r=R} \chi(r) = v \left(\frac{\partial E}{\partial v} \right)_{v=0} \chi(r). \tag{A1.7}$$

This is the equation of a one-dimensional simple harmonic oscillator with characteristic frequency ω given by

$$\omega = \left[2 \left(\frac{\partial^2 F}{\partial r^2} \right)_{r=R} \right]^{1/2} . \tag{A1.8}$$

The well known expressions for the energy eigenvalues then enable us to write

$$v \left(\frac{\partial E}{\partial v} \right)_{v=0} = (n + \tfrac{1}{2}) \left[2 \left(\frac{\partial^2 F}{\partial r^2} \right)_{r=R} \right]^{1/2} . \tag{A1.9}$$

Since we defined v in equation (2.3) to be $n + \tfrac{1}{2}$, this obviously leads to an expression identical to that of equation (3.15):

$$\left(\frac{\partial E}{\partial v} \right)_{v=0} = \left[2 \left(\frac{\partial^2 F}{\partial r^2} \right)_{r=R} \right]^{1/2} . \tag{A1.10}$$

The rest of the analysis of §§ 3 and 4 now follows identically. However, we should point out that we have actually derived these relations for a potential $V(r) = U(r) - 1/(4r^2)$, which is therefore a little different from the potential, $U(r)$, which we would really like to have treated.

Appendix 2

In this appendix we consider the constraints on a potential which supports a sequence of bound states whose energies are known up to some value E and determined by the two quantum numbers v and λ defined in equation (2.3) (see figure 4). For convenience we shall write $\Lambda = \lambda^2$ hereafter. We shall derive four equations which must be obeyed by the classical turning points r_1 and r_2 associated with the given energy $E(v, \Lambda)$ and the effective potential $F(\Lambda, r) = V(r) + \Lambda/r^2$. This amounts to two of the equations determining r_1 and r_2 while the two remaining equations act as consistency conditions (as outlined in §§ 3 and 4).

Let us begin by considering the situation sketched in figure 4 *for a fixed value of* Λ. We shall apply the Bohr–Sommerfeld quantisation rule using the energy E, labelled by the quantum numbers v and Λ. This energy E is assumed to be greater than the minimum energy, E_{min}, which occurs when $v = 0$. We thus define the minimum energy by

$$v(E_{min}, \Lambda) = 0 \tag{A2.1}$$

or equivalently

$$E_{\min} = E(0, \Lambda).$$ (A2.2)

The appropriate Bohr–Sommerfeld quantisation rule is

$$\pi v(E, \Lambda) = \int_{r_1}^{r_2} \sqrt{E - F(\Lambda, r)} \, dr.$$ (A2.3)

Let us now form

$$\int_{E_{\min}}^{E} \frac{v(E', \Lambda)}{\sqrt{E - E'}} \, dE' = \frac{1}{\pi} \int_{E_{\min}}^{E} \frac{dE'}{\sqrt{E - E'}} \int_{r_1'}^{r_2'} \sqrt{E' - F(\Lambda, r)} \, dr$$ (A2.4)

where we have made use of equation (A2.3). In this expression r_1' and r_2' are functions of E' and Λ. We now change the order of integration in equation (A2.4)

$$\int_{E_{\min}}^{E} \frac{v(E', \Lambda)}{\sqrt{E - E'}} \, dE' = \frac{1}{\pi} \int_{r_1}^{r_2} dr \int_{F(\Lambda, r)}^{E} \frac{\sqrt{E' - F(\Lambda, r)}}{\sqrt{E - E'}} \, dE'.$$ (A2.5)

The energy integral on the right-hand side may now be evaluated to yield

$$\int_{E_{\min}}^{E} \frac{v(E', \Lambda)}{\sqrt{E - E'}} \, dE' = \frac{1}{2} \int_{r_1}^{r_2} [E - F(\Lambda, r)] \, dr.$$ (A2.6)

We now integrate the left-hand side by parts to find that

$$2 \int_{E_{\min}}^{E} \frac{\partial v(E', \Lambda)}{\partial E'} \sqrt{E - E'} \, dE' = \frac{1}{2} \int_{r_1}^{r_2} [E - F(\Lambda, r)] \, dr.$$ (A2.7)

As the energy increases from $E_{\min}$ to E, the nodal quantum number increases from 0 to v, so we may rewrite this last equation in the form

$$2 \int_{0}^{v} \sqrt{E - E(v', \Lambda)} \, dv' = \frac{1}{2} \int_{r_1}^{r_2} [E - V(r) - \Lambda/r^2] \, dr.$$ (A2.8)

We now obtain our first two equations for the turning points r_1 and r_2 by differentiating equation (A2.8) with respect to E and Λ:

$$\int_{0}^{v} \frac{dv'}{\sqrt{E - E(v', \Lambda)}} = \frac{1}{2}(r_2 - r_1)$$ (A2.9)

and

$$\int_{0}^{v} \frac{\partial E(v', \Lambda)}{\partial \Lambda} \frac{dv'}{\sqrt{E - E(v', \Lambda)}} = \frac{1}{2}\left(\frac{1}{r_1} - \frac{1}{r_2}\right).$$ (A2.10)

These last two equations for the classical turning points are identical to those derived from the well known Rydberg–Klein–Rees method (see, for example, p 351 of [5]). In arriving at them, we have made use of the E (energy) dependence of v while holding the angular momentum constant. We may also obtain two other equations

for the classical turning points in an analogous manner by considering the Λ (squared angular momentum) dependence of v while *holding the energy constant.*

We define the maximum angular momentum by

$$v(E, \Lambda_{max}) = 0 \tag{A2.11}$$

or equivalently

$$\Lambda_{max} = \Lambda(0, E). \tag{A2.12}$$

Once again we shall make use of the Bohr–Sommerfeld quantisation rule of equation (A2.3). This time let us form

$$\int_{\Lambda}^{\Lambda_{max}} \frac{v(E, \Lambda')}{\sqrt{\Lambda' - \Lambda}} \, d\Lambda' = \frac{1}{\pi} \int_{\Lambda}^{\Lambda_{max}} \frac{d\Lambda'}{\sqrt{\Lambda' - \Lambda}} \int_{r_1'}^{r_2'} \sqrt{E - F(\Lambda', r)} \, dr. \tag{A2.13}$$

Changing the order of integration in equation (A2.13) as before we obtain

$$\int_{\Lambda}^{\Lambda_{max}} \frac{v(E, \Lambda')}{\sqrt{\Lambda' - \Lambda}} \, d\Lambda' = \frac{1}{\pi} \int_{r_1}^{r_2} dr \int_{\Lambda}^{\Lambda_{max}} \frac{\sqrt{E - F(\Lambda', r)}}{\sqrt{\Lambda' - \Lambda}} \, d\Lambda'. \tag{A2.14}$$

The angular momentum integral on the right-hand side may now be evaluated to yield

$$\int_{\Lambda}^{\Lambda_{max}} \frac{v(E, \Lambda')}{\sqrt{\Lambda' - \Lambda}} \, d\Lambda' = \frac{1}{2} \int_{r_1}^{r_2} [E - F(\Lambda, r)] \, r \, dr. \tag{A2.15}$$

We now integrate the left-hand side by parts to find that

$$-2 \int_{\Lambda}^{\Lambda_{max}} \frac{\partial v(E, \Lambda')}{\partial \Lambda'} \sqrt{\Lambda' - \Lambda} \, d\Lambda' = \frac{1}{2} \int_{r_1}^{r_2} (E - F(\Lambda, r)) \, r \, dr. \tag{A2.16}$$

As the squared angular momentum increases from Λ to Λ_{max}, the nodal quantum number decreases from v to 0, so we may rewrite this last equation in the form

$$2 \int_0^v \sqrt{\Lambda(v', E) - \Lambda} \, dv' = \frac{1}{2} \int_{r_1}^{r_2} (E - V(r) - \Lambda/r^2) \, r \, dr. \tag{A2.17}$$

We now obtain two more equations for the turning points r_1 and r_2 by differentiating equation (A2.17) with respect to Λ and E:

$$\int_0^v \frac{dv'}{\sqrt{\Lambda(v', E) - \Lambda}} = \frac{1}{2} \ln \left(\frac{r_2}{r_1} \right) \tag{A2.18}$$

and

$$\int_0^v \frac{\partial \Lambda(v', E)}{\partial E} \frac{dv'}{\sqrt{\Lambda(v', E) - \Lambda}} = \frac{1}{4} (r_2^2 - r_1^2). \tag{A2.19}$$

These last two equations were first deduced by Miller [6]. We may now choose any pair from equations (A2.9), (A2.10), (A2.18) and (A2.19) to determine r_1 and r_2, leaving the remaining two equations as consistency conditions.

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