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Analytic wkb energy expression for the linear plus Coulomb potential

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Received 24 August 1982

Abstract. A direct evaluation of the lowest-order WKB integral is carried out for the linear plus Coulomb potential $V(r) = \mu r - (\beta/r)$. The implicit relation for the bound-state energies defined by the WKB quantisation condition is expressed in terms of complete elliptic integrals. An approximate non-perturbative inversion of this relation provides an explicit analytic expression for the energy which reproduces known numerical results quite well. A criterion for the applicability of the approximation scheme is given.

1. Introduction

In a recent paper (Seetharaman *et al* 1982, hereafter referred to as I) we considered the direct evaluation of the lowest-order WKB integral for three-dimensional anharmonic oscillators. It was shown that the highly implicit relation for the bound-state energies defined by the WKB quantisation condition could be expressed in terms of complete elliptic integrals. Further, an approximate non-perturbative inversion of the implicit relation was performed and was found to provide explicit analytic expressions for the energy in good agreement with known values.

Motivated by the efficacy of our approximation method in the anharmonic oscillator case, in this work we analyse the case of a linear rising potential modified by the addition of an attractive Coulomb term. For this potential also the integral in the WKB quantisation condition can be expressed in terms of complete elliptic integrals. In addition to its intrinsic interest, this linear plus Coulomb potential is also of interest in the spectroscopy of charmonium levels (Eichten *et al* 1978, 1980, Quigg and Rosner 1979) whose gross features can be well accounted for by interpreting the levels as non-relativistic bound states of a heavy quark-antiquark ($c\bar{c}$) pair potential. The linear part of the interquark potential is taken to represent the confinement of quarks and the attractive Coulomb part has its origin in quantum chromodynamics.

We take the linear plus Coulomb potential in the form $V(r) = \mu r - (\beta/r)$ and, as noted earlier, evaluate the corresponding wkB integral directly in terms of complete elliptic integrals. To obtain the energies W we develop, along the lines of I, an approximation scheme in which the elliptic integrals are expanded about values (of their arguments) which depend on both the radial quantum n_r and the angular momentum l. It will be seen that our non-perturbative inversion procedure yields explicit expressions for the energy which are quite satisfactory. This paper is organised as follows. In the next section the WKB integral for the potential V(r) given above is evaluated, and the correct Coulomb spectrum is shown to follow in the limit $\mu \rightarrow 0$. Our inversion procedure is outlined in § 3 and an analytic expression for the energy W obtained from the WKB formula is also given. The results are presented and discussed in the final section.

2. Evaluation of the WKB integral

We take the Hamiltonian to be

$$H = \mathbf{p}^{2} + \mu r - (\beta/r) \qquad \mu, \beta \ge 0 \tag{2.1}$$

where we have chosen the mass to be $\frac{1}{2}$ and set $\hbar = 1^{\dagger}$. The WKB quantisation condition for the allowed bound-state energies W is

$$(n_r + \frac{1}{2})\pi = \int_b^a dr \left(W - \mu r + \frac{\beta}{r} - \frac{(l + \frac{1}{2})^2}{r^2} \right)^{1/2}$$
(2.2)

(Landau and Lifschitz 1977). Here n_r and l are non-negative integers. The integration is between the two classical turning points r = b and r = a which are (positive) roots of the cubic equation

$$r^{3} - \frac{W}{\mu}r^{2} - \frac{\beta}{\mu}r + \frac{(l+\frac{1}{2})^{2}}{\mu} = 0.$$
 (2.3)

One root of this equation is real and negative. The other two roots are real and positive for physical values of W. (In the case when the other two roots are complex conjugates, the wKB method is inapplicable.) We take the roots a, b and c to satisfy a > b > 0 and c < 0. Equation (2.2) can now be re-expressed in terms of a, b and c as

$$(n_r + \frac{1}{2})\pi = -\sqrt{\mu} \int_b^a \frac{\mathrm{d}r\{r^2 - (W/\mu)r - (\beta/\mu) + [(l + \frac{1}{2})^2/\mu r]\}}{[(a - r)(r - b)(r - c)]^{1/2}}.$$
 (2.4)

The right-hand side of this equation can be evaluated in terms of complete elliptic integrals (Byrd and Friedman 1971). We get

$$(n_{r} + \frac{1}{2})\pi = \{ [\frac{2}{3}\beta - (L^{2}/c) + \frac{1}{3}Wc] K(k) + \frac{1}{3}W(a-c)E(k) + L^{2}(c^{-1} - b^{-1})\Pi(\alpha^{2}, k) \} g/\sqrt{\mu}$$
(2.5)

where K, E and Π are complete elliptic integrals of the first, second and third kinds, respectively, in the notation of Byrd and Friedman (1971) and

$$L^{2} = (l + \frac{1}{2})^{2} \qquad k^{2} = (a - b)/(a - c) \qquad \alpha^{2} = ck^{2}/b \qquad g = 2(a - c)^{-1/2}.$$
(2.6)

It is easy to see that $0 < k^2 < 1$ and $\alpha^2 < 0$. Equation (2.5) is an implicit relation for the energy W.

It is known that the lowest-order WKB approximation is exact for the pure Coulomb potential. We therefore consider the limit $\mu \rightarrow 0$ in (2.5) and verify that the correct Coulomb energy spectrum results, thereby checking the correctness of (2.5). In this limit, the bound-state energy W is negative and the roots of the cubic equation (2.3)

[†] The analysis of this paper can easily be extended to the case $\beta < 0$, though this case does not seem to have physical interest.

are given by

$$a \rightarrow -[\beta + (4L^2W + \beta^2)^{1/2}]/2W$$

$$b \rightarrow -[\beta - (4L^2W + \beta^2)^{1/2}]/2W$$

$$c \rightarrow \frac{W}{\mu} + \frac{\beta}{W} \qquad (W < 0)$$

with the assumption that $4L^2W + \beta^2 > 0$. These expressions lead to the following limiting forms of k^2 , α^2 and g:

$$k^{2} \rightarrow (4L^{2}W + \beta^{2})^{1/2} \mu / W^{2}$$

$$\alpha^{2} \rightarrow 2(4L^{2}W + \beta^{2})^{1/2} / [-\beta + (4L^{2}W + \beta^{2})^{1/2}] \qquad g \rightarrow 2(\mu / -W)^{1/2}.$$

Since $k^2 \rightarrow 0$ as $\mu \rightarrow 0$ while α^2 remains finite, we also have

$$K(k) \to \frac{1}{2}\pi (1 + \frac{1}{4}k^2) \qquad E(k) \to \frac{1}{2}\pi (1 - \frac{1}{4}k^2) \qquad \Pi(\alpha^2, k) \to \pi/[2(1 - \alpha^2)^{1/2}]$$

(Byrd and Friedman 1971). Incorporating all these into (2.5) and evaluating the limit $\mu \rightarrow 0$, we get

$$W = -\beta^2 / 4(n_r + l + 1)^2, \qquad (2.7)$$

which gives the correct Coulomb energy spectrum for a particle of mass $\frac{1}{2}$. Note that W satisfies the inequality $4L^2W + \beta^2 > 0$, which justifies the assumption made earlier.

3. Analytic expression for W

Having expressed the WKB quantisation condition (2.2) in terms of elliptic integrals, we now consider the inversion of the resulting relation (2.5) which is an implicit function of the energy W. First we simplify matters a little by invoking a scaling of the Hamiltonian (2.1) to make the strength of the linear potential unity. Next we consider the limit $W \rightarrow \infty$ in (2.5) and obtain the leading term in the dependence of W on n_r and l. Finally we derive an analytic expression for W by improving on the above leading term, as was done in I for anharmonic oscillators.

3.1. Scaling

With the replacement $r \rightarrow \tau r$ (τ constant) in the Hamiltonian (2.1), it is easy to show that the energy eigenvalues obey the scaling relation

$$W(\mu,\beta) = \mu^{2/3} W(1,\mu^{-1/3}\beta).$$
(3.1)

This is also true of the energy W defined by the WKB condition (2.2). We can therefore set $\mu = 1$ without loss of generality and then need consider only $W(1, \lambda) \equiv W(\lambda)$ where we have defined

$$\lambda \equiv \mu^{-1/3} \beta. \tag{3.2}$$

The new Hamiltonian has the form

$$\bar{H} = p^2 + r - (\lambda/r). \tag{3.3}$$

Henceforth we shall consider this Hamiltonian and its eigenvalues $W(\lambda)$.

3.2. Leading (WKB) approximation to W

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It is not difficult to verify that, as $W \to \infty$, the roots a, b and c go as follows (with $\mu = 1$):

$$\rightarrow W \qquad b \rightarrow L/\sqrt{W} \qquad c \rightarrow -L/\sqrt{W}.$$

Hence

$$k^2 \rightarrow 1 - 2L/W^{3/2}$$
 $\alpha^2 \rightarrow -1.$

The limiting forms of the elliptic integrals are given by

$$K(k) \rightarrow \ln(4/k') + \frac{1}{4}(\ln(4/k') - 1)k'^{2}$$

$$E(k) \rightarrow 1 + \frac{1}{2}(\ln(4/k') - \frac{1}{2})k'^{2}$$

$$\Pi(\alpha^{2}, k) \rightarrow \frac{1}{2}\ln(4/k') + \frac{1}{8}\pi$$

where $k'^2 = 1 - k^2$ (Byrd and Friedman 1971). Putting these expressions, together with the changes $\mu \to 1$, $\beta \to \lambda$, in (2.5) and retaining only the leading terms, we get

$$(n_r + \frac{1}{2})\pi = \frac{2}{3}W^{3/2}[1 - (3\pi L/4W^{3/2})]$$

from which it follows that

$$W = \left(\frac{3}{4}\pi\right)^{2/3} \left(2n_r + l + \frac{3}{2}\right)^{2/3}.$$

In the rest of the paper we shall define $2n_r + l \equiv n$ and call the above leading term W_0 :

$$W_0 = \left(\frac{3}{4}\pi\right)^{2/3} \left(n + \frac{3}{2}\right)^{2/3}.$$
(3.4)

This expression for W_0 is in agreement with the known WKB limit for power law potentials (Quigg and Rosner 1979). Incidentally, we may note that the corresponding expression for W_0 in the case of Hamiltonian (2.1) will have an extra factor of $\mu^{2/3}$.

3.3. Improved approximation to W

As in I, the relation (3.4) will be the starting point for our approximation scheme from which we obtain an explicit expression for W which is better than that given by (3.4) with W_0 replaced by W. Since W_0 has no λ dependence, we clearly need an improvement to it. To this end, we suppose that W can be written as

$$W = W_0(1+x)$$
 $|x| \ll 1$ (3.5)

with W_0 given by (3.4). We then expand all W-dependent quantities on the RHS of (2.5) to order x. Thus we write the roots a, b and c as

$$a \simeq a_0 + a_1 x$$
 $b \simeq b_0 + b_1 x$ $c \simeq c_0 + c_1 x.$ (3.6)

The explicit expressions for a_0 , a_1 , etc, are easily found. We have

$$a_0 = \frac{1}{3}W_0(1+2p\,\cos\frac{1}{3}\varphi_0) \tag{3.7}$$

$$a_1 = \frac{1}{3}W_0(1 + 2p^{-1}\cos\frac{1}{3}\varphi_0 - \frac{2}{3}p\varphi_1\sin\frac{1}{3}\varphi_0)$$
(3.8)

where

$$p = (1 + 3\lambda / W_0^2)^{1/2}$$
 $\varphi_0 = \cos^{-1} A$ $\varphi_1 = -B(1 - A^2)^{-1/2}$

with

$$A = \frac{1}{p^3} \left(1 + \frac{9\lambda}{2W_0^2} - \frac{27L^2}{2W_0^3} \right) \qquad B = \frac{81L^2}{2W_0^3 p^5} \left(1 + \frac{\lambda^2}{3W_0 L^2} \right).$$

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Expressions for b_0 and c_0 (b_1 and c_1) can be obtained from (3.7) ((3.8)) by substituting $\varphi_0 \rightarrow \varphi_0 + 4\pi$ and $\varphi_0 \rightarrow \varphi_0 + 2\pi$ successively. Once *a*, *b* and *c* are known to order *x*, the remaining quantities can also be written down in a similar form:

$$k^{2} \simeq k_{0}^{2} + k_{1}^{2}x$$
 $\alpha^{2} \simeq \alpha_{0}^{2} + \alpha_{1}^{2}x$ $g \simeq g_{0} + g_{1}x$
 $K \simeq K_{0} + K_{1}x$ $E \simeq E_{0} + E_{1}x$ $\Pi \simeq \Pi_{0} + \Pi_{1}x$

where

$$K_0 = K(k_0)$$
 $E_0 = E(k_0)$ $\Pi_0 = \Pi(\alpha_0^2, k_0)$

and

$$\begin{split} & K_1 = k_1^2 [E_0 - (1 - k_0^2) K_0] / 2k_0^2 (1 - k_0^2) \\ & E_1 = k_1^2 (E_0 - K_0) / 2k_0^2 \\ & \Pi_1 = \frac{\alpha_1^2 [\alpha_0^2 E_0 + (k_0^2 - \alpha_0^2) K_0 + (\alpha_0^4 - k_0^2) \Pi_0]}{2\alpha_0^2 (1 - \alpha_0^2) (\alpha_0^2 - k_0^2)} + \frac{k_1^2 [E_0 - (1 - k_0^2) \Pi_0]}{2(1 - k_0^2) (k_0^2 - \alpha_0^2)}. \end{split}$$

Putting these in (2.5) and rearranging terms, we get the following expression for x:

$$x = N/D \tag{3.9}$$

with

$$N = \frac{3\pi(n-l+1)}{2g_0} - \left(W_0c_0 - \frac{3L^2}{c_0} + 2\lambda\right)K_0 - W_0(a_0 - c_0)E_0 - 3L^2\left(\frac{1}{c_0} - \frac{1}{b_0}\right)\Pi_0 \qquad (3.10)$$

$$D = \left[W_0\left(c_1 + c_0 + c_0\frac{g_1}{g_0}\right) + \frac{3L^2}{c_0}\left(\frac{c_1}{c_0} - \frac{g_1}{g_0} + \frac{2\lambda c_0g_1}{3L^2g_0}\right)\right]K_0 + \left(W_0c_0 - \frac{3L^2}{c_0} + 2\lambda\right)K_1 + W_0\left[\left(1 + \frac{g_1}{g_0}\right)(a_0 - c_0) + a_1 - c_1\right]E_0 + W_0(a_0 - c_0)E_1 + 3L^2\left[\frac{g_1}{g_0}\left(\frac{1}{c_0} - \frac{1}{b_0}\right) + \frac{b_1}{b_0^2} - \frac{c_1}{c_0^2}\right]\Pi_0 + 3L^2\left(\frac{1}{c_0} - \frac{1}{b_0}\right)\Pi_1. \qquad (3.11)$$

Our formula for W is defined by the relations (3.5), (3.9), (3.10) and (3.11). These give an explicit analytic expression for the energy of any state labelled by the quantum numbers n and l. For given n and l, N and D can be evaluated easily using standard tables of elliptic integrals such as those of Belyakov et al (1965). In connection with our formula the following points should be noted. First, the elliptic integrals and their derivatives are to be computed at values which are explicitly dependent on n and l. It is this feature that accounts for the success of the method. Second, as W_0 is positive and as x is small by assumption, W given by (3.5) will be positive. Therefore the entire approximation procedure outlined above will be consistent and meaningful only if, for a given value of λ , the actual energies of the system are positive. Since the potential V(r) is not positive definite, it can give rise to negative-energy bound states (in addition to positive-energy ones) for sufficiently large λ . Hence the approximation procedure cannot be good for all values of λ . We may, however, expect it to work reasonably well provided λ is such that there are no negative-energy bound states. A simple, natural way to ensure this is to require that the classical effective potential $V_{\text{eff}} = r - (\lambda/r) + (l + \frac{1}{2})^2/r^2$ has a positive value at its minimum. For any given l, a

sufficient condition for the minimum of V_{eff} to be positive is $\lambda < \frac{3}{4}(2l+1)^{4/3}$. It turns out that this condition provides a suitable criterion for determining the range of λ values over which our approximate inversion works satisfactorily.

4. Results and discussion

The energy values of several levels n, l calculated from our approximate nonperturbative expression for a typical value of $\lambda = 0.1$ are given in table 1. For comparison values of $W_{\rm WKB}$ obtained by numerical solution of (2.5) are also given. The quantities W_{exact} in this table are the actual eigenvalues of the Hamiltonian $H = p^2 + r - (\lambda/r)$ taken from the work of Eichten *et al* (1978)⁺. For $\lambda = 0.1$ (a value well below the limit $\frac{3}{4}(2l+1)^{4/3}$ for all l) our approximation to W deviates by no more than 1% from $W_{\rm WKB}$ in all cases, and provides values significantly closer to $W_{\rm WKB}$ than those given by W_0 . One can further see from the table that $W_{\rm WKB}$ itself is quite close to the exact eigenvalue even for the lowest levels. Our approximation can therefore be taken to provide reasonably good estimates of the actual energies. As noted in the previous section, our formula for the energy can be used with confidence for all levels as long as λ is restricted to low values ($\lambda < 0.75$ for S states, $\lambda < 3.25$ for P states, and so on). We observe that the restriction on λ is really of importance only for the first few levels, since it is only these levels that can have negative energies when λ is sufficiently large. This point is borne out by the results given in table 2 in which values of $W_0(1+x)$ and W_{WKB} for various values of λ are given for n = 0, l = 0 and n = 2, l = 0 levels. Comparing the difference between $W_0(1+x)$ and W_{WKB} , we note that only for the ground state does the difference vary markedly with λ .

n, l	W_0	$W_0(1+x)$	$W_{\rm WKB}$	Wexact
0,0	2.320	2.275	2.263	2.253
1, 1	3.262	3.301	3.314	3.310
3, 1	4.826	4.842	4.846	4.843
4, 2	5.517	5.578	5.598	5.597
6,0	6.784	6.752	6.748	6.746
10, 10	9.021	9.550	9.539	_
100, 50	38.529	39.213	39.444	_

Table 1. Energy values for $\lambda = 0.1$.

Finally, we make a few observations on the criterion of applicability of our approximation procedure. The limit on λ is intended only to indicate roughly the value up to which the method could be expected to give good results, and is not an absolute limit. As the limit has been derived from classical considerations, one cannot conclude that values of λ beyond the limit will necessarily result in the energies of the ground state (and its closest neighbours) becoming negative, although the ground-state energy will be negative if λ is sufficiently large. Therefore we can say that, while the method can be expected to be quite satisfactory for λ values lying well below the

[†] These are obtained by numerical solution of the Schrödinger equation.

	n = 0, l = 0		n = 2, l = 0	
λ	$\overline{W_0(1+x)}$	W _{WKB}	$\overline{W_0(1+x)}$	W _{WKB}
0.05	2.310	2.306	4.067	4.065
0.1	2.275	2.263	4.042	4.035
0.2	2.203	2,174	3.991	3.974
0.3	2.127	2.083	3.939	3.913
0.4	2.047	1.989	3.886	3.851
0.5	1.964	1.893	3.832	3.788
0.6	1.879	1.795	3.778	3.725
0.75	1.747	1.644	3.695	3.630

Table 2. λ dependence of energy values for the lowest two S states.

Table 3. Energy values for $\lambda = 1.131$ (charmonium case).

n, l	$W_0(1+x)$	$W_{ m WKB}$	W_{exact}
0,0	1.396	1.234	1.256
1, 1	2.822	2.753	2.752
2,0	3.481	3.381	3.390
2, 2	3.838	3.798	3.797
3, 1	4.486	4.406	4.405
4,0	5.027	4.960	4.967
4, 2	5.305	5.249	5.248

limit $\frac{3}{4}(2l+1)^{4/3}$, the error in calculating the energies will increase progressively with increasing λ , although the errors may not be unacceptably large for λ values not much larger than the limiting value. As an illustration of this point, we quote in table 3 the energies calculated for $\lambda = 1.131$. This value corresponds to one of the potentials used by Quigg and Rosner for fitting the charmonium levels (after a suitable scaling to bring their Hamiltonian to the form used in § 3). This value is above the S-state limit but below the P-state limit. As may be seen from the table, the error for the P states is much less than that for the corresponding S states. For comparison, we give the exact eigenvalues for the value $\lambda = 1.131$, again from the work of Eichten *et al* (1978). Our analytic expression can at best be taken to give a first approximation to the actual charmonium levels, since these levels are S and P states with low values of *n*.

Acknowledgment

One of us (MSR) wishes to thank J Pasupathy for discussions.

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