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1997 J. Phys. A: Math. Gen. 30 1719

(http://iopscience.iop.org/0305-4470/30/5/032)

J. Phys. A: Math. Gen. **30** (1997) 1719–1729. Printed in the UK PII: S0305-4470(97)77001-X

WKB expansion for the angular momentum and the Kepler problem: from the torus quantization to the exact one

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Received 26 July 1996

Abstract. We calculate the WKB series for the angular momentum and the non-relativistic three-dimesional Kepler problem. This is the first semiclassical treatment of the angular momentum for terms beyond the leading WKB approximation. We explain why the torus quantization (the leading WKB term) of the full problem is exact, even if the individual torus quantization of the angular momentum and of the radial Kepler problem separately is not exact. In this way we derive Langer's rule, calculate the first correction to the leading Langer's term and conjecture the form of all higher terms.

1. Introduction

The semiclassical methods used to solve the Schrödinger problem are of extreme importance in understanding the global behaviour of eigenfunctions and energy spectra, especially as a function of some external parameter, since usually they are the only approximation known in the form of an explicit formula.

The leading semiclassical approximation is just the first term of a certain $\hbar$-expansion. The method goes back to the early days of quantum mechanics and was developed by Bohr and Sommerfeld for one-freedom systems and separable systems, it was then generalized for integrable (but not necessarily separable) systems by Einstein (1917), which is called EBK or torus quantization. In fact, Einstein's result was corrected for the phase changes due to caustics by Maslov (1961) (see also Maslov and Fedoriuk (1981)), but the torus quantization formula thus obtained is still just a first term in a certain $\hbar$-expansion, whose higher terms are unknown in systems with more than one degree of freedom. Thus recently it was observed (Prosen and Robnik 1993, Graffi *et al* 1994) that these leading-order semiclassical approximations generally fail to predict the individual energy levels (and the eigenstates) within a vanishing fraction of the mean-energy level spacing. This conclusion is believed to be correct not only for the torus quantization of the integrable systems, but also in applying the Gutzwiller trace formula (Gutzwiller 1990) to general systems, including the completely chaotic ones, cf Gaspard and Alonso (1993). Therefore, a systematic study of the accuracy of semiclassical approximations is very important, especially in the context of quantum

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chaos (Casati and Chirikov 1995, Gutzwiller 1990). To present full generality is an almost impossible task, but in some special cases it is possible to work out the quantum corrections to higher or even all orders (Degli Esposti *et al* 1991, Graffi and Paul 1987, Salasnich and Robnik 1996, Robnik 1984, Narimanov 1995). On the other hand, in systems with one degree of freedom a systematic WKB expansion is possible, at least in principle, and in a few cases can be worked out even explicitly to all orders, resulting in a convergent series whose sum is identical to the exact spectrum (Dunham 1932, Bender *et al* 1977, Voros 1993, Robnik and Salasnich 1996).

Our goal in the present paper is to deal systematically with the WKB expansions for the angular momentum problem and for the Kepler problem. This is important not only from the point of view of mathematical physics (formal existence of the systematic series, its convergence properties and the summation), but also because the Kepler problem is so fundamental in physics. To the best of our knowledge a detailed analysis of this problem has not been undertaken in the literature so far. As will be seen, our treatment is to some extent, a derivation of the famous Langer correction (Langer 1937) together with higher corrections.

We shall work out some next to the leading terms for the Kepler problem and show—under a conjecture about the higher terms—that an exact result is obtained after all corrections have been taken into account and the resulting series has been summed. This is non-trivial, because we know that the torus quantization of the three-dimensional (3D) Kepler problem yields an exact result, whereas the individual torus quantization of the radial and of the angular momentum problems is not exact. Thus our present work is the first systematic semiclassical expansion of the angular momentum problem as a prerequisite to the full study of the 3D Kepler problem.

To define the language and to introduce the notation we first give the essential formulae of the torus quantization. The Hamiltonian of the 3D Kepler problem is given by

$$H = \frac{P_r^2}{2} + \frac{L^2}{2r^2} - \frac{\alpha}{r} \tag{1}$$

where

$$L^2 = P_\theta^2 + \frac{P_\phi^2}{\sin^2(\theta)} \tag{2}$$

and

$$P_\phi = L_z \tag{3}$$

are constants of motion. Of course, the Hamiltonian is a constant of motion, whose value is equal to the total energy E.

It is well known that the exact energy spectrum can be obtained with the Bohr–Sommerfeld (torus) quantization. To perform the torus quantization it is necessary to introduce the action variables

$$I_\phi = \frac{1}{2\pi}\oint P_\phi \,\mathrm{d}\phi = P_\phi \tag{4}$$

$$I_\theta = \frac{1}{2\pi}\oint P_\theta \,\mathrm{d}\theta = L - |I_\phi| \tag{5}$$

$$I_r = \frac{1}{2\pi}\oint P_r \,\mathrm{d}r = \frac{\alpha}{\sqrt{-2E}} - L. \tag{6}$$

The Hamiltonian as a function of the actions reads

$$H = \frac{-\alpha^2}{2[I_r + I_\theta + |I_\phi|]^2} \tag{7}$$

and after the torus quantization

$$I_r = (n_r + \tfrac{1}{2})\hbar \qquad I_\theta = (n_\theta + \tfrac{1}{2})\hbar \qquad I_\phi = n_\phi\hbar \tag{8}$$

the energy spectrum is given by

$$E_{n_r l} = \frac{-\alpha^2}{2\hbar^2[n_r + l + 1]^2} \tag{9}$$

where $l = n_\theta + |n_\phi|$. (The two quantum numbers, n_r and n_θ, are non-negative integers by construction, whilst n_ϕ can be negative, but obeys the rule $|n_\phi| \leqslant l$, where l is of course also non-negative.) This is the exact energy spectrum, which can also be obtained by solving the Schrödinger equation. Also the condition $|n_\phi| \leqslant l$ is precisely as in the exact quantum result.

Note that we have quantized the angular momentum $L = I_\theta + |I_\phi|$ with a semiclassical formula $L = (l + 1/2)\hbar$. If we use the exact quantization of the angular momentum, i.e., $L = \hbar\sqrt{l(l+1)}$, we obtain a wrong formula. How can this observation be explained?

In section 2 we treat the angular momentum problem by calculating the corrections to the leading torus quantization term, and in section 3 we then proceed with the analysis of the radial Kepler problem, again by calculating the corrections to the leading torus quantization term, now using the exact result for the quantized angular momentum. In section 4 we discuss the results and draw some general conclusions.

2. WKB expansion for the angular momentum

We consider the eigenvalue equation of the angular momentum

$$\hat{L}^2 Y(\theta, \phi) = \lambda^2\hbar^2 Y(\theta, \phi) \tag{10}$$

where $\hat{L}^2$ is formally given by the equation (2) with

$$\hat{P}_\theta^2 = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot(\theta)\frac{\partial}{\partial\theta} \right) \tag{11}$$

$$\hat{P}_\phi^2 = -\hbar^2 \frac{\partial^2}{\partial\phi^2}. \tag{12}$$

We can write the eigenfunction as

$$Y(\theta, \phi) = T(\theta)\, \mathrm{e}^{\mathrm{i}n_\phi\phi} \tag{13}$$

and we obtain

$$\hat{P}_\phi^2 Y(\theta, \phi) = n_\phi^2\hbar^2 Y(\theta, \phi) \tag{14}$$

and also

$$T''(\theta) + \cot(\theta)T'(\theta) + \left(\lambda^2 - \frac{n_\phi^2}{\sin^2(\theta)}\right) T(\theta) = 0. \tag{15}$$

Notice that $\hbar$ no longer appears in this equation. The special case $\lambda = n_\phi = 0$ can be worked out exactly, not only for the angular momentum problem but also for the radial Kepler problem (see section 3). Thus in this case no expansions are necessary.

Now we turn to the non-trivial case of $\lambda > 0$. To perform the WKB expansion we introduce a small parameter ϵ, which might be thought of as proportional to $\hbar$, and consider the eigenvalue problem

$$\epsilon^2 T''(\theta) + \epsilon^2 \cot(\theta)T'(\theta) = Q(\theta)T(\theta) \tag{16}$$

where

$$Q(\theta) = W(\theta) - \lambda^2 = \frac{n_\phi^2}{\sin^2(\theta)} - \lambda^2. \tag{17}$$

This small ϵ limit is equivalent to the large n_ϕ and/or large λ limit. The parameter ϵ helps to organize the WKB series; we set $\epsilon = 1$ when the calculation is completed. First we put

$$T(\theta) = \exp\left\{\frac{1}{\epsilon}S(\theta)\right\} \tag{18}$$

where $S(\theta)$ is a complex function that satisfies the differential equation

$$S'^2(\theta) + \epsilon S''(\theta) + \epsilon \cot(\theta) S'(\theta) = Q(\theta). \tag{19}$$

The WKB expansion for the function $S(\theta)$ is given by

$$S(\theta) = \sum_{k=0}^{\infty} \epsilon^k S_k(\theta) \tag{20}$$

and by comparing like powers of ϵ we obtain a recursion formula ($n > 0$)

$$S_0'^2 = Q \qquad \sum_{k=0}^{n} S_k' S_{n-k}' + S_{n-1}'' + \cot(\theta) S_{n-1}' = 0. \tag{21}$$

Straightforward calculations give for the first few terms

$$S_0' = -Q^{\frac{1}{2}} \tag{22}$$

$$S_1' = -\tfrac{1}{4} Q' Q^{-1} - \tfrac{1}{2}\cot(\theta) \tag{23}$$

$$S_2' = -\frac{1}{32} Q'^2 Q^{-5/2} - \frac{1}{8}\frac{\mathrm{d}}{\mathrm{d}\theta}(Q' Q^{-3/2}) - \frac{1}{8}\cot^2(\theta) Q^{-1/2} - \frac{1}{4}\left(\frac{\mathrm{d}}{\mathrm{d}\theta}\cot(\theta)\right) Q^{-1/2}. \tag{24}$$

The exact quantization of the wavefunction (18) is given by

$$\oint \mathrm{d}S = \sum_{k=0}^{\infty} \oint \mathrm{d}S_k = 2\pi \mathrm{i} n_\theta \tag{25}$$

where we have now set $\epsilon = 1$. This integral is a complex contour integral which encircles the two turning points on the real axis. Obviously, it is derived from the requirement of the uniqueness of the complex wavefunction T (Dunham 1932, Bender *et al* 1977).

The zero-order term is given by

$$\oint \mathrm{d}S_0 = 2\mathrm{i} \int \mathrm{d}\theta \sqrt{\lambda^2 - W(\theta)} = 2\pi \mathrm{i}(\lambda - |n_\phi|) \tag{26}$$

and the first term reads

$$\oint \mathrm{d}S_1 = -\tfrac{1}{4} \ln Q|_{\mathrm{contour}} = -\pi \mathrm{i}. \tag{27}$$

Evaluating $\ln Q$ once around the contour gives $4\pi\mathrm{i}$ because the contour encircles two simple zeros of Q.

All the other odd terms vanish when integrated along the closed contour because they are exact differentials (Bender *et al* 1977). So the quantization condition (25) can be written as

$$\sum_{k=0}^{\infty} \oint \mathrm{d}S_{2k} = 2\pi \mathrm{i}\left(n_\theta + \frac{1}{2}\right) \tag{28}$$

and thus it is a sum over even-numbered terms only. The next non-zero term is given by

$$\oint \mathrm{d}S_2 = -\mathrm{i}\left[\frac{1}{12}\frac{\partial^2}{\partial(\lambda^2)^2}\int \mathrm{d}\theta\, \frac{W'^2(\theta)}{\sqrt{\lambda^2 - W(\theta)}} + \frac{1}{2}\frac{\partial}{\partial(\lambda^2)}\int \mathrm{d}\theta\, \frac{W'(\theta)\cot(\theta)}{\sqrt{\lambda^2 - W(\theta)}}\right.$$
$$\left. + \frac{1}{4}\int \mathrm{d}\theta\, \frac{\cot^2(\theta)}{\sqrt{\lambda^2 - W(\theta)}}\right]. \tag{29}$$

These three integrals give (see the appendix A)

$$\oint \mathrm{d}S_2 = \frac{\pi \mathrm{i}}{4\lambda} \tag{30}$$

where, importantly, the n_ϕ dependence drops out now. Thus up to the second order in ϵ the quantization condition reads

$$\lambda + \frac{1}{8\lambda} = l + \frac{1}{2} \tag{31}$$

where $l = n_\theta + n_\phi$. The term $1/8\lambda$ is the first quantum correction to the the quantization of the angular momentum. From this result we can argue (‘conjecture by educated guess’) that the ϵ^{2k} term in the WKB series is ($k > 0$)

$$\oint \mathrm{d}S_{2k} = 2\pi \mathrm{i}\binom{\frac{1}{2}}{k} 2^{-2k}\lambda^{1-2k} \tag{32}$$

so that the WKB expansion of the angular momentum to all orders is given by

$$\sum_{k=0}^{\infty}\binom{\frac{1}{2}}{k} 2^{-2k}\lambda^{1-2k} = l + \frac{1}{2}. \tag{33}$$

This is the exact formula for the relationship between l and λ, because

$$\sum_{k=0}^{\infty}\binom{\frac{1}{2}}{k} 2^{-2k}\lambda^{1-2k} = \frac{1}{2}\sqrt{1+4\lambda^2} \tag{34}$$

and the equation $\sqrt{1+4\lambda^2}/2 = l + \frac{1}{2}$ can be inverted and gives $\lambda = \sqrt{l(l+1)}$. Please observe that this series is convergent for $\lambda > \frac{1}{2}$, which means that the series converges for all non-zero values of l.

This completes our investigation of the semiclassical expansion for the angular momentum, where it remains in general to prove the conjectured formula (32) for $k \geqslant 2$.

At this point it is necessary to give some historical comments. It was Langer’s (1937) discovery that by replacing the exact value of $L^2 = \lambda^2\hbar^2 = l(l+1)\hbar^2$ with the torus quantized value $(l+\frac{1}{2})^2\hbar^2$ in the radial Kepler problem defined by equation (35) of section 3 and performing the torus quantization of this radial eigenvalue problem one can get the exact result. However, Langer gave no deep justification for such a ‘prescription’ and it is one of the major goals of our present paper to explain Langer’s rule and to go one order beyond Langer’s term and further to formulate the well supported conjecture embodied in equation (32) about all the higher corrections. In doing so we thus demonstrate the tour from Langer’s correction to the exact result. For a discussion of the Langer’s rule see Gutzwiller’s book (1990, p 212).

3. WKB expansion for the radial Kepler problem

We consider the Schrödinger equation for the radial problem

$$\left[-\frac{\hbar^2}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V(r)\right]\psi(r)=E\psi(r) \tag{35}$$

where

$$V(r)=\frac{L^2}{2r^2}-\frac{\alpha}{r}. \tag{36}$$

We can always write the wavefunction as

$$\psi(r)=\exp\left\{\frac{\mathrm{i}}{\hbar}\sigma(r)\right\} \tag{37}$$

where the phase $\sigma(r)$ is a complex function that satisfies the differential equation

$$\sigma'^2(r)+\left(\frac{\hbar}{\mathrm{i}}\right)\sigma''(r)=2(E-V(r)). \tag{38}$$

The WKB expansion for the phase is

$$\sigma(r)=\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k\sigma_k(r). \tag{39}$$

Substituting (39) into (38) and comparing like powers of $\hbar$ gives the recursion relation ($n>0$)

$$\sigma_0'^2=2(E-V(r)) \qquad \sum_{k=0}^{n}\sigma_k'\sigma_{n-k}'+\sigma_{n-1}''=0. \tag{40}$$

The quantization condition is obtained by requiring the uniqueness of the wavefunction

$$\oint \mathrm{d}\sigma=\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^k\oint \mathrm{d}\sigma_k=2\pi n_r\hbar \tag{41}$$

where $n_r\geqslant 0$, an integer number, is the radial quantum number.

The zero-order term, which gives the Bohr–Sommerfeld formula (6), is given by

$$\oint \mathrm{d}\sigma_0=2\int \mathrm{d}r\sqrt{2(E-V(r))} \tag{42}$$

and the first odd term in the series gives the Maslov corrections (the Maslov index is equal to two)

$$\left(\frac{\hbar}{\mathrm{i}}\right)\oint \mathrm{d}\sigma_1=-\pi\hbar. \tag{43}$$

All the other odd terms vanish when integrated along the closed contour because they are exact differentials (Bender *et al* 1977). So the quantization condition (41) can be written as

$$\sum_{k=0}^{\infty}\left(\frac{\hbar}{\mathrm{i}}\right)^{2k}\oint \mathrm{d}\sigma_{2k}=2\pi\left(n_r+\frac{1}{2}\right)\hbar \tag{44}$$

thus again a sum over even-numbered terms only. The next two non-zero terms are (Bender *et al* 1977)

$$\left(\frac{\hbar}{\mathrm{i}}\right)^2\oint \mathrm{d}\sigma_2=-\hbar^2\frac{1}{12}\frac{\partial^2}{\partial E^2}\int \mathrm{d}r\frac{V'^2(r)}{\sqrt{2(E-V(r))}} \tag{45}$$

$$\left(\frac{\hbar}{\mathrm{i}}\right)^4\oint \mathrm{d}\sigma_4=\hbar^4\left[\frac{1}{240}\frac{\partial^3}{\partial E^3}\int \mathrm{d}r\frac{V'^2(r)}{\sqrt{2(E-V(r))}}\right.$$

$$- \frac{1}{576} \frac{\partial^4}{\partial E^4} \int \mathrm{d}r \frac{V'^2(r) V''(r)}{\sqrt{2(E - V(r))}} \bigg] . \tag{46}$$

A straightforward calculation of these terms gives (see appendix B)

$$\left(\frac{\hbar}{\mathrm{i}}\right)^2 \oint \mathrm{d}\sigma_2 = -\hbar^2 \frac{\pi}{4L} \tag{47}$$

and

$$\left(\frac{\hbar}{\mathrm{i}}\right)^4 \oint \mathrm{d}\sigma_4 = \hbar^4 \frac{\pi}{64L^3} . \tag{48}$$

Up to the fourth order in $\hbar$ the quantization condition reads

$$\left(\frac{\alpha}{\sqrt{-2E}} - L\right) - \hbar^2 \frac{1}{8L} + \hbar^4 \frac{1}{128L^3} = \left(n_r + \frac{1}{2}\right)\hbar . \tag{49}$$

So we have obtained the first two quantum corrections to the torus quantization of the radial Kepler problem. Obviously at this point of truncating the series we get the wrong spectrum if we use the torus quantized angular momentum $L = (l + \frac{1}{2})\hbar$, and this is still true if the series is expanded to all orders. However, for the anticipated infinite series expansion we shall obtain the exact quantized value of the eigenenergies when using the exact angular momentum $L^2 = l(l+1)\hbar^2$. To show this we note that higher-order corrections quickly increase in complexity but each integral gives a polynomial in E with leading term E^M, where M is the power of the operator $\partial^M/\partial E^M$ in front of the integral (Barclay 1993). Differentiating M times leaves a constant independent of E. Since this happens in all terms in the series (with $k > 0$), the WKB corrections to the Bohr–Sommerfeld formula have no E-dependence. From this result we can guess the general formula, based on our two correcting terms to the torus quantization, namely

$$\begin{aligned} \frac{\alpha}{\sqrt{-2E}} &= \hbar \left[\left(n_r + \frac{1}{2}\right) + \lambda + \sum_{k=1}^{\infty} \binom{\frac{1}{2}}{k} 2^{-2k} \lambda^{1-2k} \right] \\ &= \hbar \left[\left(n_r + \frac{1}{2}\right) + \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} 2^{-2k} \lambda^{1-2k} \right] \end{aligned} \tag{50}$$

where $\lambda = L/\hbar$, and so the $\hbar^{2k}$ term in the WKB series is ($k > 0$)

$$\left(\frac{\hbar}{\mathrm{i}}\right)^{2k} \oint \mathrm{d}\sigma_{2k} = -2\pi\hbar \binom{\frac{1}{2}}{k} 2^{-2k} \lambda^{1-2k} . \tag{51}$$

In conclusion, the energy spectrum of the WKB algorithm to all orders is given by

$$E_{n_r\lambda}^{\mathrm{WKB}} = \frac{-\alpha^2}{2\hbar^2 [(n_r + \frac{1}{2}) + \sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} 2^{-2k} \lambda^{1-2k}]^2} . \tag{52}$$

Now, by using the formula (33) of the WKB expansion of the angular momentum, we obtain the exact result $E_{n_r\lambda}^{\mathrm{WKB}} = E_{n_r l}$, as given in equation (9).

We can summarize the mathematical reason for the exactness of the torus quantization formula (derived in section 1) for the 3D Kepler problem: since the problem is separable, the wavefunctions (for the angular momentum and for the radial part) multiply and their phases have the additivity property, and therefore the total phase written as $(\mathrm{i}/\hbar)(\sigma - \mathrm{i}\hbar S)$ must obey the quantization condition (uniqueness of the wavefunction). From the two formulae (32) and (51) one can see that the quantum corrections (i.e. terms higher than the torus quantization terms) do indeed compensate mutually term-by-term.

In concluding this section we mention another closely related problem, namely the 3D isotropic harmonic oscillator, where the same Langer's rule must be applied to get the exact result by the torus quantization in spherical coordinates. (This problem is of course also separable in Cartesian coordinates and thus the torus quantization of each 1D oscillator leads to the exact result.) Therefore, here, we find exactly the same mathematical mechanism for mutual cancellation of all correcting terms higher than the torus quantization term. This similarity is of course not very surprising since the 3D Kepler problem is equivalent to a 4D harmonic oscillator with a constraint and thus through O(4) symmetry Kepler problem is dynamically equivalent to the harmonic oscillator.

4. Discussion and conclusions

In the present paper we offer (to the best of our knowledge) the first calculation of the higher WKB terms beyond the torus quantization leading terms for the angular momentum and the radial Kepler problem. This analysis explains the curious compensation of the higher-order quantum corrections (of the two separated problems) resulting in the exactness of the torus quantization for the entire 3D Kepler problem (see section 1). In this way we in fact derive Langer's (1937) rule but also go higher by one order or calculation, and then make the reasonable and well supported conjecture about all higher orders. We have no reason to doubt that our conjectured general formulae (32) and (51) are correct for all $k > 0$, but this still has to be proved mathematically.

We consider this kind of study as important in understanding the accuracy of the semiclassical methods, and many of the results in this context for 1D problems are known, including some more general families of 1D potentials studied by Barclay (1993) which are characterized by the factorization property (Infeld and Hull 1957, Green 1965). For related developments see (Inomata *et al* 1993, Inomata and Junker 1994) and references therein.

One important future project is to analyse a more general class of the 1D potentials and in particular to extend the results to systems with two or more degrees of freedom, even if they are integrable (but not separable). Further, it remains as an important project to assess the accuracy of much more general (although mathematically not yet completely satisfactory, due to the divergent series expansions) methods like the Gutzwiller theory (1967, 1969, 1970, 1971, 1990), applicable to non-integrable systems, including the chaotic systems (Gaspard and Alonso 1993).

Acknowledgments

LS thanks Professor Sandro Graffi (Università di Bologna) for many enlightening discussions and acknowledges the Alps-Adria Rectors Conference Grant of the University of Maribor. MR thanks Dr Evvuueni Narimanov and Professor Douglas A Stone (Yale University) for stimulating discussions and for communicating related results. The financial support by the Ministry of Science and Technology of the Republic of Slovenia is acknowledged with thanks.

Appendix A

In this appendix we show how to obtain the formula (30). In all integrals of this section the limits of integration are between the two turning points. After substitution $z = \tan(\theta)$, we have

$$\int \mathrm{d}\theta \frac{W'(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = \frac{4n_\phi^4}{\sqrt{\lambda^2 - n_\phi^2}} \int \mathrm{d}z \frac{(1+z^2)}{z^6} \sqrt{\frac{z^2}{z^2-\beta}}$$

$$= \frac{3\pi}{2|n_\phi|}(\lambda^2 - n_\phi^2)^2 + 2\pi |n_\phi| (\lambda^2 - n_\phi^2) \tag{53}$$

where $\beta = n_\phi^2/(\lambda^2 - n_\phi^2)$, so that

$$\frac{\partial^2}{\partial(\lambda^2)^2} \int \mathrm{d}\theta \frac{W'^2(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = \frac{3\pi}{|n_\phi|}. \tag{54}$$

For the other integrals we use the same procedure.

$$\int \mathrm{d}\theta \frac{W'(\theta)\cot(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = -\frac{2n_\phi^2}{\sqrt{\lambda^2 - n_\phi^2}} \int \mathrm{d}z \frac{1}{z^4} \sqrt{\frac{z^2}{z^2-\beta}} = -\frac{\pi}{|n_\phi|}(\lambda^2 - n_\phi^2) \tag{55}$$

from which we obtain

$$\frac{\partial}{\partial(\lambda^2)} \int \mathrm{d}\theta \frac{W'(\theta)\cot(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = -\frac{\pi}{|n_\phi|}. \tag{56}$$

The last integral gives

$$\int \mathrm{d}\theta \frac{\cot^2(\theta)}{\sqrt{\lambda^2 - W(\theta)}} = \frac{1}{\sqrt{\lambda^2 - n_\phi^2}} \int \mathrm{d}z \frac{1}{z^2(1+z^2)} \sqrt{\frac{z^2}{z^2-\beta}} = \pi \left(\frac{1}{|n_\phi|} - \frac{1}{\lambda}\right). \tag{57}$$

In conclusion

$$\oint \mathrm{d}S_2 = -\mathrm{i}\left[\frac{1}{12}\frac{3\pi}{|n_\phi|} + \frac{1}{2}\left(-\frac{\pi}{|n_\phi|}\right) + \frac{1}{4}\pi\left(\frac{1}{|n_\phi|} - \frac{1}{\lambda}\right)\right] = \frac{\pi \mathrm{i}}{4\lambda}. \tag{58}$$

Appendix B

In this appendix we show how to obtain formulae (47) and (48). In this section again all integrals are taken between the two turning points. For the first one, after substitution $y = 1/r$, we have

$$\int \mathrm{d}r \frac{V'^2(r)}{\sqrt{2(E - V(r))}} = \int \mathrm{d}y \frac{L^4 y^4 - 2L^2 \alpha y^3 + \alpha^2 y^2}{L\sqrt{a + by - y^2}} \tag{59}$$

where $a = 2E/L^2$ and $b = 2\alpha/L^2$. We observe that

$$I_2 = \int \mathrm{d}y \frac{y^2}{\sqrt{a + by - y^2}} = \frac{\pi}{8}(4a + 3b^2) \tag{60}$$

$$I_3 = \int \mathrm{d}y \frac{y^3}{\sqrt{a + by - y^2}} = \frac{\pi}{16}(12a + 5b^2) \tag{61}$$

$$I_4 = \int \mathrm{d}y \frac{y^4}{\sqrt{a + by - y^2}} = \frac{\pi}{128}(48a^2 + 128ab^2 + 35b^4). \tag{62}$$

Because we must apply the operator $\partial^2/\partial E^2$ and $a = 2E/L^2$, the only non-zero contribution stems from the integral I_4 and we obtain

$$\frac{\partial^2}{\partial E^2} \int \mathrm{d}r \frac{V'^2(r)}{\sqrt{2(E - V(r))}} = \frac{3\pi}{L}. \tag{63}$$

In conclusion we have

$$\left(\frac{\hbar}{\mathrm{i}}\right)^2 \oint \mathrm{d}\sigma_2 = -\hbar^2 \frac{1}{12}\frac{3\pi}{L} = -\hbar^2 \frac{\pi}{4L}. \tag{64}$$

To obtain the formula (48) we proceed in the same way.

$$\int \mathrm{d}r \frac{V''^2(r)}{\sqrt{2(E-V(r))}} = \int \mathrm{d}y \frac{9L^4y^6 - 12L^2\alpha y^5 + 4\alpha^2 y^4}{L\sqrt{a+by-y^2}} \tag{65}$$

its leading integral is

$$I_6 = \int \mathrm{d}y \frac{y^6}{\sqrt{a+by-y^2}} = \frac{\pi}{1024}(320a^3 + 1680a^2b^2 + 1260ab^2 + 231b^6) \tag{66}$$

from which we obtain

$$\frac{\partial^3}{\partial E^3}\int \mathrm{d}r \frac{V''^2(r)}{\sqrt{2(E-V(r))}} = \frac{135\pi}{L^3}. \tag{67}$$

For the last integral we have

$$\int \mathrm{d}r \frac{V'^2(r)V''(r)}{\sqrt{2(E-V(r))}} = \int \mathrm{d}y \frac{3L^6y^8 - 8L^4y^7 + 7L^2\alpha^2y^6 - 2\alpha^3y^5}{L\sqrt{a+by-y^2}} \tag{68}$$

its leading integral is

$$I_8 = \int \mathrm{d}y \frac{y^8}{\sqrt{a+by-y^2}} = \frac{\pi}{32768}(8960a^4 + 80640a^3b^2 + 110880a^2b^4 + 48048ab^6 + 6435b^8) \tag{69}$$

from which we obtain

$$\frac{\partial^4}{\partial E^4}\int \mathrm{d}r \frac{V'^2(r)V''(r)}{\sqrt{2(E-V(r))}} = \frac{315\pi}{L^3}. \tag{70}$$

In conclusion we have

$$\left(\frac{\hbar}{\mathrm{i}}\right)^4 \oint \mathrm{d}\sigma_4 = \hbar^4\left[\frac{1}{240}\frac{135\pi}{L^3} - \frac{1}{576}\frac{315\pi}{L^3}\right] = \hbar^4\frac{\pi}{64L^3}. \tag{71}$$

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