Preprint CAMTP/96-5
July 1996

WKB to all orders and the accuracy of the semiclassical quantization

Marko Robnik(*)[1] and Luca Salasnich(*)(+)[2]

(*) Center for Applied Mathematics and Theoretical Physics, University of Maribor, Krekova 2, SLO–2000 Maribor, Slovenia

(+) Dipartimento di Matematica Pura ed Applicata Università di Padova, Via Belzoni 7, I–35131 Padova, Italy
and
Istituto Nazionale di Fisica Nucleare, Sezione di Padova, Via Marzolo 8, I–35131 Padova, Italy

Abstract. We perform a systematic WKB expansion to all orders for a one–dimensional system with potential $V(x) = U_0/\cos^2(\alpha x)$. We are able to sum the series to the exact energy spectrum. Then we show that at any finite order the error of the WKB approximation measured in *the natural units of the mean energy level spacing* does not go to zero when the quantum number goes to infinity. Therefore we make the general conclusion that the semiclassical approximations fail to predict the individual energy levels within a vanishing fraction of the mean energy level spacing.

PACS numbers: 03.65.-w, 03.65.Ge, 03.65.Sq
Submitted to **Journal of Physics A: Mathematical and General**

[1]e–mail: robnik@uni-mb.si
[2]e–mail: salasnich@math.unipd.it

1 Introduction

In the last years many studies have been devoted to the transition from classical mechanics to quantum mechanics. These studies are motivated by the so–called quantum chaos (see Ozorio de Almeida 1990, Gutzwiller 1990, Casati and Chirikov 1995). An important aspect is the semiclassical quantization formula of the energy levels for integrable and quasi–integrable systems, i.e. the torus quantization initiated by Einstein (1917) and completed by Maslov (1972, 1981). As is well known, the torus quantization is just the first term of a certain $\hbar$-expansion, the so–called WKB expansion, whose higher terms can be calculated with a recursion formula at least for one degree systems (Dunham 1932, Bender, Olaussen and Wang 1977, Voros 1983).

Recently it has been observed by Prosen and Robnik (1993) and also Graffi, Manfredi and Salasnich (1994) that the leading–order semiclassical approximation fails to predict the individual energy levels within a vanishing fraction of the mean energy level spacing. This result has been shown to be true also for the leading (torus) semiclassical approximation by Salasnich and Robnik (1996).

In this paper we analyze a simple one–dimensional system for which we are able to perform a systematic WKB expansion to all orders resulting in a convergent series whose sum is identical to the exact spectrum. For this system we show that any finite order WKB (semiclassical) approximation fails to predict the individual energy levels within a vanishing fraction of the mean energy level spacing.

2 The system and the WKB expansion method

The Hamiltonian of the system is given by

$$H = \frac{p^2}{2m} + V(x) \; , \tag{1}$$

where

$$V(x) = \frac{U_0}{\cos^2(\alpha x)} \; . \tag{2}$$

Of course, the Hamiltonian is a constant of motion, whose value is equal to the total energy E. To perform the torus quantization it is necessary to introduce the action variable

$$I = \frac{1}{2\pi} \oint p dx = \frac{\sqrt{2m}}{\alpha} (\sqrt{E} - \sqrt{U_0}) \ . \tag{3}$$

The Hamiltonian as a function of the action reads

$$H = \frac{\alpha^2}{2m} I^2 + 2\alpha \sqrt{\frac{U_0}{2m}} I + U_0 \ , \tag{4}$$

and after the torus quantization

$$I = (\nu + \frac{1}{2}) \hbar \ , \tag{5}$$

where $\nu = 0, 1, 2, \ldots$, the energy spectrum is given by

$$E_\nu^{tor} = A[(\nu + \frac{1}{2}) + \frac{1}{2} B]^2 \ , \tag{6}$$

where $A = \alpha^2 \hbar^2/(2m)$ and $B = \sqrt{8mU_0}/(\alpha\hbar)$.

The Schrödinger equation of the system

$$[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)] \psi(x) = E \psi(x) \ , \tag{7}$$

can be solved analytically (as shown in Landau and Lifshitz 1973, Flügge 1971) and the exact energy spectrum is:

$$E_\nu^{ex} = A[(\nu + \frac{1}{2}) + \frac{1}{2} \sqrt{1 + B^2}]^2 \ , \tag{8}$$

where $\nu = 0, 1, 2, \ldots$. We see that the torus quantization does not give the correct energy spectrum, but it is well known that the torus quantization is just the first term of the WKB expansion. To calculate all the terms of the WKB expansion we observe that the wave function can always be written as

$$\psi(x) = \exp{(\frac{i}{\hbar} \sigma(x))} \ , \tag{9}$$

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

$$\sigma'^2(x) + (\frac{\hbar}{i}) \sigma''(x) = 2m(E - V(x)) \ . \tag{10}$$

The WKB expansion for the phase is given by

$$\sigma(x) = \sum_{k=0}^{\infty} (\frac{\hbar}{i})^k \sigma_k(x) \ . \tag{11}$$

Substituting (11) into (10) and comparing like powers of $\hbar$ gives the recursion relation $(n > 0)$

$$\sigma'^2_0 = 2m(E - V(x)), \quad \sum_{k=0}^{n} \sigma'_k \sigma'_{n-k} + \sigma''_{n-1} = 0 \ . \tag{12}$$

The quantization condition is obtained by requiring the single-valuedness of the wave function

$$\oint d\sigma = \sum_{k=0}^{\infty} (\frac{\hbar}{i})^k \oint d\sigma_k = 2\pi\hbar\ \nu \ \ , \tag{13}$$

where $\nu = 0, 1, 2, \ldots$ is the quantum number.

The zero order term, which gives the Bohr-Sommerfeld formula, is given by

$$\oint d\sigma_0 = 2 \int dx \sqrt{2m(E - V(x))} = 2\pi\hbar(\sqrt{\frac{E}{A}} - \frac{1}{2}B) \ , \tag{14}$$

and the first odd term in the series gives the Maslov corrections (Maslov index is equal to 2)

$$(\frac{\hbar}{i}) \oint d\sigma_1 = (\frac{\hbar}{i}) \frac{1}{4} \ln p|_{contour} = -\pi\hbar \ . \tag{15}$$

The zero and first order terms give the equation (6), which is the torus quantization formula for the energy levels (Bohr–Sommerfeld–Maslov). Here we want to analyze the quantum corrections to this formula. We observe that all the other odd terms vanish when integrated along the closed contour because they are exact differentials (Bender, Olaussen and Wang 1977). So the quantization condition (13) can be written

$$\sum_{k=0}^{\infty} (\frac{\hbar}{i})^{2k} \oint d\sigma_{2k} = 2\pi\hbar(\nu + \frac{1}{2}) \ , \tag{16}$$

thus again a sum over even–numbered terms only. The next two non–zero terms are (Narimanov 1995, Bender, Olaussen and Wang 1977, Robnik and Salasnich 1996)

$$(\frac{\hbar}{i})^2 \oint d\sigma_2 = -\frac{\hbar^2}{\sqrt{2m}} \frac{1}{12} \frac{\partial^2}{\partial E^2} \int dx \frac{V'^2(x)}{\sqrt{E - V(x)}} \; , \tag{17}$$

$$(\frac{\hbar}{i})^4 \oint d\sigma_4 = \frac{\hbar^4}{(2m)^{3/2}} [\frac{1}{120} \frac{\partial^3}{\partial E^3} \int dx \frac{V''^2(x)}{\sqrt{E - V(x)}} - \frac{1}{288} \frac{\partial^4}{\partial E^4} \int dx \frac{V'^2(x) V''(x)}{\sqrt{E - V(x)}}] \; . \tag{18}$$

A straightforward calculation of these terms gives (see the Appendix)

$$(\frac{\hbar}{i})^2 \oint d\sigma_2 = -\frac{2\pi\hbar}{4B} \; , \tag{19}$$

and

$$(\frac{\hbar}{i})^4 \oint d\sigma_4 = \frac{2\pi\hbar}{16B^3} \; . \tag{20}$$

Up to the fourth order in $\hbar \sim B^{-1}$ the quantization condition reads

$$E_\nu^{(4)} = A[(\nu + \frac{1}{2}) + \frac{1}{2}B + \frac{1}{4B} - \frac{1}{16B^3}]^2 \; . \tag{21}$$

The first two terms on the right side give the torus quantization formula, and the other two terms are quantum corrections. Higher–order quantum corrections quickly increase in complexity but in this specific case they can be calculated. We first verify by induction, following Bender, Olaussen and Wang (1977), that the solution to (12) has the general form

$$\sigma_n^{'}(x) = (\sigma_0^{'})^{1-3n} P_n(\cos(\alpha x)) \sin^{f(n)}(\alpha x) \; , \tag{22}$$

where $f(n) = 0$ for n even and $f(n) = 1$ for n odd, and P_n is a polynomial given by

$$P_n(\cos(\alpha x)) = \sum_{l=0}^{g(n)} C_{n,l} \cos^{2l-3n}(\alpha x) \; , \tag{23}$$

with $g(n) = (3n-2)/2$ for n even and $g(n) = (3n-3)/2$ for n odd.
The integrals in (16) are performed by substituting $z = \tan(\alpha x)$. In this

way the $2k$-term reduces to

$$(\frac{\hbar}{i})^{2k} \oint d\sigma_{2k} = (\frac{\hbar}{i})^{2k} \frac{(2m)^{1/2-3k}}{\alpha} \sum_{l=0}^{3k-1} C_{2k,l} \oint dz \frac{(1+z^2)^{3k-l-1}}{(E-U_0-U_0 z^2)^{3k-1/2}} \ . \tag{24}$$

We observe that

$$\oint dz \frac{(1+z^2)^{3k-l-1}}{(E-U_0-U_0 z^2)^{3k-1/2}} =$$
$$= (-1)^{3k-1} \frac{\Gamma(\frac{1}{2})}{\Gamma(3k-\frac{1}{2})} \frac{\partial^{3k-1}}{\partial E^{3k-1}} \oint dz \frac{(1+z^2)^{3k-l-1}}{(E-U_0-U_0 z^2)^{1/2}} \ , \tag{25}$$

so the only non–zero term is for $l=0$

$$\frac{\partial^{3k-1}}{\partial E^{3k-1}} \oint dz \frac{(1+z^2)^{3k-1}}{(E-U_0-U_0 z^2)^{1/2}} = \frac{2^{6k-1}}{U_0^{1/2}} \frac{\Gamma(3k-1/2)^2}{\Gamma(6k-1)} \frac{\partial^{3k-1}}{\partial E^{3k-1}} \beta^{3k-1} =$$
$$= \frac{2^{6k-1}}{U_0^{1/2}} \frac{\Gamma(3k-1/2)^2}{\Gamma(6k-1)} \Gamma(3k) \frac{1}{U_0^{3k-1/2}} 2\pi \ , \tag{26}$$

where $\beta = (E-U_0)/U_0$. At this stage we obtain

$$(\frac{\hbar}{i})^{2k} \oint d\sigma_{2k} = (-1)^{5k-1} \hbar^{2k} \frac{(2m)^{1/2-3k}}{\alpha} C_{2k,0} \frac{1}{U_0^{3k-1/2}} 2\pi \ . \tag{27}$$

Now we need to find the coefficient $C_{2k,0}$ explicitly. By inserting (22) with (23) in the recursion relation (12) we obtain

$$\sum_{k=0}^{n} C_{k,0} C_{n-k,0} - (2mU_0\alpha) C_{n-1,0} = \sum_{k=1}^{n-1} C_{k,0} C_{n-k,0} + 2C_{n,0} - (2mU_0\alpha) C_{n-1,0} = 0 \ , \tag{28}$$

from which we have

$$C_{k,0} = \frac{1}{2} [(2m\alpha U_0) C_{k-1,0} - \sum_{j=1}^{k-1} C_{j,0} C_{k-j,0}], \quad C_{0,0} = 1 \ . \tag{29}$$

¿From this equation one shows $C_{1,0} = m\alpha U_0$. Further, it easy to show that all higher odd coefficients vanish, $C_{2k+3,0} = 0$ for $k = 0, 1, 2, \ldots$. The solution of this equation for the remaining nonzero even coefficients is given by

$$C_{2k,0} = (-1)^k (2mU_0\alpha)^{2k} 2^{-2k} \binom{\frac{1}{2}}{k} \ , \tag{30}$$

which can be verified by direct substitution in equation (29) resulting in an identity for half integer binomial coefficients. Then the integral (27) can be written

$$(\frac{\hbar}{i})^{2k} \oint d\sigma_{2k} = (-1)\hbar^{2k} 2\pi\alpha^{2k-1}(2m)^{1/2-k}2^{-2k}\binom{\frac{1}{2}}{k}U_0^{k-1/2} = -\frac{1}{2}\binom{\frac{1}{2}}{k}\frac{2\pi\hbar}{B^{2k-1}} . \tag{31}$$

In conclusion, the WKB quantization to all orders (16) is

$$E_\nu^{(\infty)} = A[(\nu+\frac{1}{2}) + \frac{1}{2}\sum_{k=0}^{\infty}\binom{\frac{1}{2}}{k}\frac{1}{B^{2k-1}}]^2 . \tag{32}$$

Because $\sum_{k=0}^{\infty}\binom{\frac{1}{2}}{k}B^{1-2k} = \sqrt{1+B^2}$ we have $E_\nu^{ex} = E_\nu^{(\infty)}$, i.e. the WKB series converges to the exact result (8).

Now we can calculate the error in units of the mean level spacing $\Delta E_\nu = E_{\nu+1}^{ex} - E_\nu^{ex}$ between the exact level E_ν^{ex} and its WKB approximation $E_\nu^{(N)}$ to Nth order:

$$\frac{E_\nu^{ex} - E_\nu^{(N)}}{\Delta E_\nu} = \frac{1}{2}\sum_{k=N+1}^{\infty}\binom{\frac{1}{2}}{k}\frac{1}{B^{2k-1}} , \qquad \text{for } \nu \to \infty . \tag{33}$$

The limit clearly shows that even for arbitrarily small but finite $\hbar$ ($1 << B < \infty$), the relative error for any finite WKB approximation becomes constant on increasing ν, and scales as

$$\frac{E_\nu^{ex} - E_\nu^{(N)}}{\Delta E_\nu} \sim \frac{1}{2}\binom{\frac{1}{2}}{N+1}\frac{1}{B^{2N+1}} , \qquad B \to \infty . \tag{34}$$

Note that the limit $B \to \infty$ is equivalent to the limit $\hbar \to 0$.

3 Conclusions and discussion

For our present system we can conclude that to any finite order semiclassical approximation the error measured in units of the mean level spacing remains constant even if the quantum number increases indefinitely, contrary to the naive expectation, even if $\hbar$ is small but fixed and nonzero. This confirms the general statements made by Prosen and Robnik (1993). We have thus provided a clear demonstration that the semiclassical methods cannot predict the individual energy levels (and also their wavefunctions) within a vanishing fraction of the mean energy level spacing in the limit when the quantum number goes to infinity, $\nu \to \infty$, but $\hbar$ is small but fixed. Therefore we cannot expect the semiclassics at any nonzero value of $\hbar$ to correctly describe the fine structure of energy spectra manifested in the short range statistics like the energy level repulsion, which was predicted to be a purely quantum effect (Robnik 1986), later reconfirmed by Berry (1991). On the other hand Prosen and Robnik (1993) have shown that the long range statistics of the energy spectra are very well captured even by the lowest order semiclassical approximation. This is of course compatible with the very important semiclassical theory of delta statistics $\Delta(L)$ (spectral rigidity) by Berry (1985), employing the Gutzwiller periodic orbit theory (1990), where agreement with predictions of random matrix theories and with the experimental and numerical data has been obtained at large L. Also, Berry and Tabor (1977) have used torus quantization of integrable systems (with more than one degrees of freedom), predicting the Poissonian (exponential) energy level spacings distribution. Our results show that their result cannot be rigorous, especially as we know some counterexamples of integrable systems with non-Poissonian statistics (Bleher *et al* 1993), and also know that their approximation does not take into account the nonperturbative tunneling effects, but it is nevertheless a good heuristic argument explaining why *typically* we do observe Poissonian statistics in classically integrable systems. By typically we mean that the set of exceptions has a small or even vanishing measure.

We should emphasize again that the error of the torus quantization (which Berry and Tabor (1977) have used) and of the Gutzwiller trace formula (which obviously has generally the same quality as EBK quantization of classically integrable systems) scales as $\propto \hbar^2$, in the limit of fixed quantum numbers but $\hbar \to 0$. (This is the actual semiclassical limit in the strong sense.) In systems with f degrees of freedom the mean energy level spacing ΔE scales as $\hbar^f$ (due to the asymptotically exact Thomas-Fermi rule). Therefore, the error of the leading semiclassical approximation (EBK, Gutzwiller) measured in units of ΔE scales as $\hbar^{(2-f)}$. Thus it goes to zero only in one degree of freedom systems ($f = 1$), it is constant in two degrees of freedom ($f = 2$), and can even diverge for higher degrees of freedom ($f \geq 3$). Thus to improve the theoretical results we need higher corrections to the leading semiclassical terms. However, one should not forget that in order to explain quantal results $\hbar$ must be nonzero and fixed, however small, in which case the fine structure of energy spectra at scales smaller than certain characteristic range (a power of $\hbar$) cannot be correctly described.

The conclusion of this paper is that the semiclassical methods are just not good enough (at any order) to describe the fine structure of energy spectra and wavefunctions. Our approach leading to the above conclusion rests upon a systematic WKB expansion for the potential $V(x) = U_0/\cos^2(\alpha x)$ using the technique of Bender, Olaussen and Wang (1977). We are able to calculate all orders, the series is convergent and can be summed precisely to the exact result.

Acknowledgements

LS acknowledges the Alps-Adria Rectors Conference Grant of the University of Maribor. MR thanks Dr. Evgueni 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

In this appendix we show how to obtain the formulas (19) and (20). In all integrals of this section the limits of integration are between the two turning points. After substitution $z = \tan(\alpha x)$, we have

$$\begin{aligned}\int dx \frac{V'^2(x)}{\sqrt{E - V(x)}} &= \frac{4\alpha U_0^2}{\sqrt{U_0}} \int_{-\sqrt{\beta}}^{\sqrt{\beta}} dz \frac{z^2(z^2+1)}{\sqrt{\beta - z^2}} = \\ &= \frac{4\alpha U_0^2}{\sqrt{U_0}} (3\beta^2 + 4\beta)\frac{\pi}{8}) \ , \end{aligned} \tag{35}$$

where $\beta = (E - U_0)/U_0$. In conclusion we have

$$(\frac{\hbar}{i})^2 \oint d\sigma_2 = -\frac{\hbar^2 \alpha \pi}{8\sqrt{2mU_0}} = -\frac{2\pi\hbar}{4B} \ , \tag{36}$$

with $B = \sqrt{8mU_0}/(\alpha\hbar)$.

To obtain the formula (21) we proceed in the same way.

$$\begin{aligned}\int dx \frac{V''^2(x)}{\sqrt{E - V(x)}} &= \frac{4\alpha^3 U_0^2}{\sqrt{U_0}} \int_{-\sqrt{\beta}}^{\sqrt{\beta}} dz \frac{(9z^4 + 6z^2 + 1)(z^2+1)}{\sqrt{\beta - z^2}} = \\ &= \frac{4\alpha U_0^2}{\sqrt{U_0}} (45\beta^3 + 90\beta^2 + 56\beta + 16)\frac{\pi}{16} \ , \end{aligned} \tag{37}$$

¿From which we obtain

$$\frac{\partial^3}{\partial E^3} \int dx \frac{V''^2(x)}{\sqrt{E - V(x)}} = \frac{135\pi\alpha^3\sqrt{U_0}}{2U_0^2} \ . \tag{38}$$

For the last integral we have

$$\begin{aligned}\int dx \frac{V'^2(x)V''(x)}{\sqrt{E - V(x)}} &= \frac{8\alpha^3 U_0^2}{\sqrt{U_0}} \int_{-\sqrt{\beta}}^{\sqrt{\beta}} dz \frac{z^2(3z^2+1)(z^2+1)^2}{\sqrt{\beta - z^2}} = \\ &= \frac{8\alpha U_0^2}{\sqrt{U_0}} (105\beta^4 + 280\beta^3 + 240\beta^2 + 60\beta)\frac{\pi}{128} \ , \end{aligned} \tag{39}$$

from which we obtain

$$\frac{\partial^4}{\partial E^4}\int dx \frac{V'^2(x)V''(x)}{\sqrt{E-V(x)}} = \frac{315\pi\alpha^3\sqrt{U_0}}{2U_0^2} \ . \tag{40}$$

In conclusion we have

$$\begin{aligned} (\frac{\hbar}{i})^4 \oint d\sigma_4 &= \frac{\hbar^4}{(2m)^{3/2}}\frac{\alpha^3\sqrt{U_0}}{U_0^2}[\frac{1}{120}\frac{135}{2} - \frac{1}{288}\frac{315}{2}] = \\ &= \frac{\hbar^4\alpha^3\pi\sqrt{U_0}}{64(2m)^{3/2}U_0^2} = \frac{2\pi\hbar}{16B^3} \ . \end{aligned} \tag{41}$$

References

Bender C M, Olaussen K and Wang P S 1977 *Phys. Rev.* D **16** 1740

Berry M V 1985 *Proc. Roy. Soc. London A* **400** 229

Berry M V 1991 in *Chaos and Qunatum Physics*, eds. M.-J. Giannoni, A. Voros and J. Zinn-Justin (Amsterdam: North-Holland) 251

Berry M V and Tabor M 1977 *Proc. Roy. Soc. London A* **356** 375

Bleher P M, Cheng Zheming, Dyson F J and Lebowitz J L 1993 *Commun. Math. Phys.* **154** 433

Casati G and Chirikov B V 1995 *Quantum Chaos* (Cambridge: Cambridge University Press)

Dunham J L 1932 *Phys. Rev.* **41** 713

Einstein A 1917 *Verh. Dtsch. Phys. Ges.* **19** 82

Flügge S 1971 *Practical Quantum Mechanics I* (Berlin: Springer)

Graffi S, Manfredi V R and Salasnich L 1994 *Nuovo Cim.* B **109** 1147

Gutzwiller M C 1990 *Chaos in Classical and Quantum Mechanics* (New York: Springer)

Landau L D and Lifshitz E M 1973 *Nonrelativistic Quantum Mechanics* (Moscow: Nauka)

Maslov V P 1961 *J Comp. Math. and Math. Phys.* **1** 113–128; 638–663 (in Russian)

Maslov V P and Fedoriuk M V 1981 *Semi-Classical Approximations in Quantum Mechanics* (Boston: Reidel Publishing Company), and the references therein

Narimanov E 1995, private communication

Ozorio de Almeida A 1990 *Hamiltonian Systems: Chaos and Quantization* (Cambridge: Cambridge University Press)

Prosen T and Robnik M 1993 *J. Phys.* A **26** L37

Robnik M 1986 *Lecture Notes in Physics* **263** 120

Robnik M and Salasnich L 1996 "WKB Expansion for the Angular Momentum and the Kepler Problem: from the Torus Quantization to the Exact One", Preprint University of Maribor, CAMTP/96-4

Salasnich L and Robnik M 1996 "Quantum Corrections to the Semiclassical Quantization of a Nonintegrable System", Preprint University of Maribor, CAMTP/96-1

Voros A 1983 *Ann. Inst. H. Poincaré* A **39** 211