

Approximations to the eigenvalues of the Hamiltonian $P^2 + A \bmod X^{\nu}$ mod in the Weyl correspondence limit—a critical appraisal of Turschner's formula

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1979 J. Phys. A: Math. Gen. 12 L223

(<http://iopscience.iop.org/0305-4470/12/9/001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 30/05/2010 at 19:53

Please note that [terms and conditions apply](#).

LETTER TO THE EDITOR

Approximations to the eigenvalues of the Hamiltonian $P^2 + A|X^\nu|$ in the Weyl correspondence limit—a critical appraisal of Turschner's formula

B J B Crowley and T F Hill†

Department of Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, UK

Received 8 May 1979

Abstract. Accurate numerical calculations performed for the linear, quartic and square-well potentials ($V(X) = A|X^\nu|$, $\nu = 1, 4, \infty$) fail to confirm the recent claim by Turschner to have found an exact closed-form formula for the eigenvalues of the Hamiltonian $H(P, X) = P^2 + A|X^\nu|$ for any $\nu > 0$. The formula is found to be an approximation (except for $\nu = 2$). However, for the lowest eigenvalues of the potentials considered, it is found to be significantly more accurate than the simple WKB approximation based upon the Bohr-Sommerfeld integral. For $|\frac{1}{2} \ln(\frac{1}{2}\nu)|^2 \ll 1$ we suggest that Turschner's formula should be a valuable means of accurately estimating the lowest ($n \leq 2$) eigenvalues of $H(P, X)$ —particularly in view of its remarkable simplicity in these cases. For the higher eigenvalues ($n \geq 3$), the Bohr-Sommerfeld formula may be used without significant loss of accuracy. An examination of Turschner's theoretical arguments, in the light of these quantitative discrepancies, leads us to the following conclusion: the assumption that, in the Weyl correspondence, a bijective (i.e. one-to-one onto) canonical transformation in classical phase-space possesses an exact unitary representation in Hilbert space is, in general, without foundation. This leads us to associate the Weyl-correspondence limit with the semi-classical limit and to propose a criterion for a better correspondence principle. The technique used by Turschner in deriving his formula is a powerful one and should find wide application. However, in the absence of a suitable ('good') correspondence principle, the results yielded will in general be approximate.

1. Introduction

In an article recently published in this journal, Turschner (1979) claims to have derived an exact closed-form expression for the eigenvalues of the Hamiltonian $H(P, X) = P^2 + A|X^\nu|$ for $\nu > 0$. However, exact numerical calculations of the low-lying eigenvalues of the linear ($\nu = 1$) and quartic ($\nu = 4$) potentials fail to support this. In fact our calculations indicate significant errors of the order of a percent or less. Thus although Turschner's eigenvalue formula (1979 equation 4.14) (hereafter cited as T(4.14)) is undoubtedly an approximation for these cases, it is, at least for the low lying eigenvalues, an extremely good approximation. For the higher energy eigenvalues the approximations based upon the WKB (Bohr-Sommerfeld integral) formula are simpler to calculate and *may* be more reliable. A careful scrutiny of Turschner's theoretical argument has enabled us to identify the logical defect and to show that the result is, in fact, an approximation associated with the semi-classical limit.

† Permanent address: Atomic Energy Board, Pelindaba, Transvaal, South Africa.

2. Test of Turschner's formula

Using tables of zeros of the Airy function $Ai(x)$ and its derivative (Abramowitz and Stegun 1965 table 10.13) we are able to calculate with high precision the eigenvalues $E_n^{(1)}$ (for $n \leq 10$) of the linear ('V') potential as given by

$$-d^2\psi_n/dx^2 + (|x| - E_n^{(1)})\psi_n = 0 \tag{1}$$

for $x \in \mathbb{R}^{(1)}$. The results for the first three eigenvalues, $n = 0, 1, 2$, are compared with values calculated using T(4.14) in table 1. For reference, the WKB results obtained using the well-known Bohr-Sommerfeld formula,

$$\begin{aligned} (n + \frac{1}{2})\pi &= 2 \int_0^{E_n^{1/\nu}} (E_n - X^\nu)^{1/2} dX \\ &= 2E_n^{1/\nu+1/2} \int_0^1 (1 - q^\nu)^{1/2} dq, \end{aligned}$$

from which we obtain

$$E_n^{(\nu)} = \left(\left(n + \frac{1}{2} \right) \frac{\pi^{1/2}(\nu+2)\Gamma(\frac{1}{2} + \nu^{-1})}{2\Gamma(\nu^{-1})} \right)^{2\nu/(\nu+2)}, \tag{2}$$

are also given.

In the case of the quartic oscillator ($\nu = 4$) the ground-state energy $E_0^{(4)}$ calculated using T(4.14) is in disagreement with the exact result as calculated by Balian *et al* (1978) by the order of 3% (table 1).

More serious discrepancies between the exact theory and that of Turschner (1979) arise in the case of the infinite square-well potential

$$\begin{aligned} V^{(\infty)}(x) &= 0, & |x| < 1 \\ &= \infty, & |x| > 1 \end{aligned}$$

which corresponds to the limit $\nu \rightarrow \infty$, with $a = 1$, of T(4.10-4.14). For this case the exact eigenvalues $E_n^{(\infty)}$ of the Schrödinger equation expressed in units of $2m = \hbar = 1$ are well known to be given by

$$E_n^{(\infty)} = [(n + 1)\pi/2]^2,$$

Table 1. Eigenvalues of the Hamiltonian $P^2 + |X^\nu|$ in units in which $\hbar = 2m = 1$ compared with predictions of WKB and Turschner (1979) approximations.

Potential	ν	n	E_n exact	\tilde{E}_n calculated using T(4.14)	E_n^{WKB} calculated using equation (2)
Linear	1	0	1.01879297	1.00697648	1.11546024
		1	2.33810741	2.34961178	2.32025079
		2	3.24819758	3.24470198	3.26162552
Quartic	4	0	1.060	1.032	0.867
Square well	1	0	2.467	1.234	0.617
		1	9.870	6.169	5.552
		2	22.207	16.038	15.421

whereas T(4.14) which in the limit $\nu \rightarrow \infty$ takes the form

$$\tilde{E}_n^{(\infty)} = \pi^2 \frac{(-1)^n}{n!} \frac{d^n}{ds^n} \left(\frac{(2+s)^n}{s^3} \right)_{s=2}, \tag{3}$$

yields $\tilde{E}_n^{(\infty)} = \pi^2/8, 5\pi^2/8, 13\pi^2/8, \dots$ for $n = 0, 1, 2, \dots$ respectively. This is in marked disagreement with the exact eigenvalues $E_n^{(\infty)} = \pi^2/4, \pi^2, 9\pi^2/4, \dots$. It is perhaps significant that, for this potential, the WKB also yields poor results, for low values of n , in the form of $E_n^{(\infty)WKB} = [(n + \frac{1}{2})\pi/2]^2$.

In passing, we note that T(4.14) predicts that the ratio $E_n^{(\nu)}/E_m^{(\nu)}$ of any two eigenvalues of the Hamiltonian $P^2 + |X^\nu|$, where ν is a rational number, is itself a rational number (for finite m, n). This would indeed have been a surprising result were it to have been exactly true.

It is thus established beyond doubt that, in the context of non-relativistic quantum theory, Turschner's (1979) theory is, in general, approximate. This should not however detract excessively from the value of the formula T(4.14), which offers a simple means of calculating the lowest eigenvalues of a wide class of Hamiltonians (for ν not too large[†]), in an approximation which offers a significant improvement in accuracy over WKB. It would be unfortunate if our criticisms led to a failure to recognize the importance of the technique as a powerful tool in obtaining high quality semi-classical approximations to a wide range of bound-state eigenvalue problems.

3. Theoretical discussion

Evidently the theoretical arguments given in Turschner (1979) contain a flaw. This we have been able to identify, but only after carefully eliminating all other possibilities. We could find no errors[‡] of manipulation in the formalism as presented in the paper and, in view of our numerical results, this brings into question the underlying assumptions of the method.

The essence of the method is as follows: starting from a quantum-mechanical Hamiltonian, $H(P, X)$, the corresponding classical Hamiltonian $h(p, x)$ is obtained using the Weyl correspondence rules (Cahill and Glauber 1969). By means of a bijective (one-to-one and onto) canonical transformation in classical phase space, this Hamiltonian is mapped onto a new Hamiltonian, $\tilde{h}(|\tilde{p}^2 + \tilde{x}^2|)$ whose constant energy surfaces in phase space are circles. Inversion of the correspondence procedure yields, from \tilde{h} , the Hamiltonian $\tilde{H}(N)$, where $N = \frac{1}{2}(X - iP)(X + iP) = \frac{1}{2}(X^2 + P^2 - 1)$, whose eigenvalues are just $\tilde{H}(n)$ ($n = 0, 1, 2, \dots$). Thus, if the transformation $H \rightarrow \tilde{H}$ is unitary, H and \tilde{H} have the same spectrum and the eigenvalues of H are given by the function $\tilde{H}(n)$. The validity of the result thus depends only upon the existence of a linear unitary transformation connecting H and \tilde{H} . We are therefore able to conclude that, in general, such a unitary transformation does not exist.

The postulate of Turschner, that H and \tilde{H} are related by a unitary transformation, depended upon two conjectures, namely:

[†] The parameter $\gamma = \frac{1}{2} \ln \left(\frac{1}{2}\nu \right) = \tanh^{-1} [2\nu/(\nu + 2) - 1]$ provides a useful guide to the quality of the approximation. The formula is exact (all n) for $\gamma = 0$, and becomes progressively poorer as $|\gamma|$ increases. The approximation should be good for $|\gamma|^2 \ll 1$.

[‡] Other than inconsequential typographical errors such as T(2.2) which should read

$$D(\alpha) = \exp(\alpha a^\dagger - \alpha^* a)$$

(i) that the mapping $h(p, x) = \bar{h}(|\bar{p}^2 + \bar{x}^2|)$ may be achieved by a bijective canonical transformation in phase space.

(ii) that a bijective canonical transformation in classical phase-space of a classical function $f(x, p)$ is equivalent to a unitary transformation of the quantum-mechanical operator related to $f(x, p)$ by the Weyl correspondence.

In order to test assumption (i) we derived explicit forms of a canonical transformation which transforms the constant energy surfaces of $h(p, x) = p^2 + |x^\nu|$ into circles in the \bar{p}, \bar{x} plane. Using plane polar coordinates $\bar{r}, \bar{\theta}$ to span the symplectic manifold $\{\bar{p}, \bar{x}\}$, such that $\bar{x} + i\bar{p} = \bar{r} e^{i\bar{\theta}}$, these are as follows:

$$\bar{r} = (8b_\nu)^{1/2} (p^2 + x^\nu)^{(\nu+2)/4\nu} \quad (4a)$$

$$\bar{\theta} = \frac{1}{2}\pi I(p^2/(p^2 + x^\nu); \frac{1}{2}, \nu^{-1}) \quad (4b)$$

for $p \geq 0, x \geq 0, 0 \leq \bar{\theta} \leq \pi/2$, where

$$b_\nu = \frac{1}{2\pi} \int_0^1 dt (1-t^\nu)^{1/2} = \frac{1}{2\pi(\nu+2)} B(1; \frac{1}{2}, \nu^{-1})$$

and

$$I(\xi; a, b) = B(\xi; a, b)/B(1; a, b)$$

and $B(\xi; a, b)$ is the *incomplete beta function* (Abramowitz and Stegun 1965 § 6.6),

$$B(\xi; a, b) = \int_0^\xi t^{a-1} (1-t)^{b-1} dt.$$

The complete beta function (Abramowitz and Stegun 1965 § 6.2) is

$$B(1; a, b) = \Gamma(a)\Gamma(b)/\Gamma(a+b).$$

The transformation (4) maps the quadrant $p \geq 0, x \geq 0$ onto the quadrant $0 \leq \bar{\theta} \leq \pi/2$. The complete transformation which includes the remaining quadrants follows by using the reflection symmetry about the $p = 0, x = 0$ and $\bar{p} = 0, \bar{x} = 0$ axes. From (4a) it is clear that this transformation maps the constant energy surfaces $p^2 + |x^\nu|$ onto circles ($\bar{r} = \text{constant}$) in $\{\bar{p}, \bar{x}\}$. It is straightforward to show that the Jacobian

$$|\partial(\bar{x}, \bar{p})/\partial(x, p)| = \bar{r} |\partial(\bar{r}, \bar{\theta})/\partial(x, p)|$$

is everywhere equal to unity, thus demonstrating that the transformation is area preserving and therefore canonical. The transformation and its inverse are one-to-one, and are defined for all $\{x, p\} \in \mathbb{R}^{(2)}$ and $\{\bar{x}, \bar{p}\} \in \mathbb{R}^{(2)}$. It is therefore bijective. Having thus demonstrated assumption (i) to be justified for all Hamiltonians $h(p, x)$ of the form $h(p, x) = p^2 + |x^\nu|$, we deduce that assumption (ii) cannot in general be justified.

We conclude therefore that the conjecture 'that a bijective canonical transformation in classical phase-space possesses, in the Weyl correspondence, an exact unitary representation in quantum-mechanical Hilbert space', is not in general true.† However the quantum-mechanical operators corresponding to bijective canonical transformations are, as they must be, unitary in the semi-classical limit. This suggests that approximating the quantum-mechanical operators by unitary ones is a kind of semi-classical approximation (see Appendix), and accounts for the observed correlation between the errors arising from use of the WKB approximation (2) and those arising from use of T(4.14). However it is not clear that the 'Weyl correspondence limit' is

† See Appendix.

equivalent to the 'semi-classical limit', particularly as the theories appear incompatible in so far as the treatment of complex trajectories (e.g. Balian *et al* 1978) is concerned. We do note however that the result of applying T(4.14) to the ground state of the quartic oscillator (table 1) is in good agreement with the zero-order semi-classical calculation of Balian *et al* (1978) when the contribution δ from complex trajectories is included.

Finally, we propose that the criterion for a 'good' correspondence principle (should it exist) be that all bijective canonical mappings in classical phase-space should possess a unitary representation in quantum mechanics. With such a correspondence principle, the basic method of Turschner (1979) (as outlined above) would be exact.

The authors are grateful to Brian Buck for discussions. This work was carried out with support from the Science Research Council (UK) and the South African Council for Scientific and Industrial Research.

Appendix

The defect in Turschner's 'proof' of the unitary equivalence of the Hamiltonians H and \bar{H} is as follows. (Following Turschner, we let $\mathcal{H}^{(2)}$ denote the Hilbert space of Hilbert-Schmidt operators acting on $\mathcal{H}^{(1)}$, $\mathcal{H}^{(1)}$ being the Hilbert space of quantum states of the system.) Although it is shown by Turschner (1979 (4.7 *et seq.*)) that the operator U which relates H and \bar{H} is a unitary operator on $\mathcal{H}^{(2)}$, it is not shown that U is equivalent to a unitary operator on $\mathcal{H}^{(1)}$. This requires establishing the existence of a unitary operator A acting on $\mathcal{H}^{(1)}$ such that $\bar{H} (=UH) = AHA^\dagger$. In general, such an operator A cannot be found.

The Weyl correspondence is defined by the set of operators $\{T(\alpha)\}$ which, for α spanning $\{p, x\}$, comprise a complete orthonormal basis spanning $\mathcal{H}^{(2)}$. This provides a representation of an operator $F \in \mathcal{H}^{(2)}$ in terms of the corresponding classical function $f(\alpha)$ in the manner of T(2.5a and 2.8). The operator U on $\mathcal{H}^{(2)}$ is defined by the relation (T(3.4))

$$UT(\alpha) = T(\bar{\alpha}) = T(g(\alpha)) \forall \alpha$$

where $\bar{\alpha} = g(\alpha)$ defines a bijective canonical transformation in classical phase space. For the operator U to be equivalent to a unitary transformation on $\mathcal{H}^{(1)}$ there must exist an operator A acting on $\mathcal{H}^{(1)}$ such that

$$UT(\alpha) = AT(\alpha)A^\dagger \quad \forall \alpha, \tag{5}$$

i.e. A must be independent of α .

The operator T is defined by (T(2.1))

$$T(\alpha) = 2D(\alpha)(-1)^{a^\dagger a}D(-\alpha) \tag{6}$$

where $D(\alpha)$ is the displacement operator (Cahill and Glauber 1969 equation 2.11) and a is the operator $2^{-1/2}(Q + iP)$. Using the unitary property of $D(\alpha)$ (Cahill and Glauber 1969 equation 2.12) an operator $A(\alpha)$ satisfying (5) above is easily deduced to be

$$\begin{aligned} A(\alpha) &= D(g(\alpha))D^\dagger(\alpha) \\ &= D(\bar{\alpha})D(-\alpha) \\ &= D(\bar{\alpha} - \alpha) \exp[i \operatorname{Im}(\bar{\alpha}^* \alpha)] \end{aligned}$$

(using Cahill and Glauber 1969 equations 2.12 and 2.19). Note that the unitary operator $A'(\alpha) = A(\alpha) \exp(i\Phi(\alpha))$, where $\text{Im } \Phi(\alpha) = 0$, is equivalent to A . In general it is not possible to find an operator A , independent of α , that satisfies (5). However, we note the following exceptions:

(i) $g(\alpha) = \alpha + c$ (constant displacement in phase-space) when $A = D(c)$;

(ii) $g(\alpha) = \alpha \exp i\phi$ (fixed rotation in phase-space) when $A = \exp(i\phi a^\dagger a)$;

(iii) $g(\alpha) = \alpha^*$ when A is the time-reversal operator which is *anti-unitary* but which preserves the spectrum of a time-reversal invariant Hamiltonian.

(iv) In the semi-classical limit, it follows from Cahill and Glauber (1969 equation 6.35) (with $s = 0$) that $T(\alpha)$ is diagonal in the representation defined by the eigenstates ($\in \mathcal{H}^{(1)}$) of the operator a , and that the matrix elements of $T(\alpha)$ are then δ -functions in α . That is, the matrix elements of $T(\alpha)$ are of the form

$$\langle \beta | T(\alpha) | \gamma \rangle \underset{\hbar \rightarrow 0}{\sim} \delta(\beta - \gamma) \delta(\beta - \alpha) T_\beta.$$

A unitary operator A that is independent of α is then easily found to be

$$\begin{aligned} A &= \int D(g(\beta)) D^\dagger(\beta) |\beta\rangle\langle\beta| \pi^{-1} d^2\beta \\ &= \int |g(\beta)\rangle\langle\beta| \pi^{-1} d^2\beta, \end{aligned}$$

where $|\beta\rangle \in \{|\beta\rangle \in \mathcal{H}^{(1)} | a|\beta\rangle = \beta|\beta\rangle\}$ which is the complete set of eigenstates of a and which provides a representation of the identity operator through

$$1 = \int |\beta\rangle\langle\beta| \pi^{-1} d^2\beta$$

(Cahill and Glauber 1969 equation 2.27). We have also made use of the following properties of D :

$$D(\beta)|0\rangle = |\beta\rangle \quad \text{and} \quad D^\dagger(\beta)|\beta F\rangle = |0\rangle$$

(Cahill and Glauber 1969 equations 2.12 and 2.19–20). The existence of a unitary operator A (that is independent of α) in the semi-classical limit explains why the method yields good results consistent with the semi-classical approximation.

References

- Abramowitz M and Stegun I A 1965 *Handbook of Mathematical Functions* (New York: Dover)
 Balian R, Parisi G and Voros A 1978 *Phys. Rev. Lett.* **41** 1141–4
 Cahill K E and Glauber R J 1969 *Phys. Rev.* **177** 1857–81
 Turschner H 1979 *J. Phys. A: Math. Gen.* **12** 451–7