# WKB wave functions without matching

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A method is presented for the construction of WKB wave functions that avoids explicit consideration of any matching between results pertaining to classically allowed and classically forbidden regions. The formalism is based on the maximization of a suitably defined quantal pseudoentropy, subject to the constraints posed by the expectation values of a reduced number of operators, which are evaluated according to special WKB techniques that consider expansions up to orders $\hbar$ and $\hbar^2$. The algorithm is tested with reference to the harmonic and quartic anharmonic oscillators.

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## I. INTRODUCTION

Semiclassical methods, although already introduced in the early days of quantum mechanics, enjoy still wide popularity [1–6], as they are usually able to provide us with analytical expressions that pave the way for an approximate description of the mechanisms underlying some physical phenomena. Foremost among these methods is the WKB approximation [7], which still receives the attention of different investigators because it constitutes one of the most useful available tools in facing a variety of problems [1], and has even found some place among quite contemporary developments [8–16].

Recently, a detailed review of the WKB method has been presented [5] that enables one to appropriately relate it to other semiclassical approaches such as the Wigner-Kirkwood (WK) approach [17,18]. As it is well known, the WKB approximation constitutes a valid theoretical tool as long as characteristic actions of the problem at hand are large in relation to $\hbar$. In the study referred to above [5], the "smallness" of $\hbar$ is exploited in two different fashions, namely, (i) to obtain an explicit $\hbar^2$ expansion, and (ii) to "smooth" the level density. The first aspect corresponds to the usual WKB expansion which has been treated according to the Dunham formalism [19–21]. The second facet provides the connection between WKB and WK.

From a practical point of view, the treatment developed in Ref. [5] yields a quite convenient recipe for evaluating expectation values, something which, as remarked by Landau and Lifschitz, constitutes a serious difficulty in dealing with semiclassical approaches [7]. Nevertheless, this treatment does not allow for an explicit semiclassical expansion of the wave function. It is true that the usual WKB formulation does yield such an expansion, by recourse to the pertinent connection formulas at the turning points. However, the concomitant effort to be invested is often greater than the one related to dealing with the exact quantal derivation [5].

It would be of interest to have at our disposal the advantages of the WKB formulation derived in Ref. [5], while, at the same time, being able to obtain a corresponding semiclassical wave function. This is just the motivation of the present effort. It has recently been shown [22] that starting with the knowledge of a few expectation values, application of information-theory (IT) tools enable one to *infer* reasonably good wave functions. By recourse to a suitable defined "quantal" entropy that measures the lack of information associated with the probability distribution of a quantum state over a given known basis, this inference approach allows for a variety of interesting applications [22–25].

The objective of the present paper is to incorporate to the developments of Ref. [5] the IT tools advanced in Ref. [22] so as to obtain inferred WKB one-dimensional wave functions that will not exhibit any kind of divergence at the turning points. In addition, the techniques for incorporating corrections of the order of $\hbar^2$ can easily be accommodated within the scheme to be presented and help one to understand their significance.

The paper is organized as follows. A brief review of WKB concepts is presented in Sec. II. A summary of the method for inferring wave functions by maximizing the quantal pseudoentropy is given in Sec. III. Our present proposal is introduced in Sec. IV and applied to the harmonic oscillator and the anharmonic one in Sec. V. Finally, some conclusions are drawn in Sec. VI.

## II. WKB EXPECTATION VALUES

Following the method proposed in Refs. [5,21] and using a first-order perturbation theory, the expectation value of a given one-body operator for a given level of en-

 

ergy $\varepsilon$ can be computed as

$$\langle F\rangle_\varepsilon = \lim_{\lambda\to 0}\frac{1}{\lambda}[\varepsilon(V+\lambda F)-\varepsilon(V)]\ , \tag{2.1}$$

where $\varepsilon(V+\lambda F)$ is the eigenvalue of the energy when a term $\lambda F$ is added to the potential $V$.

The eigenvalues of the energy are determined by requiring

$$S(\varepsilon_n,V,\hbar)=(n+\tfrac{1}{2})h\ , \tag{2.2}$$

where $n$ is the number of zeros of the exact wave function. The $S$ function is defined as

$$S=\oint(\chi+i\hbar\chi_1)dz\ , \tag{2.3}$$

where $\chi$ is the solution of the Ricatti equation, and the contour integration in the complex $z$ plane encloses the segment of the real axis between the turning points.

The semiclassical WKB approximation is recovered by assuming that $\chi$ (therefore also $S$ and $\varepsilon_n$) admits a power expansion in $\hbar$,

$$S=\sum_{m=0}^{\infty}(i\hbar)^{2m}S_m(\varepsilon_n,V,\hbar)\ , \tag{2.4}$$

and

$$\varepsilon=\varepsilon_0+\hbar^2\varepsilon_1+\ \cdots\ . \tag{2.5}$$

Equation (2.1) can be rewritten as

$$\langle F\rangle_\varepsilon=\frac{-\delta S(F,\varepsilon)}{\dfrac{\partial S}{\partial\varepsilon}} \tag{2.6}$$

with

$$\delta S(F,\varepsilon)=\lim_{\lambda\to 0}[S(\varepsilon,V+\lambda F)-S(\varepsilon,V)]/\lambda\ . \tag{2.7}$$

The expansion of $S$ and $\varepsilon_n$ can be truncated at order $\hbar^2$ and allowing for the explicit expressions of $S$ [5], the expectation value of one-body operators for one-dimensional systems can be written as

$$\langle F\rangle_\varepsilon=\frac{\oint\dfrac{F}{\sqrt{\varepsilon_0-V}}dz}{\oint\dfrac{1}{\sqrt{\varepsilon_0-V}}dz}-\hbar^2\left\{\frac{\frac{1}{16}\oint\dfrac{V''F}{(\varepsilon_0-V)^{5/2}}dz+\frac{5}{64}\oint\dfrac{V'^2F}{(\varepsilon_0-V)^{7/2}}dz+\frac{1}{2}\dfrac{d}{d\varepsilon_0}\left[\varepsilon_1\oint\dfrac{F}{(\varepsilon_0-V)^{1/2}}dz\right]}{\oint\dfrac{1}{(\varepsilon_0-V)^{1/2}}dz}\right\}$$
$$+O(\hbar^4)+\ \cdots\ , \tag{2.8}$$

where $\varepsilon_0$ is the eigenenergy (order $\hbar$), determined using (2.2),

$$\oint\sqrt{\varepsilon_0-V}\ dz=(n+1/2)h\ , \tag{2.9}$$

and $\varepsilon_1$ is the correction of order $\hbar^2$ of the eigenenergy

$$\varepsilon_1=-\frac{1}{24}\frac{\oint\dfrac{V''}{(\varepsilon_0-V)^{3/2}}dz}{\oint\dfrac{1}{(\varepsilon_0-V)^{1/2}}dz}\ . \tag{2.10}$$

All the contour integrations of (2.8) and (2.10) can be computed in the real axis, evaluating derivatives with respect to the energy:

$$\frac{d}{d\varepsilon_0}\oint(\varepsilon_0-V)^{-n/2}dz=-n/2\oint(\varepsilon_0-V)^{-(n+2/2)}dz\ , \tag{2.11}$$

and using

$$\oint dz=2\int_{x_-}^{x_+}dx\ , \tag{2.12}$$

where $x_\pm$ are the turning points.

If the integrals in the real axis are not analytical, the $\hbar^2$ corrections of $\langle F\rangle_\varepsilon$ [cf. Eq. (2.8)], imply the numerical computation of fourth-order derivatives, with the subsequent loss of accuracy. In that case we compute all the integrals of (2.8) in the complex $z$ plane. As in Ref. [26], for a potential with two turning points, $z_1$ and $z_2$, one chooses a path $C$ that encloses $z_1$ and $z_2$. It is assumed that the potential $V$ is both single valued and analytic on $C$ and in all regions enclosed by $C$. We have tested this method for the harmonic-oscillator potential. In this case the integrals of (2.8) for an operator $x^n$ are analytical. We have also controlled that the results are independent of the integration contour.

## III. ON INFERRING QUANTUM WAVE FUNCTIONS

Consider a system described by a Hamiltonian $\hat{H}$. Let $\{\hat{O}_\alpha,\alpha=1,\ldots,m\}$ be a set of (relevant) independent commuting operators, diagonal in the common basis $\{|j\rangle,j=1,\ldots,k\}$. It has been shown in Ref. [22] that the ground state of the system denoted by $|0\rangle$ can be *inferred* to be of the form

$$|0\rangle=\sum_j C_j^{(0)}|j\rangle\ , \tag{3.1}$$

with

$$|C_j^{(0)}|^2=\exp\left\{-\left[\lambda_0+\sum_{\alpha=1}^{n}\lambda_\alpha O_\alpha(j)\right]\right\}\ , \tag{3.2}$$

where $O_\alpha(j)=\langle j|\hat{O}_\alpha|j\rangle$ and the $\lambda_\alpha$ constitute a set of optimizable parameters. Normalization is ensured by setting

$$\lambda_0=\ln\sum_j \exp\left[-\sum_\alpha \lambda_\alpha O_\alpha(j)\right] . \tag{3.3}$$

The square moduli (3.2) have the functional form that maximizes the so-called *quantal* entropy [22–25] (not to be confused with the ordinary, thermodynamic entropy, which vanishes for a pure state)

$$S=-\sum_j |C_j^{(0)}|^2 \ln|C_j^{(0)}|^2 , \tag{3.4}$$

subject to the constraints

$$\langle \hat{O}_\alpha\rangle \equiv \langle 0|\hat{O}_\alpha|0\rangle = o_\alpha . \tag{3.5}$$

The information entropy (3.4) obviously differs from the conventional one and measures the lack of information concerning the probability distribution over the common basis, vanishing only if $|0\rangle$ coincides with one of the basis states. It has been shown in Refs. [23] and [25] that a very accurate description of the ground state of various many-body systems can be achieved in this way by recourse to just a few relevant one-body and two-body operators $\hat{O}_\alpha$ for all values of the pertinent coupling constants, *including* transitional regions. Application of this method to one-dimensional problems is made in Ref. [22]. The discussion of how to deal with energy spectra and excited states can be found in Refs. [24] and [27]. The main point of the method reviewed here is to infer an appropriate wave function on the basis of a few pertinent expectation values by recourse to the maximum- (quantal) entropy principle (MEP).

In the one-dimensional case one assumes to know the ground-state expectation values $g_i$ of $n$ linearly independent functions $G_i$ of the coordinate $x$,

$$g_i=\langle G_i(x)\rangle=\int_{-\infty}^{\infty}\psi^2(x)G_i(x)dx . \tag{3.6}$$

The least biased wave function (for the ground state) adopts the appearance [22]

$$\psi(x)=\exp\left\{-\tfrac{1}{2}\left[\lambda_0+\sum_{i=1}^{n}\lambda_i G_i(x)\right]\right\} , \tag{3.7}$$

with

$$\lambda_0=\ln\left\{\int_{-\infty}^{\infty}\exp\left[-\sum_{i=1}^{n}\lambda_i G_i(x)\right]dx\right\} , \tag{3.8}$$

where the Lagrange multipliers $\lambda_i$ are to be obtained as the solutions of the system of equations

$$\frac{\partial\lambda_0}{\partial\lambda_i}=-g_i . \tag{3.9}$$

For additional details the reader is referred to Refs. [22–25]. In what follows the figures $g_i$ will correspond to expectation values of powers of $x$ evaluated according to the WKB0 (order $\hbar$) and WKB2 (order $\hbar^2$) prescriptions of Krivine, Casas, and Martorell [5], out of which we shall infer quantum wave functions in the fashion described in the present section.

## IV. PRESENT APPROACH

We shall consider one-dimensional potentials $V(x)$ and Hamiltonians of the form $\hat{H}=\frac{1}{2}\hat{p}^2+V(x)$. We follow the WKB prescriptions of Krivine, Casas, and Martorell [5] and obtain pertinent expectation values of $\hat{x}^{2n}$ ($n$ integer) both to order $\hbar$ (WKB0) and to order $\hbar^2$ (WKB2). With these values for the moments of the powers of $x$ we can infer ground-state wave functions by recourse to the ideas expounded in the previous section [22]. For excited states, we consider the series of functions $\psi_0(x)$, $x\psi_0(x)$, $x^2\psi_0(x)$, $x^3\psi_0(x),\ldots$, with $\psi_0$ of the form (3.7). By recourse to Schmidt's orthonormalization procedure we obtain a concomitant series of orthogonal wave functions and the approximate positions of the pertinent zeros for the excited states. The new wave functions are of the familiar form (polynomial in $x$) times (exponential) which satisfy a relative maximum-entropy principle [27]. By recourse to the appropriate WKB0 and WKB2 expectation values, we optimize the wave functions inferred for the excited states by suitably adjusting the Lagrange multipliers $\lambda_i$. Some loss of orthogonality (which is mainly due to the fact that we employ as input information the WKB mean values) ensues, which is largely compensated, as we shall see below, by the quality of the inferred wave functions.

The simple procedure here outlined yields semiclassical wave functions for the ground and excited states *without any "quantum" input.* All the information provided is of a semiclassical origin. We thus extend here the methodology of Krivine, Casas, and Martorell [5], by dealing with WKB wave functions that are obtained without any consideration to the position of the turning points. No "matching" of any kind is necessary [7]. With the rather small effort of evaluating a few WKB expectation values we infer a corresponding wave function, whose quality will be discussed in what follows, by reference to some concrete (and important) examples.

## V. APPLICATIONS

### A. Harmonic oscillator

Any decent approach to the quantum problem should work quite well when applied to the harmonic oscillator (HO). As the concomitant energies are well predicted by the WKB approach, some people tend to believe that this technique is indeed successful here. This belief is actually unjustified.

Let us consider the orthodox WKB treatment of the HO, as expounded, for example, in Ref. [29]. We find the following anomalies concerning the concomitant wave functions for the different HO states. (i) They are defined only between the turning points. A quite complicated matching procedure is necessary in order to have a wave function defined over the whole coordinate range. (ii) The virial theorem is violated as the $\langle x^2\rangle$ value is wrong.

The WKB described by Krivine, Casas, and Martorell, although not able to provide us with a wave function, does yield the exact value for $\langle x^2\rangle$ (the virial theorem holds).

TABLE I. Harmonic oscillator. The overlap $\langle\psi(N=1)|\psi(N=3)\rangle$ and the transition probability $|\langle\psi(N=1)|x^2|\psi(N=3)\rangle|^2$ evaluated in different WKB environments are compared to the exact values. $N$ is the phonon number.

| Method | Overlap (%) | Transition probability |
|---|---|---|
| Orthodox WKB | 14 | 0.0803 |
| Present approach (WKB0) | 0.20 | 1.0513 |
| Present approach (WKB2) | 0.3 | 1.2299 |
| Quantal (exact) | 0.0 | 1.50 |

Table I neatly illustrates some of the shortcomings of the orthodox WKB approach. It is clearly seen that the present approach undoubtedly yields much better results.

A few remarks are in order here. It is well known that the inferred wave functions become exact if one provides, for the HO, the IT algorithm with just the correct expectation value of $\hat{x}^2$ [22]. We have evaluated the (inferred) WKB0 (order $\hbar$) and WKB2 (order $\hbar^2$) wave functions by introducing, as inputs, the pertinent (WKB0 and WKB2) expectation values of both $\hat{x}^2$ and $\hat{x}^4$. This entails, of course, the introduction of partially wrong information into our inference scheme, as the WKB0 and WKB2 predictions for $\langle x^4\rangle$ do not coincide with the exact ones.

A more complete set of results is displayed in Table II, where expectation values evaluated in different WKB environments are compared. We exhibit here the moments $\langle x^2\rangle$, $\langle x^4\rangle$, $\langle x^6\rangle$, and $\langle x^8\rangle$, evaluated according to (i) the orthodox WKB approach (as outlined, for example, in Ref. [28]), to (ii) the WKB0 and WKB2 recipes of Krivine, Casas and Martorell [5], and to (iii) the inference procedure that constitutes the leitmotiv of the present effort. In this last case, the appropriate WKB0 and WKB2 expectation values of $\hat{x}^2$ and $\hat{x}^4$ constitute the input to the inference algorithm described in Sec. III.

As a general conclusion it can be fairly stated that our methodology does provide, in most cases, better results than the alternative techniques discussed here. Excited states are better described than the ground state, as a consequence of the fact that WKB fares poorly, as it is well known, in this particular instance [5]. It is also seen that inferences based upon WKB results evaluated up to order $\hbar^2$ are almost always better than those based upon expectation values evaluated just up to order $\hbar$. Notice also that present inferred results approach the quantum ones in a closer fashion than the original WKB values (except for two instances corresponding to the ground state).

### B. Anharmonic oscillator

We consider now the celebrated one-dimensional quartic anharmonic oscillator

$$\hat{H}=\tfrac{1}{2}(\hat{p}^2+\hat{x}^2)+\gamma\hat{x}^4\ , \tag{5.1}$$

TABLE II. Harmonic oscillator. Expectation values of several powers of the coordinate evaluated according to different WKB prescriptions are compared to the exact results. IW denotes an inferred wave function.

| | Expectation value | | | | | |
|---|---|---|---|---|---|---|
| Moment | WKB orthodox | Quantal (exact) | WKB0 (Ref. [5]) | WKB0 (IW) | WKB2 (Ref. [5]) | WKB2 (IW) |
| | | | $N=0$ | | | |
| $\langle x^2\rangle$ | 0.410 71 | 0.50 | 0.50 | 0.50 | 0.50 | 0.50 |
| $\langle x^4\rangle$ | 0.290 62 | 0.750 | 0.375 | 0.375 | 0.5625 | 0.5625 |
| $\langle x^6\rangle$ | 0.236 09 | 1.875 | 0.3125 | 0.336 79 | 1.093 75 | 0.878 26 |
| $\langle x^8\rangle$ | 0.203 79 | 6.5625 | 0.273 44 | 0.341 56 | 2.187 50 | 1.679 20 |
| | | | $N=1$ | | | |
| $\langle x^2\rangle$ | 1.542 78 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 |
| $\langle x^4\rangle$ | 3.222 11 | 3.75 | 3.375 | 3.375 | 3.5625 | 3.5625 |
| $\langle x^6\rangle$ | 7.667 52 | 13.125 | 8.4375 | 9.764 98 | 10.7812 | 11.3200 |
| $\langle x^8\rangle$ | 19.5068 | 59.0625 | 22.1484 | 33.8262 | 39.3750 | 44.4018 |
| | | | $N=2$ | | | |
| $\langle x^2\rangle$ | 2.658 33 | 2.5 | 2.5 | 2.5 | 2.5 | 2.5 |
| $\langle x^4\rangle$ | 9.676 15 | 9.75 | 9.375 | 9.375 | 9.5625 | 9.5625 |
| $\langle x^6\rangle$ | 38.6282 | 46.875 | 39.0625 | 41.4318 | 42.9687 | 44.0726 |
| $\langle x^8\rangle$ | 163.170 | 269.063 | 170.898 | 209.546 | 218.750 | 237.161 |
| | | | $N=3$ | | | |
| $\langle x^2\rangle$ | 3.762 83 | 3.5 | 3.5 | 3.5 | 3.5 | 3.5 |
| $\langle x^4\rangle$ | 19.5953 | 18.75 | 18.375 | 18.375 | 18.5625 | 18.5625 |
| $\langle x^6\rangle$ | 111.017 | 118.125 | 107.188 | 112.405 | 112.656 | 115.231 |
| $\langle x^8\rangle$ | 659.180 | 846.563 | 656.523 | 775.373 | 750.312 | 810.048 |

TABLE III. Anharmonic quartic oscillator ($\gamma=1$). Expectation values of $x^2$, $x^4$, $x^6$, and $x^8$ evaluated according to different prescriptions. $N$ is the principal quantum number. IW denotes an inferred wave function.

| | Expectation value | | | | | |
|---|---|---|---|---|---|---|
| Moment | Quantal (exact) | Quantal (IW) | WKB0 (Ref. [5]) | WKB0 (IW) | WKB2 (Ref. [5]) | WKB2 (IW) |
| | | | $N=0$ | | | |
| $\langle x^2\rangle$ | 0.257 15 | 0.257 15 | 0.295 57 | 0.295 57 | 0.295 12 | 0.295 12 |
| $\langle x^4\rangle$ | 0.182 21 | 0.182 21 | 0.136 21 | 0.136 21 | 0.142 40 | 0.142 40 |
| $\langle x^6\rangle$ | 0.201 13 | 0.200 56 | 0.070 40 | 0.076 09 | 0.135 93 | 0.084 57 |
| $\langle x^8\rangle$ | 0.293 93 | 0.291 07 | 0.038 33 | 0.048 32 | 0.167 98 | 0.057 55 |
| | | | $N=1$ | | | |
| $\langle x^2\rangle$ | 0.662 93 | 0.662 93 | 0.657 90 | 0.657 90 | 0.659 55 | 0.659 55 |
| $\langle x^4\rangle$ | 0.691 66 | 0.691 66 | 0.681 86 | 0.681 86 | 0.684 56 | 0.684 56 |
| $\langle x^6\rangle$ | 0.962 35 | 0.960 90 | 0.794 44 | 0.941 70 | 0.863 62 | 0.946 06 |
| $\langle x^8\rangle$ | 1.650 47 | 1.641 59 | 0.976 24 | 1.600 26 | 1.295 13 | 1.607 66 |
| | | | $N=2$ | | | |
| $\langle x^2\rangle$ | 0.942 47 | 0.942 47 | 0.942 29 | 0.942 29 | 0.943 40 | 0.943 40 |
| $\langle x^4\rangle$ | 1.412 27 | 1.412 27 | 1.403 52 | 1.403 52 | 1.405 47 | 1.405 47 |
| $\langle x^6\rangle$ | 2.513 88 | 2.515 15 | 2.351 89 | 2.479 53 | 2.421 99 | 2.484 38 |
| $\langle x^8\rangle$ | 5.157 11 | 5.161 66 | 4.157 85 | 5.042 43 | 4.626 42 | 5.053 30 |
| | | | $N=3$ | | | |
| $\langle x^2\rangle$ | 1.190 59 | 1.190 59 | 1.190 31 | 1.190 31 | 1.191 11 | 1.191 11 |
| $\langle x^4\rangle$ | 2.250 61 | 2.250 61 | 2.243 64 | 2.243 64 | 2.245 23 | 2.245 23 |
| $\langle x^6\rangle$ | 4.923 42 | 4.895 50 | 4.759 81 | 4.865 48 | 4.830 35 | 4.867 36 |
| $\langle x^8\rangle$ | 11.9336 | 11.7052 | 10.6547 | 11.6017 | 11.2540 | 11.5979 |
| | | | $N=4$ | | | |
| $\langle x^2\rangle$ | 1.415 74 | 1.415 74 | 1.415 54 | 1.415 54 | 1.416 15 | 1.416 15 |
| $\langle x^4\rangle$ | 3.182 61 | 3.182 61 | 3.176 70 | 3.176 70 | 3.178 06 | 3.178 06 |
| $\langle x^6\rangle$ | 8.189 93 | 8.169 09 | 8.025 75 | 8.137 47 | 8.096 56 | 8.139 32 |
| $\langle x^8\rangle$ | 22.9304 | 22.6396 | 21.3969 | 22.5108 | 22.1151 | 22.5074 |

with $[\hat{x},\hat{p}\,]=i$. This sort of potential has been the subject of considerable work during the past years (see, for instance, Refs. [30–39]), due to its relevance in the description of molecular vibrations and to its importance in the modeling of nonlinear quantum field theories. Attempts made recently to tackle the Hamiltonian (5.1) with the WKB weaponry [39], have not been regarded as successful [28].

In order to apply the procedure described in Sec. IV we have found it convenient to base the orthonormalization procedure upon the wave function inferred for the first excited state. In Table III we present results for $\gamma=1$ and in Table IV the corresponding ones for $\gamma=10$. None of these situations can be regarded, obviously, as a perturbative one. We compare the expectation values $\langle x^2\rangle$, $\langle x^4\rangle$, $\langle x^6\rangle$, and $\langle x^8\rangle$ evaluated within the framework of the diverse WKB environments of the previous subsection and compare them to the exact quantal results. In all cases the inferred wave functions are built up with two Lagrange multipliers, corresponding to the prior information [cf. Eq. (3.5)] provided by the expectation values $\langle x^2\rangle$ and $\langle x^4\rangle$. These are either the WKB0 (order $\hbar$) or the WKB2 (order $\hbar^2$) computed according to the recipes described in Sec. II. We have checked that the same ground-state wave function is obtained if one uses more complicated information as, for instance, the expectation values $\langle x^2\rangle$ and $\langle \ln(x^2+1)\rangle$ instead of $\langle x^2\rangle$ and $\langle x^4\rangle$. Notice that we also include figures under the label "inferred quantum results." These correspond to MEP inferred wave functions constructed with the input provided by the (exact) quantum expectation values $\langle x^2\rangle$ and $\langle x^4\rangle$. The inferred wave functions do not coincide with the exact ones [22], although the inferred expectation values $\langle x^6\rangle$ and $\langle x^8\rangle$ are quite reasonable ones.

The inferred results compare better, in general, to the quantum ones than the original semiclassical values, except for the ground-state figures, where it is well known that the WKB technique fares rather poorly [5]. As expected, predictions inferred with WKB2 inputs are of a better quality than these in which the semiclassical expansion is stopped at order $\hbar$ (WKB0).

The figures display some typical densities $\rho(x)=|\psi(x)|^2$ for the first and the fourth excited state. Figures 1 and 3 display results for the first excited state while Figs. 2 and 4 show the values corresponding to the fourth excited states. Figures 1 and 2 are drawn for the anharmonic well with $\gamma=1$ and Figs. 3 and 4 depict situations corresponding to $\gamma=10$. Within the scales of the figures it is somewhat hard to distinguish between the different approximations and the exact quantum results

TABLE IV. Anharmonic quartic oscillator ($\gamma=10$). Details are identical to those of Table III. IW denotes an inferred wave function.

| Moment | Expectation value | | | | | |
|---|---|---|---|---|---|---|
| | Quantal (exact) | Quantal (IW) | WKB0 (Ref. [5]) | WKB0 (IW) | WKB2 (Ref. [5]) | WKB2 (IW) |
| | | | $N=0$ | | | |
| $\langle x^2\rangle$ | 0.130 02 | 0.130 02 | 0.152 18 | 0.152 18 | 0.157 60 | 0.157 60 |
| $\langle x^4\rangle$ | 0.045 83 | 0.045 83 | 0.036 78 | 0.036 78 | 0.038 00 | 0.038 00 |
| $\langle x^6\rangle$ | 0.024 91 | 0.024 82 | 0.009 98 | 0.010 81 | 0.017 07 | 0.011 04 |
| $\langle x^8\rangle$ | 0.017 79 | 0.017 57 | 0.002 86 | 0.003 62 | 0.010 60 | 0.003 63 |
| | | | $N=1$ | | | |
| $\langle x^2\rangle$ | 0.326 52 | 0.326 52 | 0.321 45 | 0.321 45 | 0.322 91 | 0.322 91 |
| $\langle x^4\rangle$ | 0.166 50 | 0.166 50 | 0.164 42 | 0.165 05 | 0.165 05 | 0.165 05 |
| $\langle x^6\rangle$ | 0.112 59 | 0.112 39 | 0.094 76 | 0.112 97 | 0.101 92 | 0.112 85 |
| $\langle x^8\rangle$ | 0.093 45 | 0.092 85 | 0.057 64 | 0.961 30 | 0.074 32 | 0.095 23 |
| | | | $N=2$ | | | |
| $\langle x^2\rangle$ | 0.453 92 | 0.453 92 | 0.453 73 | 0.453 73 | 0.454 50 | 0.454 50 |
| $\langle x^4\rangle$ | 0.329 77 | 0.329 77 | 0.327 89 | 0.327 89 | 0.328 35 | 0.328 35 |
| $\langle x^6\rangle$ | 0.283 61 | 0.283 84 | 0.267 03 | 0.282 17 | 0.274 21 | 0.281 77 |
| $\langle x^8\rangle$ | 0.280 21 | 0.280 67 | 0.229 56 | 0.280 33 | 0.253 23 | 0.278 50 |
| | | | $N=3$ | | | |
| $\langle x^2\rangle$ | 0.569 25 | 0.569 25 | 0.568 99 | 0.568 99 | 0.569 49 | 0.569 49 |
| $\langle x^4\rangle$ | 0.517 36 | 0.517 36 | 0.515 86 | 0.515 86 | 0.516 23 | 0.516 23 |
| $\langle x^6\rangle$ | 0.543 87 | 0.540 66 | 0.527 13 | 0.538 12 | 0.534 32 | 0.538 08 |
| $\langle x^8\rangle$ | 0.632 29 | 0.619 58 | 0.568 62 | 0.616 41 | 0.598 38 | 0.615 45 |
| | | | $N=4$ | | | |
| $\langle x^2\rangle$ | 0.673 78 | 0.673 78 | 0.673 61 | 0.673 61 | 0.673 97 | 0.673 97 |
| $\langle x^4\rangle$ | 0.724 50 | 0.724 50 | 0.723 23 | 0.723 23 | 0.723 54 | 0.723 54 |
| $\langle x^6\rangle$ | 0.891 94 | 0.890 03 | 0.875 21 | 0.889 30 | 0.882 40 | 0.888 94 |
| $\langle x^8\rangle$ | 1.193 61 | 1.179 30 | 1.118 12 | 1.180 09 | 1.153 40 | 1.178 03 |

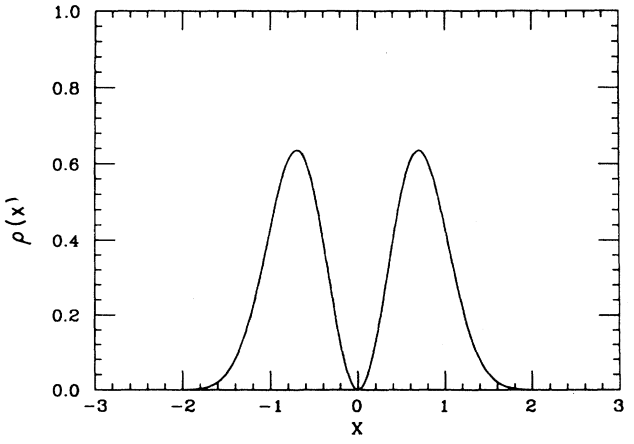


FIG. 1. Densities $\rho(x)=|\psi|^2$, for the quartic oscillator with $\gamma=1$, corresponding to the first excited state. The solid line represents the quantal (exact) result. The dashed line exhibits the results inferred from WKB0 expectation values. Dotted-dashed lines do the same for the WKB2 situation.

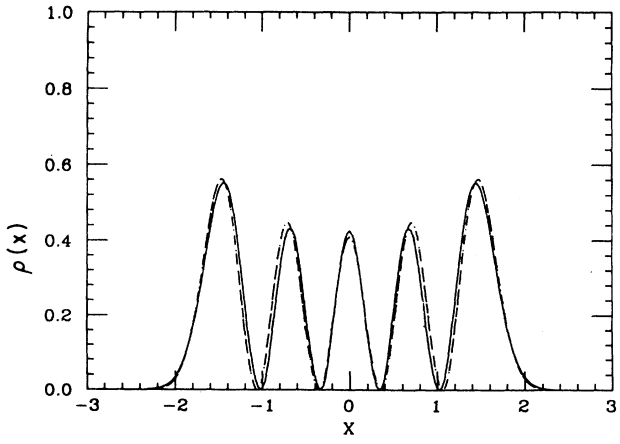


FIG. 2. Densities, for the quartic oscillator with $\gamma=1$, for the fourth excited state. Additional details are as in Fig. 1.

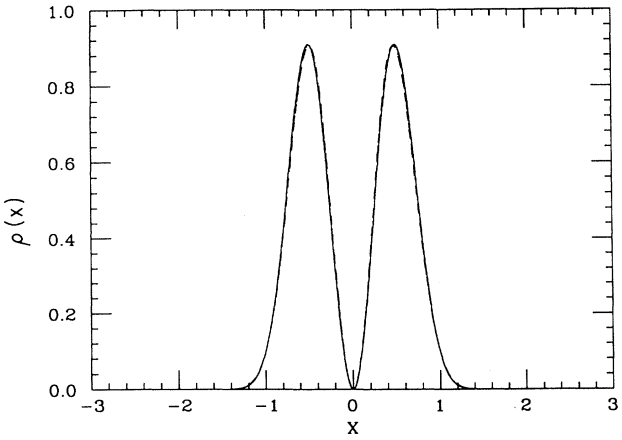


FIG. 3. Densities, for the quartic oscillator with $\gamma=10$ corresponding to the first excited state. Additional details are as in Fig. 1.

(solid line). Both inferred WKB wave functions compare quite well with the exact result. The densities inferred with exact quantal results are known to excellently match the exact ones [22] and are not depicted here in order to simplify the drawings. It is worth mentioning that earlier efforts directed towards obtaining WKB wave functions without matching do fail precisely in dealing with excited states [28].

## VI. CONCLUSIONS

An information-theory-based algorithm that is able to yield WKB wave functions on the basis of a few easily evaluated expectation values has been presented. These "input" expectation values are calculated within the WKB structures described by Krivine, Casas, and Martorell [5], and allow for the incorporation of $\hbar^2$ effects

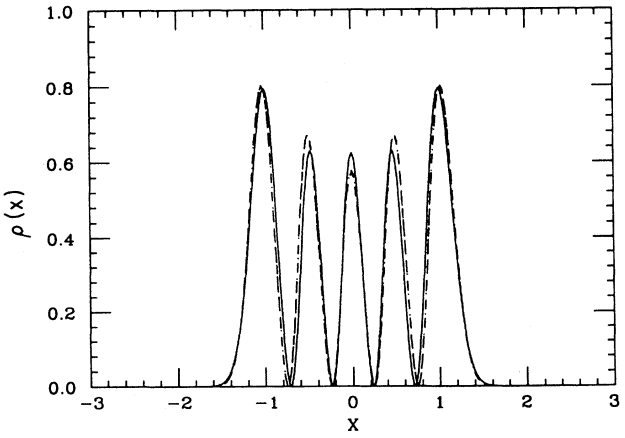


FIG. 4. Densities, for the quartic oscillator with $\gamma=10$, corresponding to the fourth excited state. Additional details are as in Fig. 1.

TABLE V. Ground-state quantal entropy for the harmonic oscillator ($\gamma=0$) and for the anharmonic quartic oscillator (cases $\gamma=1$ and 10) obtained with the quantal, WKB0, and WKB2 inferred wave functions.

| | Entropy | | |
|---|---|---|---|
| $\gamma$ | Quantal | WKB0 | WKB2 |
| 0 | 1.072 36 | 0.795 14 | 1.047 11 |
| 1 | 0.738 30 | 0.577 75 | 0.624 14 |
| 10 | 0.396 59 | 0.262 84 | 0.241 94 |

(WKB2). The present procedure yields wave functions whose validity is not (at all) restricted to the classical, permitted regions. No problems of any kind arise at the turning points. No matching of any type is required. The inferred wave functions are of rather good quality, as illustrated by Figs. 1–4. The worst results are those pertaining to the ground state, where the WKB approach *is known to fare poorly* [5]. For excited states our method does a rather good job, as opposed to what happens with other semiclassical techniques recently proposed [28]. Notice also that these work reasonably well only for small anharmonicities, while our approach is not restricted in this sense.

A few comments are here in order with reference to the behavior of the quantal pseudoentropy [cf. Eq. (3.4)], which is illustrated by the figures of Table V. $S$ (which is maximized within the framework of the present algorithm, subject to the constraint imposed by the input values $\langle x^2\rangle$ and $\langle x^4\rangle$) measures the lack of information concerning the probability distribution of the inferred wave function over the position eigenstates.

It is clear that as $\gamma$ increases, this probability distribution exhibits a tendency towards concentrating near the origin as the potential well becomes steeper, and this is reflected in the behavior of $S$ if one looks at the pertinent figures. Additionally the quantal input concerning $\langle x^2\rangle$ and $\langle x^4\rangle$ carries with it the information that the pertinent wave function is not restricted by any consideration relative to turning points, which, instead, is indeed the case when these inputs refer to WKB calculations. Consequently $S$ is larger in the quantal case than for the wave functions inferred on the basis of WKB information.

The main drawback of our approach concerns the nonorthogonality of the inferred wave functions, although this is already the case for the orthodox WKB treatment, where a quick glance to the pertinent analytical forms already suffices to detect their nonorthogonal character [29].

Summing up, good quality WKB wave functions can be inferred without much numerical work with just a couple of semiclassically obtained expectation values. Based on a mere consideration of ratios of cost to benefit, we have shown that a great deal of information can be extracted, without undue effort, from a rather modest informational input. The present results should encourage further efforts towards dealing with more complex situations.

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