WKB wave functions without matching: A self-consistent procedure

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A method is presented for the construction of Wentzel-Kramers-Brillouin (WKB) wave functions that avoids explicit consideration of any matching between results pertaining to classically allowed and forbidden regions. The formalism is based on the maximization of a suitable 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. A self-consistent procedure is developed that simultaneously yields the nodes of the wave function and the information theory parameters.

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I. INTRODUCTION

Semiclassical methods, although already introduced more than 60 years ago, enjoy still an enormous popularity [1–4]. Of course, foremost among these methods is the celebrated Wentzel-Kramers-Brillouin (WKB) one [5–8] (with more than 100 references in 1994).

The WKB expansion, treated according to the Dunham formalism [9,10], provides one with a practical recipe for evaluating expectation values with very little effort. However, if one wishes for WKB *wave functions* (WF's), matters become quite involved, as already noted by Landau and Lifschitz [11]. A complicated matching procedure must be followed that becomes more cumbersome than trying to solve Schrödinger's equation itself.

This matching problem has been attacked in various ways, but only within "perturbative environments" [12]. Recently, however, an approach has been proposed that entirely bypasses the matching procedure by recourse to information theory (IT) [13] concepts.

This IT methodology, however, was restricted only to symmetric potentials, and, moreover, the different excited states failed to be mutually orthogonal. In addition, not all the different excited states were treated on an equal footing. There was always a "privileged" one.

The goal of the present effort is that of overcoming these difficulties. As a result, we will be led to an easy-to-handle IT-based algorithm that preserves all the conveniences of the WKB approach, yields good wave functions, and is not marred either by orthogonality problems or by restrictions on the nature of the potential functions.

The paper is organized as follows. Our formalism is introduced in Sec. II and applied to symmetric and asymmetric potentials in Sec. III. Finally, some conclusions are drawn in Sec. IV.

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II. THEORY

A. Introductory remarks

1. Generalities

IT-based approximate wave functions (ITWF's) have been extensively discussed in recent years [14–19]. They provide one with a reasonable alternative to the celebrated Gutzwiller ansatz in relation to the Hubbard model of superconductivity [20] and allow for an extremely simple approximation with reference to the Dicke model of quantum optics [21]. In the many-body problem they have been shown to advantageously compete with those approximate WF's provided by the Hartree-Fock [16], the BCS [17], or the random-phase approximation (RPA) [19] treatments. Some reasons that underlie the apparently surprising success of these WF's have been discussed in [15]. If the state vector $|\psi\rangle$ is expanded in the basis $|j\rangle$ (with coefficients C_j), the maximum entropy recipe assigns to these components C_j a typical IT exponential form [14–19]. The concomitant exponents are sums of products of Lagrange multipliers (arising out of the entropy extremalization process) times diagonal matrix elements of the form $\langle j|\hat{O}_\mu|j\rangle$. The $\hat{O}_\mu$ belong to a set of M linearly independent, commuting operators whose expectation values are assumed to be known.

These M expectation values constitute our input information, and constrain the extremalization procedure, in the usual way, via the associated Lagrange multipliers λ_μ [14–19].

In the one-dimensional case we deal with a continuous basis labeled by the coordinate x and with multiplicative operators (powers of the coordinate). The components C_j become the ordinary wave functions $\psi(x)$ and the above mentioned diagonal matrix elements are (because of the multiplicative character of the operators involved) just appropriate powers of the coordinate, evaluated at x. Thus, the ITWF's are of the general appearance (for a state with n nodes) [14,15]

$$\psi_n(x) = P_n(x) \exp\left[-\frac{1}{2}\sum_{\mu=1}^{M} \lambda_\mu x^\mu\right] \equiv P_n(x)\omega_n(x) \quad , \quad (1)$$

where P_n is an nth-order polynomial and the λ's are the Lagrange parameters, characteristic of the IT approach [14–19], that are determined by the input information.

In building up an ITWF one faces the problem of determining two types of unknown quantities, which an appropriately devised IT inference methodology must provide. We need the values of the polynomial coefficients, on the one hand, and those of the Lagrange multipliers entering ω_n, on the other one.

In the case of ground-state (g.s.) wave functions, Jaynes's original IT methodology [14,15] by itself, without further ado, is able to provide the latter, by recourse to appropriate input information (expectation values of M relevant operators $\hat{O}_\mu$). One does not require, of course, to solve Schrödinger's equation in order to obtain an approximate g.s. wave function [14–19]. The main advantage of such an approach lies in the fact that it enables one to undertake the description of systems for which important (or even all) details of the pertinent interactions may be missing (how would one then write down Schrödinger's equation?).

2. *WKB wave functions without matching*

As stated in Sec. I, one wishes to take advantage of the WKB treatment following Dunham [22,23], which, although yielding without much work any expectation value, is not able to provide one with a semiclassical wave function. Such a goal was certainly achieved in Ref. [13].

The essence of the method introduced in [13] is to employ WKB expectation values (instead of experimental ones) as input information. Full advantage is thus taken of a quite convenient reformulation of the Dunham approach effected in Refs. [22,23]. This information supply, by recourse to elementary IT concepts, readily fixes the λ's in (1). However, somewhat more elaborate considerations are needed in order to fix the coefficients in $P_n(x)$. The resulting approach of Ref. [13], although providing one with quite reasonable results, exhibits, however, some drawbacks, as, for instance, lack of orthogonality and applicability restricted to even potentials. These problems can be overcome as indicated below.

B. Present formalism

A definite IT algorithm [to be referred to as the Lagrange multipliers algorithm (LMA)] yields the Lagrange multipliers [14,15] on the basis of a set of expectation values $\langle \hat{O}_\mu \rangle$ corresponding to some relevant operators $\hat{O}_\mu$, $\mu = 1, ..., M$ [15]. A standard well-known numerical method is available [24]. In order to build up our WKB formalism we will now (i) describe first a self-consistent approach to determine the zeros of the $P_n(x)$ [let us abbreviate it as the zeros determination algorithm (ZDA)] and (ii) discuss afterwards how to combine the LMA with the ZDA.

(i) We have

$$P_n(x) = x^n + \sum_{\alpha=1}^{n-1} a_\alpha^{(n)} x^\alpha \quad , \quad (2)$$

where, of course, the $a_\alpha^{(n)}$ are unknown quantities. In order to fix them we shall require strict orthogonality (in order to improve upon the approach of Ref. [13]). We face the set of conditions

$$\langle \psi_j | \psi_k \rangle = 0, \quad j = 1, ..., N-1, \quad k < j \quad , \quad (3)$$

which, under the assumption that the $\omega_n(x)$ are known (by recourse to the LMA), *can be regarded as a linear system in the* $a_\alpha^{(n)}$.

(ii) In order to combine our two techniques (LMA and ZDA) we (a) start with an arbitrary set of $P_n(x)$, (b) determine the $\omega_n(x)$ by recourse to the LMA, on the basis of some relevant informational input (the $\langle \hat{O}_\mu \rangle$), and (c) fix the zeros of the $P_n(x)$ by solving the linear system Eq. (3). At this stage one goes back to (a) and restarts the process until convergence is achieved. This self-consistent procedure neatly solves our problem.

III. APPLICATIONS

A. The harmonic oscillator

As might be expected, the self-consistent inference procedure of Sec. II yields the exact WF in the case of the harmonic oscillator (HO). The only informational input here required is that of $\langle \hat{x}^2 \rangle_n$ (for each n-phonon state), computed according to the WKB0 prescription [13,23] (the last zero tells us that we are employing a WKB prescription up to order $\hbar$ [23]).

B. Anharmonic oscillator

As in [13] we shall concentrate efforts upon symmetric potentials of the type

$$V(x) = \frac{\alpha}{2} x^2 + \gamma x^4 \quad , \quad (4)$$

which have been the subject of much interesting work (in several disciplines) [25–28].

We shall take M, the number of relevant input operators, equal to 2 and consider the expectation values $\langle \hat{x}^2 \rangle$ and $\langle \hat{x}^4 \rangle$, which are evaluated up to order $\hbar$ (WKB0) or up to order $\hbar^2$ (WKB2) [13,23]. With our self-consistent inference technique we *predict* then $\langle \hat{x}^{2n} \rangle$ values with n=3, 4, and 5.

For the sake of definiteness we adopt the values α =1 and γ =2 in (4), so that a clearly nonperturbative situation is to be confronted. Table I displays the concomitant results. The inferred results corresponding to odd states closely resemble the exact (quantal) ones. This is not the case for the even states (see the first column). Here, the well-known fact that WKB fares rather poorly for the ground state [23] is amplified by our self-consistent procedure. In order to overcome this difficulty, recourse can be

TABLE I. Anharmonic quartic oscillator (γ=2). The overlap deficiency D is evaluated according to different prescriptions. The inferred expectation values of $\langle x^6\rangle$, $\langle x^8\rangle$, and $\langle x^{10}\rangle$ are compared to the quantal results. IW denotes an inferred wave function. Notice that the Comtet *et al.* approach [29] is not employed here for the g.s.

	D	x^6	x^8	x^{10}
		$n=0$		
IWKB0	5.6×10^{-2}	0.04464	0.02385	0.01405
IWKB2	2.0×10^{-2}	0.06642	0.04640	0.03653
Quantal		0.11094	0.13180	0.19147
		$n=1$		
IWKB0	5.0×10^{-5}	0.51231	0.71541	1.17633
IWKB2	2.0×10^{-4}	0.53672	0.78028	1.34803
Quantal		0.51749	0.71824	1.17198
		$n=2$		
IWKB0	8.0×10^{-4}	1.29585	2.07635	3.70943
IWKB2	2.0×10^{-3}	1.30678	2.09257	3.72677
Quantal		1.32971	2.20263	4.11752
		$n=3$		
IWKB0	5.0×10^{-5}	2.56224	4.98466	10.6009
IWKB2	8.0×10^{-5}	2.58043	5.04674	10.8030
Quantal		2.57901	5.03806	10.7678
		$n=4$		
IWKB0	4.1×10^{-2}	4.06387	8.57062	19.1120
IWKB2	2.0×10^{-2}	4.13361	8.90435	20.3636
Quantal		4.26193	9.60159	23.2107

made to an idea introduced (within a different context) by Comtet, Bandrauk, and Campbell [29]. They suggest replacing, *just for the ground state*, the WKB g.s. by a variational one. The idea of Comtet *et al.* translates here into considering (for n= 0) λ_2 and λ_4 as variational parameters, chosen so as to minimize $\langle H\rangle_{\text{g.s.}}$. We insist: this is done just for the zero-phonon g.s. (not for excited states). The results are displayed in Table II. A clear improvement with respect to the figures of Table I is easily appreciated (for even states). Indeed, comparison of the concomitant overlap deficiencies D

$$D = 1 - |\langle\psi_{\text{exact}}|\psi_{\text{inferred}}\rangle| \ , \tag{5}$$

which is quickly effected by glancing at the first columns of Table I and Table II, respectively, clearly illustrates the fact that the "Comtet idea" [29] allows for a big improvement of the concomitant "even" results (the results corresponding to odd states remain unchanged). We adopt then, throughout, the Comtet *et al.* approach [29]. Ta-

TABLE II. Anharmonic quartic oscillator (γ=2). In this case the Comtet *et al.* approach [29] is employed for the g.s. Additional details are the same as in Table I.

	D	x^6	x^8	x^{10}
		$n=0$		
Comtet	1.0×10^{-6}	0.11067	0.13059	0.18749
Quantal		0.11094	0.13180	0.19147
		$n=1$		
IWKB0	5.0×10^{-5}	0.51231	0.71541	1.17633
IWKB2	2.0×10^{-4}	0.53672	0.78028	1.34803
Quantal		0.51749	0.71824	1.17198
		$n=2$		
IWKB0	2.0×10^{-5}	1.30874	2.13694	3.92003
IWKB2	3.0×10^{-5}	1.32809	2.19335	4.07921
Quantal		1.32971	2.20263	4.11752
		$n=3$		
IWKB0	5.0×10^{-5}	2.56224	4.98466	10.6009
IWKB2	8.0×10^{-5}	2.58043	5.04674	10.8030
Quantal		2.57901	5.03806	10.7678
		$n=4$		
IWKB0	8.0×10^{-6}	4.24158	9.51324	22.8570
IWKB2	5.0×10^{-6}	4.25831	9.57512	23.0747
Quantal		4.26193	9.60159	23.2107

TABLE III. Anharmonic quartic oscillator (γ=20). Additional details are the same as in Table II.

	D	x^6	x^8	x^{10}
		$n=0$		
Comtet	1.6×10^{-6}	0.01271	0.00719	0.00493
Quantal		0.01274	0.00726	0.00504
		$n=1$		
IWKB0	2.0×10^{-4}	0.05758	0.03921	0.03156
IWKB2	4.0×10^{-4}	0.05991	0.04213	0.03527
Quantal		0.05724	0.03787	0.02939
		$n=2$		
IWKB0	2.0×10^{-5}	0.14145	0.10984	0.09566
IWKB2	3.0×10^{-6}	0.14332	0.11237	0.09901
Quantal		0.14359	0.11303	0.10024
		$n=3$		
IWKB0	1.4×10^{-4}	0.27327	0.25248	0.25496
IWKB2	1.7×10^{-4}	0.27501	0.25520	0.25905
Quantal		0.27475	0.25438	0.25738
		$n=4$		
IWKB0	8.0×10^{-6}	0.44785	0.47507	0.53941
IWKB2	6.0×10^{-6}	0.44949	0.47788	0.54401
Quantal		0.44991	0.47932	0.54752

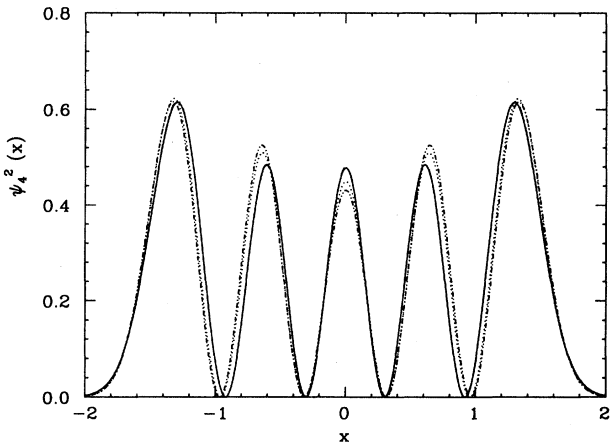

FIG. 1. Densities $\rho(x) = |\psi|^2$, for the quartic oscillator with γ=2, corresponding to the fourth excited state. The solid line represents the quantal (exact) result. The dotted-dashed and the dashed lines correspond to the inferred results from WKB0 and WKB2 expectation values, respectively, which coincide with the exact result. For comparison the WKB0 (dotted line) and the WKB2 (dashed-dotted-dotted line) results corresponding to Ref. [13] are also superimposed.

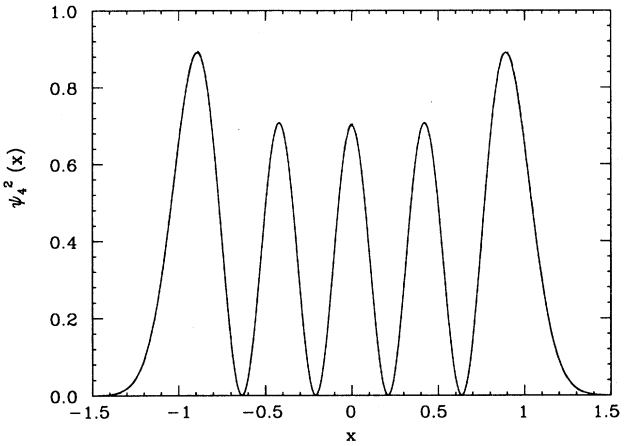

FIG. 2. Densities, for the quartic oscillator with γ=20, corresponding to the fourth excited state. The solid line represents the quantal (exact) result. The dotted-dashed and the dashed lines correspond to the inferred results from WKB0 and WKB2 expectation values, respectively, which coincide with the exact result.

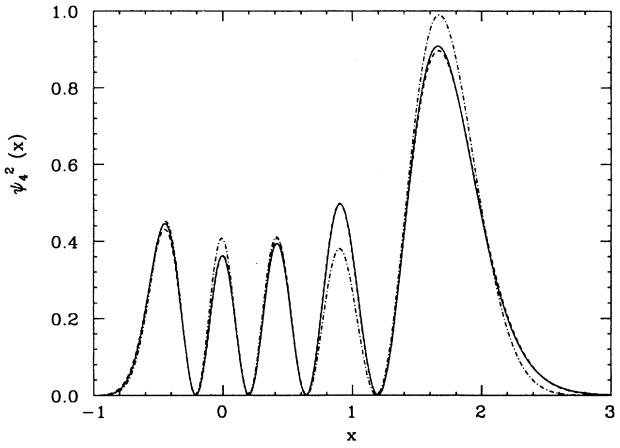

FIG. 3. Densities, for the Morse potential with A=40. Additional details are the same as in Fig. 2.

ble III exhibits results similar to those of Table II, but evaluated for a much larger anharmonicity ($\gamma = 20$).

Figures 1 and 2 depict the densities $\rho(x) = |\psi(x)|^2$ for the fourth excited state corresponding to, respectively, γ=2 and $\gamma = 20$. Exact and inferred densities resemble each other in quite a close fashion. In Fig. 1 we also depict, for the sake of comparison, the results obtained with the method of Ref. [13]. The superiority of the present approach is easily appreciated. Notice that our WF's are everywhere defined, *even beyond the turning points.*

TABLE IV. Morse potential (A=40). Overlap deficiency D and expectation values of several powers of the coordinate are compared to the exact ones. IW denotes an inferred wave function.

	D	x^8	x^{10}
		$n = 0$	
Comtet	3.0×10^{-7}	0.00415	0.00352
Quantal		0.00423	0.00367
		$n = 1$	
IWKB0	9.4×10^{-3}	0.04840	0.03683
IWKB2	3.0×10^{-6}	0.11628	0.14888
Quantal		0.11946	0.15800
		$n = 2$	
IWKB0	5.7×10^{-3}	1.01683	1.53438
IWKB2	1.0×10^{-5}	1.55663	3.07494
Quantal		1.58547	3.20980
		$n = 3$	
IWKB0	4.7×10^{-3}	10.8954	28.6256
IWKB2	3.6×10^{-5}	13.9716	42.3157
Quantal		14.2098	44.0644
		$n = 4$	
IWKB0	4.0×10^{-3}	83.3114	341.658
IWKB2	1.2×10^{-4}	102.904	476.675
Quantal		104.886	499.095

C. Morse potential

As a typical example of an *asymmetric* potential we shall employ the celebrated Morse one, used in modeling the interaction potential of diatomic molecules [30,31]. We have

$$V(x) = A\left[1 - \exp(-x)\right]^2 \quad , \tag{6}$$

and we take $A = 40$.

We construct our informational input with the first four moments $\langle x^n \rangle$ (n=1,...,4) and display the main results in Table IV, where inferred (predicted) $\langle x^8 \rangle$ and $\langle x^{10} \rangle$ moments are compared to the exact ones.

The corresponding densities are depicted in Fig. 3. Notice that in the case of the Morse potential recourse to a WKB2 input noticeably improves upon a WKB0 one.

IV. CONCLUSIONS

We have here developed a *self-consistent* algorithm, based upon information theory that is able to yield WKB wave functions on the basis of a few easily evaluated expectation values. These "input" expectation values are obtained within the WKB framework, by following the recipes described by Krivine *et al.* [23], and allow for the incorporation of $\hbar^2$ effects (WKB2) (in addition to the textbook, customary $\hbar$ ones). The g.s. input is obtained following the ideas of Ref. [29].

Our procedure yields wave functions whose validity is not (at all) restricted to the classical, permitted regions, *which constitutes its main advantage with relation to the orthodox WKB treatment.* No problems of any sort arise at the turning points. No messy matchings of any kind are required and the resulting wave functions are indeed of a rather good quality.

The methodology introduced in the present effort exhibits clear-cut advantages over that of Ref. [13]. This claim can be justified on the following grounds.

(i) The present is *a global* inference procedure. The totality of the states to be described is inferred as a *sin-*

gle entity. The approach of Ref. [13] follows, instead, a "state-by-state" inference philosophy.

(ii) The techniques of Ref. [13] are unable to deal with asymmetric potentials. Only even ones can be tackled. Our present treatment does not suffer from limitations of this sort (as illustrated here by the Morse example).

(iii) In Ref. [13] recourse is made to the Gram-Schmidt (GS) orthogonalization method. It is well known that the GS algorithm often presents one with a number of difficulties from the numerical standpoint. Moreover, it forces one to select a "privileged" state as the "starting" one. We entirely bypass here the GS procedure. Instead, we face a simple *linear* system. As a consequence, there are no privileged states.

(iv) The present results are of better quality than those provided by the methodology of Ref. [13] (see Fig. 1).

(v) The approach here described is in a better position (see Fig. 3 and Table IV) than the one of Ref. [13] to take advantage of the superiority of the expansion up to $\hbar^2$ (WKB2) over the textbook one (order $\hbar$, WKB0).

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