Wentzel-Kramers-Brillouin-type approximations for bound states in short-range nonsingular potentials

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A recently proposed matrix formulation of the WKB quantization rule and the usual WKB quantization rule are tested in the case of short-range potentials in one dimension which are nonsingular at the origin. Such potentials simulate optical potentials in nuclear physics. We compare the results for the bound states of these two semiclassical quantization rules with the exact solution of the Schrödinger equation and find that usually both of these approximations yield good results. In particular, the newly proposed matrix formulation of the WKB quantization rule produces results either comparable to or better than results obtained with the usual WKB quantization rule for the low-lying states which are very interesting from a physical point of view as they simulate the ground and a couple of excited states of the nuclear optical potential.

I. INTRODUCTION

The Wentzel-Kramers-Brillouin (WKB) quantization rule[1] has proven to be very useful for finding an approximate solution of the Schrödinger equation for a diverse class of problems for a variety of potentials. The class of problems range from[2] the eigenvalue-eigenfunction problem for the bound state to the calculation of transmission probability or phase-shift for the continuum states. In the bound-state study the WKB approximation scheme has been applied to (harmonic oscillator-type) confining potentials suitable for some quantum-mechanical models or the Coulomb or screened Coulomb-type potentials appropriate to problems in atomic and molecular physics. The latter class of potentials always has a singularity at the origin which is common to many effective potentials in atomic and molecular physics.

The original WKB approximation for solving the one-dimensional wave equation is simple and transparent but has different shortcomings. A number of variants[2] have been introduced since the early days of quantum mechanics to overcome these defects. More recently, a matrix formulation of the original WKB (mWKB) quantization rule has been suggested[3] and applied to one-dimensional confining polynomial potentials of the type[3,4] $V(q) \sim |q|^{2\mu}$, $\mu > 0$, and to the one-dimensional Coulomb potential[4] $V(q) \sim |q|^{-1}$. Though the mWKB quantization rule is numerically easier to apply than the usual WKB quantization rule, for calculating binding energy, in the cases studied[3,4] the WKB method always yielded results superior to the mWKB method. It is well known that the WKB-type approximations should yield good results when the potential is varying slowly, at least for the highly excited states.[1]

In this work we apply the WKB and mWKB quantization rules to a new class of potentials in one-dimension—short-range potentials with no singularity at the origin. These potentials simulate optical potentials or effective interactions in nuclear physics.[5] They are finite at the origin and support a small number of bound states in contrast to confining potentials or long-range potentials with or without screening, which usually have a large or sometimes infinite number of bound states. The WKB-type approximations have not been extensively applied to study the bound states in short-range nonsingular potentials. We find that both WKB and mWKB approximations yield good results for bound states in these potentials. In particular, for the low-lying states the mWKB method yields results which are either comparable to or superior to those obtained with the WKB quantization rule.

We find it appropriate to mention a few words about the role of effective interaction or optical potential in nuclear physics.[5] They can reproduce certain bound and continuum states of a quantum-mechanical nuclear system where only a relatively few degrees of freedom are active. For example, a ^{2}H-^{4}He or a ^{4}He-^{12}C optical potential should be able to explain the bound states where ^{2}H, ^{4}He, and ^{12}C clusters dominate and such bound states are relatively few in number. They are easily described well by an effective interaction and not so easily by, for example, a shell-model-type description. In this paper we concentrate on a numerical study of the WKB and the mWKB quantization rules for these states. The superior results obtained by the mWKB in certain cases suggests its usefulness in dealing with these types of problems.

We also artificially varied the range parameter of these effective interactions to generate a large number of excited states—sometimes even ten in number—and calculated the binding energies of these states by the WKB and mWKB approximation schemes and by the exact solution of the Schrödinger equation. Even in this single-channel one-dimensional problem, numerically it was extremely tedious and time consuming to find these excited states via an exact solution of the Schrödinger equation unless one could make a good initial guess about the binding energies. No such guess is needed in the WKB or the mWKB approximation schemes, and the WKB or the

mWKB energy, while used as an estimate for the exact solution of the Schrödinger equation, greatly facilitate the task of the numerical solution of the Schrödinger equation, especially for the excited states.

It is well known that the one-dimensional Schrödinger equation has both symmetric and antisymmetric solutions for potentials satisfying the property $V(q)=V(-q)$, the antisymmetric solutions being identical with the solution of the s-wave three-dimensional Schrödinger equation with a local potential $V(r)$. Hence our conclusion and results are applicable to the case of the three-dimensional s-wave effective interaction in nuclear physics.

In Sec. II we present a brief summary of the WKB and the mWKB approximation schemes. In Sec. III we present and compare the mWKB, WKB, and the exact Schrödinger energy spectra for some short range-model potentials of finite depth, which are of interest in nuclear physics. In Sec. IV we present a brief discussion of our results.

II. THE mWKB FORMULATION

In a recent paper the mWKB quantization rule[3] was introduced and applied to the case of a particle of mass m subject to some (confining) potential $V(q)$. The usual WKB quantization rule is given by[1]

$$\oint p\, dq=(n+\tfrac{1}{2})h \ , \tag{1}$$

where p and q are canonical momentum and position variables and

$$p^2=2m[E-V(q)] \ , \tag{2}$$

where E is the total energy. The usual solution of Eq. (2) of interest in Eq. (1) is

$$p=\{2m[E-V(q)]\}^{1/2} \ . \tag{3}$$

The WKB energies are calculated from Eqs. (1) and (3) and they are quite accurate for large quantum numbers or the excited states.

The solution of Eq. (2) of interest in mWKB formulation is taken to be

$$\hat{p}=(2mE)^{1/2}\hat{\alpha}_j+i[2mV(q)]^{1/2}\hat{\alpha}_k, \quad j\neq k \ , \tag{4}$$

where the carets over the variables denote matrix representations, $\hat{\alpha}$'s satisfy the $D_2 s$ Clifford algebra

$$\hat{\alpha}_j\hat{\alpha}_k+\hat{\alpha}_k\hat{\alpha}_j=2\delta_{jk}\hat{I} \ , \tag{5}$$

with $j,k=1,2,\ldots,s$, s being the number of generators of the algebra, δ_{jk} the Kronecker δ symbol, $\hat{I}$ the identity matrix. From Eqs. (4) and (5) we have

$$\hat{p}^2=2m[E-V(q)]\hat{I} \ , \tag{6}$$

which should be considered as a matrix realization of Eq. (2). In view of Eqs. (4)–(6), $\hat{p}$ in this approach may be expressed in terms of the Pauli matrices which define the D_4 Clifford algebra of two generators, which readily provides the two-dimensional representation of the mWKB formulation. The WKB quantization rule (1) for finding energy is now replaced by

$$\oint \hat{p}\, dq=(n+\tfrac{1}{2})h\hat{A} \ , \tag{7}$$

where $\hat{A}^2=\hat{I}$.

The relationships between the mWKB and the WKB energy spectra for the power-law potentials $V(q)=|q|^{2\mu}$, $\mu>0$, for the binomial interaction $V(q)=q^2+\lambda q^{2\mu}$, $\mu=2$, 3, 4, 5, and 6, and for the one-dimensional Coulomb interaction $V(q)=|q|^{-1}$ has been previously studied and the results were compared[3,4] with the supersymmetric WKB[6,7] and the exact solution of the Schrödinger equation whenever applicable and available. It is interesting to observe that supersymmetric quantum mechanics has reviewed fresh interest in the study of the WKB quantization rule.[8] Though a systematic comparison of WKB and mWKB results with the exact solution of the Schrödinger equation was made only in some selected cases because of the unavailability of the exact results in all the cases, the usual WKB formulation yielded[4] more accurate results than the mWKB formulation whenever such comparison was possible.

III. NUMERICAL INVESTIGATIONS

In this work we calculate the WKB, mWKB, and the exact energy spectrum of the following nonpolynomical interactions

$$V_1(q)=\begin{cases} V_0, & |q|<R \ , \\ \tilde{V}_{01}\exp(-\mu|q|)/q^2, & q\geq R \ , \end{cases} \tag{8}$$

$$V_2(q)=\begin{cases} V_0, & |q|<R \ , \\ \tilde{V}_{02}\exp(-\mu|q|)/|q|, & q\geq R \ , \end{cases} \tag{9}$$

$$V_3(q)=V_0\exp(-\mu q^2) \ , \tag{10}$$

with $V_0=-100$ MeV, $R=1.6275$ fm, $\tilde{V}_{01}=V_0R^2\exp(\mu R)$, $\tilde{V}_{02}=V_0R\exp(\mu R)$, and μ varies from[9] 0.01 to 9. The value of m is taken as the reduced mass of the deuteron-neutron system, e.g., $m=2m_n/3$, where m_n is a nucleon mass. All three interactions (8)–(10) are of short range, finite everywhere, and are similar to effective interactions[5] of nuclear physics. Interaction (8) with $V_0=-30.325$ MeV, $R=1.6275$ fm, and $\mu=0.2$ fm^{-1} is the realistic neutron-deuteron effective interaction fitted to experimental trinucleon observables.[10] Interaction (9) is similar to a typical effective interaction in nuclear physics in being constant for $|q|<R$ and having a Yukawa tail. Interaction (10) is the Gaussian potential which also simulates effective interaction in nuclear physics.[5]

Now, remembering that the energies and the potentials are negative, Eq. (4) is rewritten as

$$\hat{p}=i(2m|E|)^{1/2}\hat{\alpha}_j-(2m|V(q)|)^{1/2}\hat{\alpha}_k \ . \tag{11}$$

In Eqs. (4) and (11) the subscripts j and k are arbitrary, $j\neq k$. If we substitute the representation (11) for the momentum in Eq. (7) and square the resultant equation we obtain

$$2m\left\{\left[\oint |V(q)|^{1/2}dq\right]^2-\left[\oint |E|^{1/2}dq\right]^2\right\}=(n+\tfrac{1}{2})^2h^2\ , \tag{12}$$

where use has been made of Eq. (5). The WKB energies are given by

$$\sqrt{2m}\oint[|V(q)|-|E|]^{1/2}dq=(n+\tfrac{1}{2})h\ . \tag{13}$$

Equations (12) and (13) were solved numerically for calculating the mWKB and the WKB energies. The exact solution of the Schrödinger equation was also found for the bound states.

In Tables I–III we show the WKB, mWKB, and the exact energies for the three potentials for some values of the parameter μ. It can be proved[3,4] that for any confining potential or for any potential of finite depth the relation $E_n(\text{mWKB})\leq E_n(\text{WKB})$ holds, i.e., the nth mWKB energy level is lower or equal to the nth WKB energy level. Since both WKB and mWKB schemes are nonvariational in nature, the associated energy levels could be above or below the exact energy levels.[4] This is clearly seen in Tables I–III and in Fig. 1 below. We see from Tables I–III that the energies of the (antisymmetric) first excited ($n=1$) states calculated via the mWKB method are closer to the exact solutions than those calculated via the usual WKB method. These states are of greatest relevance as they correspond to the ground states in the three-dimensional s-wave model. The symmetric states do not have a three-dimensional counterpart. For the (symmetric) ground state ($n=0$) both the WKB and mWKB methods yield good results and the mWKB energies are very similar to the WKB energies. Depending on the potential model used the mWKB ground state ($n=0$) energies could be a little better or a little worse than their WKB counterparts, as can be seen from Tables I–III. For the (symmetric) second excited state ($n=2$) the mWKB energies are usually a better approximation of the exact energies than the WKB energies except for the smallest values of μ, where the WKB energies are better. The smaller μ corresponds to a potential of longer range. For the higher excited states ($n\geq 3$) the WKB result is a better approximation of the exact result unless μ is increased sufficiently without destroying these levels. For a reasonably large μ only few levels exist and the mWKB is a better approximation of the exact result than the WKB. Such a μ corresponds to a range of a few Fermi which is the range typical in nuclear physics. For longer range potentials the WKB method reproduces the higher excited states ($n\geq 3$) better than the mWKB method.

To illustrate these results better we plot in Fig. 1 the energy ratios

$$R_n^{\text{mWKB}}(\mu)\equiv E_n^{\text{EXA}}(\mu)/E_n^{\text{mWKB}}(\mu)\ ,$$
and
$$R_n^{\text{WKB}}(\mu)\equiv E_n^{\text{EXA}}(\mu)/E_n^{\text{WKB}}(\mu)\ , \tag{14}$$

as functions μ for $n=0$, 1, and 2. Here EXA, WKB, and mWKB refer to the exact, WKB, and mWKB calculations for a particular μ, respectively. Consistent with Tables I–III, for $n=0$ and 1 the mWKB results (denoted by solid circles in Fig. 1) are, in general, closer to unity than the WKB results (denoted by squares in Fig. 1) and

TABLE I. The WKB, mWKB, and the exact Schrödinger energy spectrum (s) for certain values of μ and n for potential V_1. The (?) means that this state could not be calculated reliably because of numerical problems.

μ	n	0	1	2	3
	s	−89.07478	−59.52378	−24.61283	−7.93954
0.01	WKB	−93.08536	−55.23027	−23.48366	−8.49354
	mWKB	−93.12316	−56.39535	−25.53936	−10.01412
	s	−88.89598	−58.68878	−22.54694	−5.39497
0.1	WKB	−93.06390	−54.33830	−21.14496	−5.95432
	mWKB	−93.09945	−55.47916	−23.14683	−7.23537
	s	−88.52759	−57.11252	−18.79204	−1.70994
0.3	WKB	−93.02494	−52.65477	−16.81925	−2.19487
	mWKB	−93.05635	−53.74743	−18.68910	−2.91480
	s	−88.08688	−55.25524	−14.60504	(?)
0.6	WKB	−92.98196	−50.67523	−11.88486	−0.04774
	mWKB	−93.00872	−51.70327	−13.53481	−0.08708
	s	−87.63603	−53.38454	−10.68971	
1	WKB	−92.94212	−48.68950	−7.17839	
	mWKB	−92.96448	−49.64289	−8.50648	
	s	−86.42668	−48.50048		
3	WKB	−92.90434	−43.51206		
	mWKB	−92.90434	−44.21350		
	s	−85.67028	−45.54832		
6	WKB	−92.84223	−40.45653		
	mWKB	−92.84223	−40.96040		

TABLE II. Same as Table I for potential V_2.

μ \ n		0	1	2	3
	s	−90.79118	−66.74322	−41.01292	−27.55223
0.01	WKB	−93.37342	−63.58259	−41.07883	−27.69289
	mWKB	−93.43844	−64.80279	−43.13004	−29.84159
	s	−90.38780	−64.98377	−36.53937	−20.90136
0.1	WKB	−93.30209	−61.60567	−36.34083	−21.14427
	mWKB	−93.36064	−62.81457	−38.41187	−23.21451
	s	−89.69296	−61.98737	−29.29231	−11.00909
0.3	WKB	−93.19097	−58.26731	−28.46462	−11.38065
	mWKB	−93.23903	−59.44217	−30.50824	−13.09005
	s	−88.95274	−58.85872	−22.04803	−3.01801
0.6	WKB	−93.08941	−54.79681	−20.32906	−3.39921
	mWKB	−93.12737	−55.91287	−22.24476	−4.33828
	s	−88.28313	−56.00601	−15.77825	(?)
1	WKB	−93.01010	−51.65979	−13.03507	−0.00404
	mWKB	−93.03979	−52.69838	−14.70499	−0.00858
	s	−86.66921	−49.44695	−3.63842	
3	WKB	−92.92911	−44.55471	−0.01514	
	mWKB	−92.92911	−45.30959	−0.03077	
	s	−85.77311	−45.96972		
6	WKB	−92.85043	−40.87702		
	mWKB	−92.85043	−41.40934		

hence are better approximations to the exact calculation. Even for $n=2$, for most of the μ's of interest in nuclear physics [$\mu > 0.3$ fm^{-1} for potentials (8) and (9), and $\mu > 0.1$ fm^{-2} for potential (10)] the mWKB method produces better results than the WKB method. The same is true for the antisymmetric ($n=3$) state provided that μ is slightly increased and the potential is still similar to a nuclear optical-model interaction. This last state corresponds to the first excited state in the three-dimensional s-wave model. As we have pointed out before, the results for $n=1$ corresponds to the three-dimensional s-wave ground state, and in this case [Fig. 1(b)] both the approximations produce very good results and consistently the mWKB method produces better result than the WKB method. This is true for the $n=3$ state provided that μ is not too small. This demonstrates the usefulness of the

TABLE III. Same as Table II for potential V_3.

μ \ n		0	1	2	3
	s	−94.53543	−83.84877	−73.65004	−63.95295
0.01	WKB	−94.47964	−83.79532	−73.59751	−63.90132
	mWKB	−94.68653	−84.38165	−74.51573	−65.10152
	s	−83.51833	−53.12932	−28.21536	−9.76740
0.1	WKB	−82.94955	−52.57078	−27.66074	−9.23066
	mWKB	−83.56461	−54.04788	−29.43022	−10.57320
	s	−72.94080	−27.18644	−1.59784	
0.3	WKB	−71.23770	−25.54394	−0.58374	
	mWKB	−72.22783	−27.30657	−0.85543	
	s	−63.77637	−9.61010		
0.6	WKB	−60.41666	−6.81799		
	mWKB	−61.70872	−7.99515		
	s	−55.79634			
1	WKB	−50.33599			
	mWKB	−51.85956			
	s	−36.51927			
3	WKB	−22.62047			
	mWKB	−24.36099			
	s	−24.86801			
6	WKB	−4.41229			
	mWKB	−5.36250			

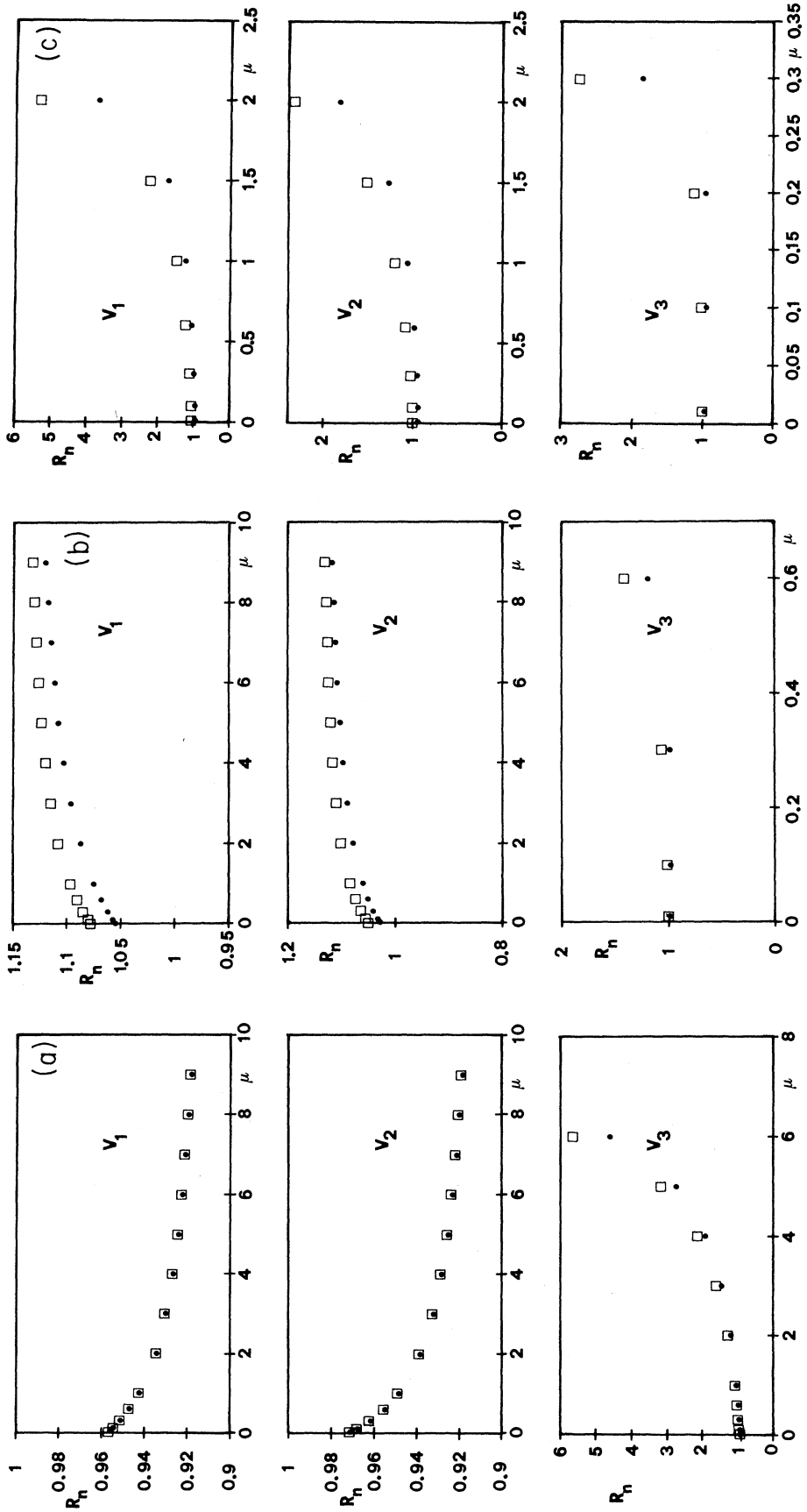

FIG. 1. The energy ratio $R_n(\mu)$ of Eq. (14) for the mWKB (●) and WKB (□) as a function of μ for the potentials V_1, V_2, and V_3 for the ground ($n=0$) (a), the first ($n=1$) (b), and the second ($n=2$) (c), excited states.

mWKB method in nuclear physics problems.

Finally, we compared the mWKB, the WKB and the exact energy spectra for the Yukawa potential simulated with the function

$$V_4(q)=\begin{cases} V_0\exp(-\mu|q|)/|q|, |q|>R \\ V_0\exp(-\mu R)/R, q\le R \end{cases}, \quad (15)$$

with $V_0=-100$ MeV and $R=10^{-20}$ fm. The value $R=0$ gives the usual Yukawa potential. The cutoff at $R=10^{-20}$ was introduced for avoiding accidental numerical difficulties with the integrals in Eqs. (12) and (13). Otherwise, our results are the same as those of the Yukawa potential (15) with $R=0$. In this case we found that the WKB results were either comparable to or better than the mWKB results for $n=0$ and $n=1$, regardless of the value of μ, contrary to the results for nonsingular potentials given by Eqs. (8)–(10). However, for $\mu\ge 0.05$ fm^{-1} the mWKB spectrum is better than the WKB spectrum for all even quantum numbers $n\ge 2$. Additionally, for $\mu>0.1$ fm^{-1}, the mWKB results are better than the WKB results for all $n\ge 2$. This shows that even in the case of a singular potential like the Yukawa interaction the mWKB method may give a good account of the energy spectrum for certain values of the potential parameters. We do not show detail of these results as the present work concentrates on the study of nonsingular potentials only.

IV. DISCUSSION

In this paper we have computed the energy levels of some nonpolynomial, nonsingular, short-range potentials of physical interest. They are supposed to simulate optical potentials in nuclear physics. The exact solution of the Schrödinger energy spectrum has been compared with that obtained by the usual WKB (Refs. 1 and 2) and a recently proposed mWKB (Ref. 3) method.

The mWKB method is simple numerically and uses a different (matrix) representation of the classical momentum. In general, both WKB and mWKB methods produce good approximations to the exact energy eigenvalues. One may have some advantage with the mWKB method over the WKB method in the case of short-range nonsingular interactions. Usually the mWKB energies of the ground and the first two excited states lie closer to the exact energies than the corresponding WKB energies. Furthermore, if the range of the interaction is reduced without destroying the energy levels, the mWKB spectrum approximates the exact spectrum better than the WKB spectrum even for higher excited states ($n>2$). In this respect the mWKB method should be considered to be complementary to the WKB method. The latter should normally be used to calculate the energy spectrum for higher excited states, while the former appears to be advantageous to estimate the energies of the ground and the lowest excited states of a short-range nonsingular interaction, and this advantage increases as the range of the interaction is decreased. The low-lying states of a nonsingular potential simulate the optical-model states of nuclear physics and this demonstrates the usefulness of the mWKB method in problems of nuclear physics. We have also used the WKB and mWKB methods for finding the bound states in Yukawa-type potentials singular at the origin and both the methods yielded good results. Specially, for ranges of interest in nuclear physics [$\mu>0.1$ fm^{-1} in Eq. (15)] the mWKB method was very promising. Hence the mWKB method deserves systematic analyses for other types of potentials.

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