

An Improved Semi-Classical Approximation Based on Heisenberg's Matrix Mechanics

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We have previously shown that the WKB and the Einstein-Brillouin-Keller (EBK) semiclassical quantization methods can be derived within a framework provided by Heisenberg matrix mechanics. Based on the relationship between quantum mechanical matrix elements and classical Fourier components, in a form emphasized in our earlier work, we suggest a modification of the semiclassical calculation that yields markedly improved values for the matrix elements of the elementary position and momentum operators, especially for low-lying states where the WKB values are poorest. The computational framework also provides quantum-mechanical sum rules for the energies that yield similarly improved values when evaluated with the new matrix elements. The scheme is illustrated by application to the quartic oscillator.

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I. Introduction

Semi-classical approximations such as the WKB and Einstein-Brillouin-Keller (EBK) quantizations have played an important role in various fields of physics. They are useful both as a practical computation tool and as a means to gain a better understanding of the problems relevant to the quantum-classical correspondence. Earlier, we studied the connection between classical periodic or multi-periodic motions and Heisenberg matrix mechanics [1, 2]. Prior and subsequent related work on EBK quantization can be found, e.g., in Refs. [3-9]. More recently we have shown that Heisenberg's matrix mechanics provides a vantage point for studying the problem of the quantum-classical correspondence [10-12]. In this note, we show how the same framework can be exploited to yield considerably improved values for matrix elements and energies compared to the standard semi-classical approximation with minimal increase of computational effort. The method exploits the connection between the matrix elements of physical operators and the Fourier components of their corresponding classical variables. For the purpose of illustration, we shall utilize several special cases of the quartic oscillator.

The paper is organized as follows. In Sec. II, we review briefly how the WKB quantization is carried out for one-dimensional classical systems using Fourier series expansions. In Sec. III, the quantum-classical correspondence and the relation to the WKB approximation within the framework of Heisenberg's matrix mechanics are examined more closely. Taking advantage of

the connection between the physical matrix elements of operators and the Fourier components of the corresponding classical variables, an improved version of the semi-classical approximation is proposed in Sec. IV. Some numerical results supporting the merits of the improved semi-classical approximation are also presented there. Finally, a summary and concluding remarks are given in Sec. V.

II. Semi-classical quantization in Fourier representation

In this section we first examine how the semi-classical quantization of periodic motions in the form of the WKB approximation is carried out through the use of Fourier series expansions. Since most of the important elements to be illustrated are already present for a system with one degree of freedom, we therefore consider here the Hamiltonian

$$H = \frac{1}{2m} p^2 + V(x); \quad (2.1)$$

for the one-dimensional system of a particle of mass m moving in the potential $V(x)$. Assume that the potential supports only periodic motions in classical mechanics so that we only have to worry about the quantization of bound states. The classical position variable $x(t)$ may then be expanded as a Fourier series,

$$x(t) = \sum_{\circ} x_{\circ} e^{i\circ! t}; \quad (2.2)$$

where $!$ is the angular frequency of the periodic motion and the summation index \circ runs over both positive and negative integers. Using Eq. (2.2) one can readily derive from Newton's second law the following equation of motion for its Fourier components x_{\circ} ,

$$m\circ^2!^2 x_{\circ} = V_{\circ}^{\circ}; \quad (2.3)$$

where $V_{\circ}^{\circ} \sim (V^{\circ})_{\circ}$ is the \circ^{th} Fourier coefficient of $V^{\circ} = \frac{d}{dx}V(x)$. To quantize the system, we adjoin the WKB quantization condition $\int p dx = (n + \frac{1}{2})\hbar$, which after appropriate Fourier expansions takes the form ($\sim = 1$),

$$m! \sum_{\circ} \circ^2 x_{\circ} x_{i-\circ} = n + \frac{1}{2}; \quad (2.4)$$

where n is an integer representing the quantum number.

As we explain more fully below, Eqs. (2.3) and (2.4) constitute the semi-classical WKB approximation for the one-dimensional system defined by the Hamiltonian (2.1) when expressed in the Fourier representation. As for the Fourier coefficients V_{\circ}° in Eq. (2.3), they can be readily calculated in terms of x_{\circ} for polynomial potentials. For instance, for a quartic potential they can be obtained by using relationships such as

$$(x^3)_{\circ} = \sum_{\circ_1 \circ_2 \circ_3} x_{\circ_1} x_{\circ_2} x_{\circ_3}; \quad (2.5)$$

For a given quantum number n ($n = 0, 1, 2, \dots$), Eqs. (2.3) and (2.4) comprise a set of algebraic equations to be solved for x_\circ , the Fourier coefficients of the position variable, and the angular frequency $!$. However, this set of equations are not only non-linear but also infinitely coupled. Fortunately, for most systems of interest there is a hierarchy of the Fourier coefficients such as

$$|x_{\circ 1}| \gg |x_{\circ 3}| \gg |x_{\circ 5}| \gg \dots \quad (2.6)$$

whereas x_\circ with even \circ vanishes for systems with even-parity potentials. Thus, for practical applications, one can usually truncate the summations such as those in Eqs. (2.4) and (2.5) so that one only sums over, *e.g.*, $|j| \leq j_{\max}$. If the hierarchy of Fourier coefficients such as that given in Eq. (2.6) really holds, one can solve the semi-classical equations (2.3) and (2.4) in successive orders with $j_{\max} = 1, 3, 5$, and so on, until convergence to the desired numerical accuracy is obtained.

For a given quantum number n , the WKB approximation to the energy of the system, which is simply the constant term of the Fourier expansion of Eq. (2.1), is given by

$$E_n = \frac{1}{2} m \dot{x}_\circ^2 + V_0 \quad (2.7)$$

Here, V_0 is the constant term in the Fourier expansion for the potential $V(x)$, which can be readily evaluated in the same fashion as what is shown in Eq. (2.5). To distinguish the above semi-classical WKB energy from the exact quantum energy eigenvalue E_n below, it should have been denoted as E_n^{WKB} instead. Also, since the solutions for x_\circ and $!$ obtained from Eqs. (2.3) and (2.4) depend on the quantum number n , they should be denoted as $x_\circ(n)$ and $!(n)$.

III. Heisenberg's matrix mechanics and quantum-classical correspondence

Heisenberg's matrix mechanics, together with the idea that sum rules are often saturated by just a few collective states, was first developed and applied in the context of the nuclear many-body problem [13, 14]. In this method, where exact eigenstates of the Hamiltonian are used, the matrix elements of operators are unknown quantities to be solved from the relevant matrix element equations of the equations of motion and commutation relations. The practical aspects as well as the numerical structure of Heisenberg's matrix mechanics were further expounded [15, 16] through applications to various one-dimensional anharmonic oscillator applications. More recently [10-12], we have also used this framework to study the Einstein-Brillouin-Keller (EBK) quantization and the associated problem of quantum-classical correspondence for nonseparable systems possessing a phase-space structure of invariant tori. Below, we follow Ref. [16] for the presentation of our version of Heisenberg's matrix mechanics.

In this framework, one works in the energy-diagonal representation formed by the exact eigenstates $|j\rangle$ of the Hamiltonian, in which

$$H|j\rangle = E_j|j\rangle; \quad (3.1)$$

where E_j are the energy eigenvalues. In this section as well as in later sections, we set $m = 1$ for the Hamiltonian given in Eq. (2.1) and work in units with $\hbar = 1$. Thus, from the commutation

relationship $[x; p] = i$ and the fact that $[x; H] = ip$, one can easily obtain the equation of motion in the form

$$\mathbf{f}_{[x; H]; H}^{\mathbf{x}} = V'(x): \quad (3.2)$$

Furthermore, the commutation relationship can be written as

$$\mathbf{f}_{[x; H]; x}^{\mathbf{x}} = 1: \quad (3.3)$$

One then takes the matrix elements of Eq. (3.2) between the two eigenstates $|j_n\rangle$ and $|j_n + \nu\rangle$ of the Hamiltonian to obtain

$$(E_{n+\nu} - E_n)^2 \langle j_n + \nu | x | j_n \rangle = \hbar \nu V'(x) \langle j_n + \nu | j_n \rangle: \quad (3.4)$$

If one adjoins the diagonal matrix elements of the commutation relation, Eq. (3.3), which yield

$$2 \sum_{\nu=j_n}^{\infty} (E_{n+\nu} - E_n) \langle j_n + \nu | x | j_n \rangle \langle j_n | j_n + \nu \rangle = 1: \quad (3.5)$$

these two sets provide just enough independent algebraic equations to solve for $\langle j_n + \nu | x | j_n \rangle$, the matrix elements of the position operator, as well as the various excitation energies. As for the matrix elements of $V'(x)$, they can be evaluated by using the sum rules for polynomial potentials. Equations (3.4) and (3.5) constitute the main set of equations in Heisenberg's matrix mechanics for the present one-dimensional system and may be viewed as the quantum generalization of the semi-classical system, Eqs. (2.3) and (2.4). The question of how the above matrix element equations can be applied to various one-dimensional quantum systems has been discussed in detail in Ref. [16].

Next, to make contact with the classical limit, we use the method of Ref. [1] in deriving the semi-classical WKB approximation in the framework of Heisenberg's matrix mechanics. For this, we first write the matrix element of x between the two eigenstates $|j_n\rangle$ and $|j_n + \nu\rangle$ of the Hamiltonian as

$$\langle j_n + \nu | x | j_n \rangle \sim x_{\nu} \left(n + \frac{\nu}{2} \right): \quad (3.6)$$

This is motivated by the observation that, while the matrix elements of x between any two eigenstates of the Hamiltonian are peaked as functions of ν , the difference between the two quantum numbers of the eigenstates, they are smooth functions of the average of the two quantum numbers involved. This is especially the case when the quantum number n is large. Thus, for large enough n , it is justifiable to make the expansion

$$\langle j_n + \nu | x | j_n \rangle = x_{\nu}(n) + \frac{1}{2} \nu x'_{\nu}(n) + \dots: \quad (3.7)$$

Similarly, for large enough quantum numbers, we also expand the energy differences,

$$E_{n+\nu} - E_n = \nu E'(n) + \frac{1}{2} \nu^2 E''(n) + \dots: \quad (3.8)$$

where $! (n) \sim @_n E_n$.

For large enough quantum number n , each differentiation with respect to the quantum number yields a derivative smaller than the original quantity by an order of $1/n$. Thus, in the large n limit, $\langle n | x | n + \circ \rangle \cong x_\circ(n)$ and $E_{n+\circ} - E_n \cong \circ! (n)$. Using these properties, neglecting terms of relative order of $1/n^2$ or smaller, and extending the lower summation limits such as $\circ = j - n$ in Eq. (3.5) to $\circ = j - 1$, the large- n expansions of Eqs. (3.7) and (3.8) enable one to derive the semi-classical equations (2.3) and (2.4) from Eqs. (3.4) and (3.5) in a straightforward manner. The correspondence between the quantum and classical mechanics is made complete by further identifying the $x_\circ(n)$ and $! (n)$ in Eqs. (3.7) and (3.8) with those x_\circ and $!$ in Eqs. (2.3) and (2.4). Details of the procedure described, as well as some practical applications can be found in Refs. [1, 2, 16].

IV. Improved semi-classical approximation

In this section we present an improved version of the semi-classical approximation that combines features of the schemes described in Secs. II and III. We shall see, however, that the basic calculation involves the same steps needed in the standard semi-classical approximation, and that with only a minimal increase of computational effort we obtain a great increase in numerical accuracy.

As mentioned previously in Sec. II, for a given quantum number the semi-classical calculation is done by solving for $x_\circ(n)$ and $! (n)$ from Eqs. (2.3) and (2.4). These solutions in turn allow one to compute the semi-classical energy eigenvalues through Eq. (2.7). Once the energy eigenvalues are evaluated, the task of performing the semi-classical calculation seems complete. However, very often one is also interested in the values of the physical matrix elements such as $\langle n | x | n + \circ \rangle$ of the position operator, which are not exactly $x_\circ(n)$. Thus, there is more to be done.

In fact, with $n! - n | \circ=2$, Eq. (3.6) can be rewritten as

$$x_\circ(n) = \frac{D}{n} \frac{\circ}{2} \langle n | x | n + \frac{\circ}{2} \rangle + \frac{\circ E}{2} \quad (4.1)$$

These Fourier coefficients of the classical position variable are what one obtains by solving Eqs. (2.3) and (2.4) for a given quantum number n . They clearly are not the desired physical matrix elements $\langle n | x | n + \circ \rangle$ because in comparison n has been shifted downward by an amount $\circ=2$. In other words, the physical matrix element $\langle n | x | n + \circ \rangle$ actually corresponds to the \circ^{th} Fourier coefficient of the position variable but with its argument n replaced by $n + \circ=2$. It is not difficult to see that the n -dependence of $x_\circ(n)$ and $! (n)$ is dictated by the quantum number given on the right-hand side of Eq. (2.4). Thus, to obtain (better approximations to) the desired physical matrix elements $\langle n | x | n + \circ \rangle = x_\circ(n + \frac{\circ}{2})$, it appears reasonable to replace the quantum number n on the right-hand side of Eq. (2.4) by $n + \circ=2$ (\circ here not to be confused with the summation index on the left hand side of Eq. (2.4)) and solve the semi-classical equations (2.3) and (2.4) all over again for $n! - n + \circ=2$. Note that $\circ=2$ is not an integer if \circ is not an even integer. Therefore, in addition to the usual set of semi-classical quantization conditions for $n = 0, 1, 2, \dots$, one also has to solve them for $n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$ in order to obtain the desired physical matrix elements such as $\langle 0 | x | 1 \rangle = x_1(\frac{1}{2})$, $\langle 1 | x | 2 \rangle = x_1(\frac{3}{2})$, ..., $\langle 0 | x | 3 \rangle = x_3(\frac{3}{2})$, $\langle 1 | x | 4 \rangle = x_3(\frac{5}{2})$, etc.

In Table I, we show the semi-classical WKB results for the energy eigenvalues, the various Fourier coefficients $x_\circ(n)$ and physical matrix elements $x_\circ(n + \frac{\circ}{2})$ and compare them with the

exact quantum values for the anharmonic oscillator $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4$. Exactly the same thing is done in Table II for the anharmonic oscillator $H = \frac{1}{2}p^2 + \frac{1}{4}x^4$.

As is well known, semi-classical approximations such as the WKB approximation yield better results for states with higher quantum numbers. As can be easily seen from the above tables, for the ground state, which is the worst case for the WKB approximation, the errors in energy eigenvalues can be as large as 8% to 18%. However, in the corresponding cases, the errors for the physical matrix elements $x_1(\frac{1}{2}) = \langle 0|x|1 \rangle$ are only 1% to 3%. Overall, WKB calculation with $n + \frac{1}{2}$ yields much better results for the physical matrix elements $x_0(n + \frac{1}{2}) = \langle n|x|n + 1 \rangle$ than the standard WKB calculation with n does for the energy eigenvalues E_n . The main errors in energy eigenvalues for low-lying states to a large extent lie in the truncations made to the expansions such as Eqs. (3.7) and (3.8) in the semi-classical approximation. This suggests that improved accuracy for the energy eigenvalues may be achieved if we use the more accurate semi-classical results for $x_0(n + \frac{1}{2})$ and $\langle n + \frac{1}{2} | \dots | n + \frac{1}{2} \rangle$ directly to evaluate E_n in the quantum fashion. In this way one avoids the usual semi-classical truncations in evaluating the energies. As can be seen in what follows, one indeed obtains much more accurate results for the energy eigenvalues.

TABLE I. Semi-classical results are compared with their exact quantum values for the Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4$.

Quantities	WKB	Exact
E_0	0.573	0.620927
E_1	2.003	2.02597
E_2	3.682	3.69845
E_3	5.544	5.55758
E_4	7.557	7.56846
$x_1(0)$	0.444	
$x_1(\frac{1}{2}) = \langle 1 x 2 \rangle$	0.589	0.5953
$x_1(1)$	0.689	
$x_1(\frac{3}{2}) = \langle 1 x 2 \rangle$	0.768	0.7709
$x_1(\frac{5}{2}) = \langle 2 x 3 \rangle$	0.893	0.8945
$x_1(\frac{7}{2}) = \langle 3 x 4 \rangle$	0.9916	0.9925
$x_3(0)$	0.00716	
$x_3(1)$	0.0179	
$x_3(\frac{3}{2}) = \langle 0 x 3 \rangle$	0.0218	0.02013
$x_3(\frac{5}{2}) = \langle 1 x 4 \rangle$	0.0281	0.02723
$x_3(\frac{7}{2}) = \langle 2 x 5 \rangle$	0.0331	0.03256
$x_5(\frac{5}{2}) = \langle 0 x 5 \rangle$	0.000855	0.000711
$x_5(\frac{7}{2}) = \langle 1 x 6 \rangle$	0.00107	0.000982

TABLE II. Semi-classical WKB results are compared with their exact quantum values for the Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{4}x^4$.

Quantities	WKB	Exact
E_0	0.344	0.420805
E_1	1.489	1.5079
E_2	2.942	2.9588
E_3	4.608	4.6212
E_4	6.442	6.4536
$x_1(0)$	0.517	
$x_1(\frac{1}{2}) = h1jxj2i$	0.652	0.6744
$x_1(1)$	0.746	
$x_1(\frac{3}{2}) = h1jxj2i$	0.821	0.8243
$x_1(\frac{5}{2}) = h2jxj3i$	0.940	0.9416
$x_1(\frac{7}{2}) = h3jxj4i$	1.034	1.0362
$x_3(0)$	0.0233	
$x_3(1)$	0.0336	
$x_3(\frac{3}{2}) = h0jxj3i$	0.0370	0.03644
$x_3(\frac{5}{2}) = h1jxj4i$	0.0424	0.04170
$x_3(\frac{7}{2}) = h2jxj5i$	0.0466	0.04622
$x_5(\frac{5}{2}) = h0jxj5i$	0.00183	0.00171
$x_5(\frac{7}{2}) = h1jxj6i$	0.00201	0.00193

To illustrate how this improved semi-classical (ISC) approximation for the energy eigenvalues is actually carried out, we take as an example the following anharmonic oscillator Hamiltonian ($\epsilon > 0$)

$$H = \frac{1}{2}p^2 + \frac{k}{2}x^2 + \frac{\epsilon}{4}x^4; \quad (4.2)$$

Using the WKB results for $x_0(n + \frac{\epsilon}{2})$ and $! (n + \frac{\epsilon}{2})$ obtained from solving Eqs. (2.3) and (2.4) with the replacement $n ! n + \frac{\epsilon}{2}$ for the quantum numbers, the ISC energy eigenvalues are given by

TABLE III. Comparison of WKB and ISC results with exact quantum values for $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \frac{1}{4}x^4$.

	WKB	ISC	Exact
E_0	0.573	0.623	0.620927
E_1	2.004	2.026	2.02597
E_2	3.682	3.697	3.69845
E_3	5.544	5.5579	5.55758
E_4	7.557	7.5687	7.56846

TABLE IV. Comparison of WKB and ISC results with exact quantum values for $H = \frac{1}{2}p^2 + \frac{1}{4}x^4$.

	WKB	ISC	Exact
E_0	0.344	0.425	0.420805
E_1	1.489	1.503	1.5079
E_2	2.942	2.949	2.9588
E_3	4.608	4.620	4.6212
E_4	6.442	6.4532	6.4536

$$\begin{aligned}
 E_n^{ISC} = & \frac{1}{2} \sum_{i=0}^n \langle n | x^2 | i \rangle \langle i | p^2 | n \rangle + \frac{1}{4} \sum_{i=0}^n \langle n | x^4 | i \rangle \langle i | n \rangle \\
 & + \frac{1}{2} \sum_{i=0}^{n-1} \langle n | x^2 | i \rangle \langle i | x^2 | n \rangle + \frac{1}{2} \sum_{i=0}^{n-1} \langle n | x^2 | i \rangle \langle i | x^2 | n \rangle \\
 & + \frac{1}{4} \sum_{i=0}^{n-1} \langle n | x^2 | i \rangle \langle i | x^2 | n \rangle + \frac{1}{4} \sum_{i=0}^{n-1} \langle n | x^2 | i \rangle \langle i | x^2 | n \rangle + \frac{1}{4} \sum_{i=0}^{n-1} \langle n | x^2 | i \rangle \langle i | x^2 | n \rangle :
 \end{aligned}
 \tag{4.3}$$

The first term on the right-hand side in the above equation is the kinetic energy evaluated by using the matrix element form of the relationship $[x; H] = ip$. Namely,

$$\langle n+1 | ip | n \rangle = (E_{n+1} - E_n) \langle n+1 | x | n \rangle
 \tag{4.4}$$

which in the present ISC approximation becomes

$$\langle n+1 | ip | n \rangle = \langle n+1 | x | n \rangle (E_{n+1} - E_n)
 \tag{4.5}$$

The numerical results of the ISC approximation for the quartic anharmonic oscillator of Eq. (4.2) with $k = \nu = 1$ and that with $k = 0$ and $\nu = 1$ are given in Table III and Table IV, respectively. As can be easily seen there, the ISC approximation E_n^{ISC} given in Eq. (4.3) is much more accurate than the standard semi-classical approximation E_n^{WKB} . Note that the ISC energy given by Eq. (4.3) reduces to the standard WKB energy if all the various arguments of x_0 and $!$ therein are all replaced by the quantum number n .

In actual numerical calculations for the ISC approximation for the anharmonic oscillators, we have taken advantage of the hierarchy of the matrix elements (or equivalently the Fourier coefficients) of the position operator as given in Eq. (2.6). This suggests that one may do the calculations order by order. In each order, the summations in Eq. (4.3) are carried out in such a fashion that only those x_0 with $|j^0| \cdot \rho_{\text{max}}$ are retained. We have thus carried out successive orders of calculation with $\rho_{\text{max}} = 1, 3, 5$, and so on, until the desired accuracy is obtained. We have found that $\rho_{\text{max}} \cong 5$ is usually good enough for most purposes.

V. Concluding remarks

In this paper we have presented an improved version of the semi-classical approximation based on the quantum-classical correspondence in the framework of Heisenberg matrix mechanics. We have shown that this improved approximation can be readily obtained from the standard semi-classical approximation with only minimal increase of computational effort but with great increase of numerical accuracy. Namely, instead of just solving the standard semi-classical equations for quantum number $n = 0, 1, 2, \dots$, one also solves the equations for $n = \text{half odd integers}$. In this way, through the quantum-classical correspondence such as $\hbar n |x| n + \rho_i = x_0 (n + \frac{\rho_i}{2})$, much more accurate results for the physical matrix elements than the energies can be obtained. The improved semi-classical approximation proposed in this paper then consists of using these more accurate matrix elements directly to evaluate the energies in the quantum fashion. Numerical results for applications to the one-dimensional anharmonic oscillator systems indeed confirm the merit of this improved version of semi-classical approximation.

We emphasize here that the improvement over the standard semi-classical WKB approximations presented here seems to be only possible in the framework of Heisenberg's matrix mechanics. From the encouraging results for the one-dimensional systems obtained here, it is warranted to apply the same modification to improve on the EKB approximation for systems with two or more degrees of freedom which possess the phase-space structure of invariant tori. This further application of the present method is currently under investigation.

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