CHINESE JOURNAL OF PHYSICS VOL. 37, NO. 6 DECEMBER 1999

# A Modification of the Quasi-Classical Approximation of Expectation Values for Harmonic Oscillator Stationary States

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(Received May 31, 1999)

I introduce, for one degree-of-freedom harmonic oscillator stationary states, a modification of the quasi-classical approximation for expectation values of observables which are polynomial functions of the position and momentum. After time averaging a suitable function determined by the observable, instead of evaluating the average at the energy eigenvalue, if one then averages over the energy with a certain gamma distribution, one gets more accurate expectation values for large quantum numbers. I consider Monte Carlo evaluations of the averages with the random phase points chosen according to the respective distributions. Although the Monte Carlo error is greater for the modification than for the quasi-classical approximation when the same number of phase points is used, it is less than that for a Monte Carlo evaluation of a certain exact expression in which the same time averaged function is averaged over the energy with Wigner's quasiprobability distribution.

PACS. 03.65.Sq – Semiclassical theories and applications.
PACS. 02.70.Lq – Monte Carlo and statistical methods.

## I. Introduction

**I first** consider two well-known phase space integral expressions for the quantum mechanical expectation value of an operator *A* for one degree-of-freedom harmonic oscillator (HO) stationary states of quantum number n. They have the form

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} A_w(q,p) f_n[E(q,p)]dqdp, \tag{1}$$

where $q$ and $p$ are position and momentum, $E$ is the energy,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f_n(E)dqdp = 1, \tag{1a}$$

and $A_w$ is Wigner's function [1] corresponding to an operator:

$$A_w = \int_{-\infty}^{\infty} dy \exp(ipy/\hbar)\langle q - y/2|\hat{A}|q + y/2\rangle. \tag{1b}$$



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I only consider operators $\hat{A}$ which are polynomial functions of $\hat{q}$ and $\hat{p}$, of degree N. Such an operator can always be written as a linear combination of the products $\hat{p}^s\hat{q}^r$, $r$ and s being non-negative integers. Wigner's function $A$ for such a product is

$$p^s p^r - (i\hbar/2)srp^{s-1}q^{r-1} - (\hbar/2)^2\frac{1}{2}s(s-1)r(r-1)p^{s-2}q^{r-2} + O(\hbar^3)$$

as $\hbar \to 0$. Hermitian operators have a real-valued $A$,. The first expression I consider is the quasi-classical (QC) approximation [2] for large n, in which $f_n$ is

$$\delta[E/\omega - \hbar(n+1/2)]/(2\pi),$$

where w is the angular frequency. It is simply an average of $A$, over the time $t$ since $dqdp = dEdt$. The second expression is Wigner's exact one in which $f_n$ is the quasi-probability density

$$W_n = (-1)^n \exp[-2E/(\hbar\omega)]L_n[4E/(\hbar\omega)]/(2h)$$

[1], $L_n$ being the Laguerre polynomials.

Multiple degree-of-freedom generalizations of the QC expression are often evaluated by the Monte Carlo (MC) method, the random times $t$ being chosen according to a uniform distribution. This is done, for example, in Ref. [3]. There, an expectation value is computed for a certain time evolution of a stationary HO state. In Ref. [4], a phase space integral expression for a transition probability is evaluated by the MC method. Like the aforementioned exact expression, its integrand contains $W_n$ as a factor. In this paper, $I$ consider MC evaluations of the two expressions for expectation values, the random phase points being chosen with density $|f_n|$. In addition to the QC expression being conceptually simpler than the exact one, its MC error is less than that for the latter when the same number of phase points are used in both, provided that n is sufficiently large. This is proved in this paper for Hermitian $\hat{A}$.

The main feature of this paper is the introduction of a new expression obeying equation (1). For sufficiently large n, it has the following properties. It is approximate, but more accurate than the QC expression. Although its MC error, when random phase points are chosen with density $|f_n|$, is greater than that of the QC expression, it is less than that of the exact one when the same number of random phase points is used for all three evaluations, at least for Hermitian $A$. With the new expression, the energy has a gamma distribution with mean equal to the eigenenergy $\hbar\omega(n+1/2)$ and a standard deviation of $\hbar\omega/2$. Thus the dependence of $f_n$ on $E$ is given by the proportionality

$$f_n \propto [E/(\hbar\omega)]^{4n(n+1)} \exp[-(4n+2)E/(\hbar\omega)].$$

Random gamma deviates are easily generated by the rejection method [5].

## II. Results

Evaluating the exact expression, one finds integrals of the form

$$I_\ell = \frac{2\pi}{\omega}\int_0^\infty \left(\frac{E}{\hbar\omega}\right)^\ell W_n(E)dE,$$

for non-negative integers $\ell$. An integral table expresses these in terms of the hypergeometric function and using one of the Gauss recursion relations for that function [6], one finds

$$I_{\ell+1} = (n + 1/2)I_\ell + \frac{\ell^2}{4}I_{\ell-1}.$$

Using the facts $I_0 = 1$ and $I_1 = n+1/2$, it follows that both $\langle \hat{A} \rangle$ and the QC approximation $\langle \hat{A} \rangle_{QC}$ are polynomial functions of n with degree $M$, the greatest integer less than or equal to N/2. The relative error of the QC approximation is found to be

$$(\langle \hat{A} \rangle - \langle \hat{A} \rangle_{QC})/\langle \hat{A} \rangle = \frac{M(M-1)(2M-1)}{24(n+1/2)^2} + O(n^{-3}), \tag{2}$$

as $n \to \infty$. The variance of the distribution of random numbers which get averaged to produce the MC estimate is $O(n^N)$ for the QC expression and is bounded below by a function which is $O(n^N)$ for the exact one. For sufficiently large n, the variance for the exact expression $V_w$ is greater than that for the QC one $V_{QC}$:

$$V_w/V_{QC} \geq 1 + \frac{\gamma}{24}\frac{N(N-1)(2N-1)}{(n+1/2)^2} + O(n^{-3}),$$

as $n \to \infty$, where $\gamma \geq 1$. The aforementioned statement about the comparison of the MC errors follows immediately.

The proposed expression of this paper $\langle \hat{A} \rangle_G$ is easily found to be a linear combination of integral powers of $n + 1/2$, the largest power being $M$. The relative error is

$$(\langle \hat{A} \rangle - \langle \hat{A} \rangle_G)/\langle \hat{A} \rangle = \frac{M(M-1)(M-2)}{12(n+1/2)^2} + O(n^{-3}),$$

as $n \to \infty$, which for sufficiently large n is less than equation (2). $V_G$ is $O(n^N)$ with

$$V_G/V_{QC} = 1 + \frac{\gamma}{8}\frac{N(N-1)}{(n+1/2)^2} + O(n^{-3}),$$

as $n \to \infty$, where $\gamma \geq 1$, and

$$V_w/V_G \geq 1 + \frac{\gamma}{12}\frac{N(N-1)(N-2)}{(n+1/2)^2} + O(n^{-3}),$$

as $n \to \infty$, where $\gamma \geq 1$.

## III. Conclusion

For MC evaluations with the highest accuracy requirements, clearly the exact expression is the only choice among the three. As one decreases this requirement, evaluations of the proposed expression of this paper may become more efficient than those of the other two. In Ref. [4], the authors found that the MC evaluation of the transition probabilities in a certain problem required many more phase points for an exact phase space integral expression than it did for a QC approximate phase space integral expression.

As for possible generalizations of the new expression, I note that Wigner has expressed the expectation value of any operator for any state with any number of degrees-of-freedom as a phase space average of $A$, with a quasi-probability distribution [1]. The QC approximation has been generalized to include anharmonic oscillators, in which case the action is assigned the value $(n+1/2)\hbar$ [2]. The QC approximation also applies to non-polynomial observables [2] and is commonly applied to oscillators with many degrees-of-freedom [3].

**Acknowledgement**

This work was funded by the National Science Council of the Republic of China through grants 84-2113-M030-001 and 85-2113-M030-004. I thank Prof. F. Budenholzer for useful discussions and encouragement.

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