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Roles of phase cancellation removing spuriously quantized states in semiclassical mechanics

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Two types of destructive interference among quantum phases are discussed that play an essential role in canceling out the unquantized states and thereby leaving only the correct projection of true eigenstates behind. Without these mechanisms, the Fourier spectra of the autocorrelation function, from which the energy spectra can be deduced numerically, can suffer from spurious features. We show two such examples: One is a spurious spectrum that appears in the negative energy domain of the Fourier frequencies for a positive potential. The other is a family of harmonic and subharmonic frequencies that are born from the ''quantizing orbits,'' which are responsible for forming eigenstates like the periodic orbits or those satisfying the Einstein-Brillouin-Keller condition. The mechanisms for the spurious spectra to appear are analyzed, emphasizing their relationship to the quality of semiclassical wave functions. [S1050-2947(99)05707-8]

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I. INTRODUCTION

In the study of energy spectra of a system where quantum nature is fading away (or surviving), there can exist two physical situations presupposed; one is a case where the Planck constant is very small compared with the system action integrals [1–5], and the other one is a many particle system in which random cancellation among quantum phases exposes only the particle (classical) nature [6]. It is vital to investigate therefore what the essential factors giving birth to quantum eigenstates in these semiclassical systems are. For instance, the spectra of vibrationally excited states of relatively large molecules in a large amplitude motion [7] are among the most interesting subjects in this aspect. Semiclassical quantization of bound states has long been studied since the Bohr-Sommerfeld quantization condition. This condition has been rebuilt so as to quantize tori in a canonically invariant form. Further, the so-called Maslov index has been taken into account, and the resultant expression is now known as the Einstein-Brillouin-Keller (EBK) quantization condition [2,6]. For a case where a classical dynamics has no tori in phase space, namely, the case of a nonintegrable system, the periodic orbit theory due to Gutzwiller has been established to quantize the density of states [8,9]. Since then, many studies have been made to extract the quantum spectra from classically chaotic systems [5,8–11].

The monumental studies mentioned above are all concerned with identifying the quantizing orbits (or paths), along which constructive interference among quantum phases represented in terms of the action integral can form a standing wave surviving eternally. We call these relevant trajectories and paths the ''quantizing orbits'' throughout the present paper. The explicit forms of the quantization conditions or the density of states, which have been basically derived through the stationary phase argument in application of the Wentzel-Kramers-Brillouin (WKB) theory or the semiclassical kernel, are represented exclusively in terms of the relevant information about the quantizing orbits only.

Yet, there can exist another general and more straightforward method to calculate the quantum spectra (eigenvalues), that is, the numerical evaluation of the Fourier transform of the autocorrelation function (see [12] for a method to extract eigenfunctions directly). In this less analytical approach, many anonymous classical trajectories other than the quantizing orbits are also to be included in the semiclassical evaluation. In comparing this kind of numerical approach to the above analytical theories, a natural question arises as to what is the role of the anonymous nonquantizing orbits in the quantization process. Also, what pathological phenomena can result, if their contributions are not appropriately taken into account? We would like to address these subjects in this paper. This kind of study seems not as ''useful'' as those giving the quantization conditions in that it is not intended to locate the correct eigenvalues. Nonetheless, the present study could facilitate understanding of one aspect of quantum-classical correspondence.

The results we are going to present here have been obtained through our study of semiclassical mechanics [13,14] based on the Maslov-type wave packet [3]. We have established a class of semiclassical approximation that has a hierarchical structure below or equal to the semiclassical Feynman kernel [1,2]: A continuous class of semiclassical wave functions has been constructed, which are represented in terms of different numbers of classical trajectories. Some of them are more accurate but require many classical trajectories, the semiclassical Feynman kernel being an extreme example. The others are less accurate but demand far fewer trajectories. We have shown that the latter type of wave function must be quite promising in an application to large-dimensional systems. With the help of these characteristics, we have scanned a relationship between quantum and classical mechanics in an approach that has not been done before

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*Author to whom correspondence should be addressed. Electronic address: KazTak@mns2.c.u-tokyo.ac.jp to our knowledge. In an application to a system which lies beyond the validity of the present semiclassical scheme, we have found spurious spectra; negative energy spectra for a positive potential. In the present paper, we ascribe this pathological appearance to the breakdown of the stationary phase condition in the Fourier time integral of the correlation function, which in turn originates from the breakdown of random phase cancellation among the anonymous nonquantizing orbits. Conversely, with this mechanism of the stationary phase in time, quantum mechanics removes the unnecessary components of the spectra.

We show another example of a spurious spectrum that also has to be canceled out in quantum mechanics. Suppose that only one quantizing orbit can dominate an eigenvalue, which can be generally seen in a one-dimensional system. If one then represents approximately a correlation function only with a single quantizing orbit without other general trajectories, many harmonics and subharmonics of this energy appear in the Fourier spectrum in addition to the true eigenvalue. This example also directly suggests the role of destructive interference of nonquantizing orbits in removing the spurious frequencies.

Although these spurious spectra have been found in applications of our Maslov-type semiclassical theory [13,14], we want to stress that the essential role of the destructive interference is generic. In other words, although the patterns of spurious spectra can depend on the semiclassical method one uses, the role of anonymous trajectories in cancellation of the unnecessary components is intrinsic. That this is really the case can be confirmed by a poor application of the semiclassical kernel, which can also yield similar spurious spectra.

This paper is organized as follows. After briefly reviewing our semiclassical scheme in Sec. II, which is based on the Maslov-type wave packet, we discuss how the negative (spurious) spectrum arises and a mechanism of how these spurious components are canceled in Sec. III A. Section III B shows the role of anonymous trajectories that cancel out the harmonics and subharmonics of a true eigenvalue. Section IV concludes this paper.

II. MASLOV-TYPE SEMICLASSICAL WAVE FUNCTIONS

A. General

It is well known that Maslov and Feodoriuk [3] have established a systematic theory to generate a class of wave functions in the form of

$$\Psi(q,t)=F(q,t)\exp\left[\frac{i}{\hbar}S_{\mathrm{cl}}\right], \tag{2.1}$$

where S_{cl} denotes the classical action satisfying the Hamilton-Jacobi equation [15,16]

$$\frac{\partial S_{\mathrm{cl}}}{\partial t}+H\left(q,\frac{\partial S_{\mathrm{cl}}}{\partial q},t\right)=0. \tag{2.2}$$

The semiclassical equation of motion for the amplitude function $F(q,t)$ is

$$\frac{\partial F}{\partial t}+\nu\cdot\boldsymbol{\nabla}F+\frac{1}{2}(\boldsymbol{\nabla}\cdot\nu)F=0, \tag{2.3}$$

which has neglected $(i\hbar/2)\nabla^2F$ from the full (rigorous) equation of motion for F [13,14]. An explicit solution to Eq. (2.3) can be readily obtained such that

$$\begin{aligned}F(q_t,t)&=F(q_0,0)\left(\frac{\partial q_t}{\partial q_0}\right)^{-1/2}\\&=F(q_0,0)\left|\frac{\partial q_t}{\partial q_0}\right|^{-1/2}\exp\left[-\frac{i\pi M}{2}\right],\end{aligned} \tag{2.4}$$

where the derivative $\partial q_t/\partial q_0$ is taken under a fixed initial momentum p_0, and M is the Maslov index in this representation that counts the number of zeros of $\partial q_t/\partial q_0$ up to degeneracy [2]. The classical action in Eq. (2.1) has naturally been chosen as the F_2-type generating function of Goldstein [15] (denoted as S_2 hereafter). In other words, all the classical paths representing Eq. (2.1) share a single action surface, the initial momentum of which is p_0 everywhere. This is why we call this function the action decomposed function (ADF). Having this action function as a phase, the initial form of ADF at $t=0$ is rewritten as

$$\Psi_{p_0}(q,t)=F(q,0)\exp\left[\frac{i}{\hbar}p_0q\right]. \tag{2.5}$$

An arbitrary wave function can be continuously expanded in terms of the ADF's (see below). A wave function which consists of a single ADF, denoted by $\Psi^{p_0}_{\mathrm{local}}(q_t,t)$, is specified as single ADF (SADF) throughout this paper. A SADF is rewritten in a little more global form as

$$\begin{aligned}\Psi_{p_0}(q,t)=&\int dq_0\,\delta(q-q_t(q_0,p_0))F(q_0,t)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2}\\&\times\exp\left[\frac{i}{\hbar}S_2(q_t,p_0;t)-\frac{i\pi M}{2}\right].\end{aligned} \tag{2.6}$$

Although the local solution $F(q_t,t)$ in Eq. (2.4) diverges at every caustic point, where the Jacobian determinant $\partial q_t/\partial q_0$ becomes zero, the global solution Eq. (2.6) does not suffer from the divergence [13,14,17].

The time-correlation function represented in a SADF is

$$\begin{aligned}C(t)&=\langle\Psi_{p_0}(0)|\Psi_{p_0}(t)\rangle\\&=\int dq_0F^*(q_t,0)F(q_0,0)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2}\\&\quad\times\exp\left[-\frac{i}{\hbar}p_0q_t+\frac{i}{\hbar}S_2(q_t,p_0;t)-\frac{i\pi M}{2}\right].\end{aligned} \tag{2.7}$$

As was stressed in the previous paper [14], this expression involves only an N-dimensional integral. This is in marked contrast to the correlation function represented in terms of the semiclassical Feynman kernel [2,17], which consists of at least $2N$-fold integrals. Therefore, a SADF is anticipated to provide quantum spectra with far fewer classical trajectories.

It has been evidenced through our numerical calculations that this is really the case [14]. On the other hand, SADF has a clear limitation beyond which the theory is not valid. Hence, SADF can be a very powerful tool to calculate spectra of a rather large system, if care to its limitation is taken.

B. Propagation of an arbitrary wave function in terms of ADF's

Suppose we have a decomposition for an arbitrary wave function such that

$$\Psi(q,0)=F(q)G(q), \tag{2.8}$$

under a condition that $G(q)$ has a momentum representation

$$\tilde{G}(p)=\frac{1}{(2\pi\hbar)^N}\int G(q)\exp\left(-\frac{i}{\hbar}pq\right)dq. \tag{2.9}$$

We assume that $F(q)$ is a slowly varying function in q space. The total wave function thus decomposed is rewritten as

$$\Psi(q,0)=\int dp_0\tilde{G}(p_0)F(q)\exp\left(\frac{i}{\hbar}p_0q\right), \tag{2.10}$$

which is regarded as a superposition of many ADF's of Eq. (2.5). The semiclassical time propagation of this wave function is straightforward such that

$$\Psi(q,t)=\int\int dq_0dp_0\delta(q-q_t)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2}F(q_0,0)\tilde{G}(p_0)\times\exp\left(\frac{i}{\hbar}S_2(q_t,p_0;t)-\frac{i\pi M}{2}\right), \tag{2.11}$$

where $q_0=\partial S_2(q,p_0;t=0)/\partial p_0$.

1. The kernel limit

The semiclassical Feynman kernel $\langle q|\exp[-(i/\hbar)Ht]|p_0\rangle=K(q,p_0;t)$ is reproduced by setting

$$F(q)=1 \quad \text{(constant);}$$

$$G(q)=\Psi(q) \quad \text{(wave function itself)} \tag{2.12}$$

and hence

$$\tilde{G}(p)=\tilde{\Psi}(p) \quad \text{(momentum representation of the wave function)}. \tag{2.13}$$

We then have

$$\Psi(q,t)=\frac{1}{(2\pi\hbar)^N}\int\int dq_0dp_0\delta(q-q_t)\left|\frac{\partial q_t}{\partial q_0}\right|^{-1/2}\times\exp\left(-\frac{i\pi M}{2}\right)\exp\left(\frac{i}{\hbar}S_2(q_t,p_0;t)\right)\tilde{\Psi}(p_0). \tag{2.14}$$

This is nothing but

$$\Psi(q,t)=\int dp_0K(q,p_0;t)\tilde{\Psi}(p_0) \tag{2.15}$$

except for a minor difference in the constant phase factor [17(c)].

2. Single ADF (SADF)

A SADF, Eq. (2.5), can be readily reproduced with an almost trivial procedure by setting

$$F=F(q) \quad \text{and} \quad G=\exp\left(\frac{i}{\hbar}p_0q\right), \quad \tilde{G}(p)=\delta(p-p_0). \tag{2.16}$$

The most significant difference between the kernel and SADF is in the distribution in momentum space, namely, Eqs. (2.13) and (2.16).

3. A pathological extreme of the SADF

The quality of a SADF depends strongly on the smoothness of the initial wave function. Suppose that $F(q)$ is a Gaussian function. If the exponent is small enough [and hence $F(q)$ is smooth enough], the level of accuracy of such a SADF is not deteriorated so much. On the other hand, in the limit of the large exponent (fixing the magnitude of the Planck constant), it gets off the boundary of the semiclassical validity. To be more precise, let us set

$$F(q)=\delta(q-q_c), \quad G(q)=\exp\left(\frac{i}{\hbar}p_cq\right), \quad \tilde{G}(p)=\delta(p-p_c). \tag{2.17}$$

We then have

$$\Psi(q,t)=\int dq_0dp_0\delta(q-q_t)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2}\times\exp\left(-\frac{i\pi M}{2}\right)\exp\left(\frac{i}{\hbar}S_2(q_t,p_0;t)\right)\times\delta(q_0-q_c)\,\delta(p_0-p_c). \tag{2.18}$$

This expression is stimulating to think about a ''classical limit'' of a quantum wave function, since a point (q_c,p_c) is specified in phase space in Eq. (2.18), determining a single classical trajectory along which the wave function is to be propagated. Thus it just seems to give a classical limit of a wave function. It also seems to have violated the uncertainty principle. However, specification at (q_c,p_c) in phase space is in a keen contradiction with the initial wave function

$$\Psi(q,0)=F(q)G(q)=\delta(q-q_c)\exp\left(\frac{i}{\hbar}p_cq\right)=\delta(q-q_c)\exp\left(\frac{i}{\hbar}p_cq_c\right), \tag{2.19}$$

in which information about p_c is already lost to the phase factor $\exp[(i/\hbar)p_cq_c]$. Thus the semiclassical limit of Eq. (2.18) is simply wrong. The point is that the Gaussian func-

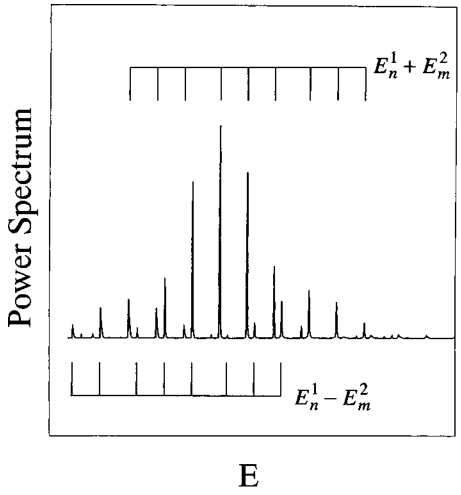

FIG. 1. Spectrum for a direct product of two anharmonic systems with use of the single action decomposed function. $\hbar=1.0$. Negative energies have arisen in one of the oscillators, for which anharmonicity is very weak.

tion should not have been brought to the δ function with fixing the magnitude of the Planck constant at a finite value.

III. ROLE OF PHASE CANCELLATION

A. Negative energies

1. Negative spectrum for a positive potential

In a previous paper [14], we have shown that the correlation function represented in terms of a SADF can produce quantum spectra very well with a much smaller number of classical trajectories. However, if a SADF is applied to a system in which quantum (classical) nature is significantly strong (weak) such as dynamics of electrons, for which the Planck constant is relatively large, the resultant correlation function for a positive potential can produce spurious spectra in the negative frequency domain [14]. Let us take an example in a very simple system composed of a direct product of two independent Morse oscillators

$$H=\left(\frac{p_1^2}{2}+D[1-\exp(-\lambda_1 q_1)]^2\right)+\left(\frac{p_2^2}{2}+D[1-\exp(-\lambda_2 q_2)]^2\right). \tag{3.1}$$

The parameters are set to $D=50$, $\lambda_1=0.1$, and $\lambda_2=0.03$. We here deliberately choose a large Planck constant $\hbar=1.0$, which brings the system far beyond the semiclassical domain. With an initial wave packet given as a Gaussian,

$$\Psi_0(q_1,q_2)=\left(\frac{1}{\pi}\right)^{1/2}\exp\left[-\frac{1}{2}(q_1^2+q_2^2)\right], \tag{3.2}$$

we have obtained a spectrum as shown in Fig. 1. Spurious combination bands arising from a negative energy like $E_0^1-E_1^2$ are observed, where E_j^i is the jth energy of the ith oscillator. The negative spectrum occurs only for the second oscillator, which is very close to a harmonic oscillator due to the small anharmonicity parameter $\lambda_2=0.03$. The first oscillator, on the other hand, does not give such a negative spectrum because of the higher anharmonicity [14].

The negative spectra for a positive potential can be suppressed by lessening the magnitude of the Planck constant. The present situation is simply summarized that this oscillator system is not in the domain where the present semiclassical approximation is valid enough. Our concern here is not to improve the semiclassical theory for removing the spurious spectrum but to analyze how the negative spectrum has appeared in the present context and how quantum mechanics suppresses the unnecessary components leaving only the correct eigenvalues. Since it is not unusual for negative frequencies to arise from a Fourier spectrum of a general time-reversal quantity, it is not trivial how the correct quantum correlation function does not generate the negative frequency.

2. A stationary phase condition on the Fourier time integral

Let us consider a Fourier spectrum of a correlation function

$$\begin{aligned}P(E)&=\int dtC(t)\exp\left(\frac{i}{\hbar}\varepsilon t\right)\\&=\int\int dtdq\Psi^*(q,0)\Psi(q,t)\exp\left(\frac{i}{\hbar}\varepsilon t\right)\\&=2\pi\hbar\sum_i|c_i|^2\delta(\varepsilon-E_i),\end{aligned} \tag{3.3}$$

where c_i is the coefficient of a true eigenfunction having the energy E_i in a trial function $\Psi(q,t)$. Here in this Fourier spectrum $\varepsilon/\hbar$ serves simply as a frequency covering $[-\infty,\infty]$ and ε does not have to be regarded as an energy at this moment.

a. Case of the kernel in the trace formula. Let us begin with the density of states that has been extensively studied by Gutzwiller in his periodic orbit theory [8,9],

$$\begin{aligned}\mathrm{Tr}\,\delta(\varepsilon-H)&=(2\pi\hbar)^{-1}\int dt\int dqK(q,q;t)\exp\left(\frac{i}{\hbar}\varepsilon t\right)\\&=(2\pi i\hbar)^{-N/2}\int dt\int dq\left|\frac{\partial q}{\partial p_0}\right|^{-1/2}\\&\quad\times\exp\left(\frac{i}{\hbar}S_1(q,q;t)-\frac{i\pi\mu}{2}+\frac{i}{\hbar}\varepsilon t\right),\end{aligned} \tag{3.4}$$

where μ is the Maslov index. We now apply the stationary phase argument to this Fourier time integral. Since q is an independent variable and therefore independent of time, and also due to the property of the Hamilton principal function [15], we simply have

$$\frac{\partial}{\partial t}\{S_1(q,q;t)+\varepsilon t\}=-E_{\mathrm{cl}}+\varepsilon=0. \tag{3.5}$$

Thus ε must be one of the classical energies, which are never negative for a positive potential. We would like to emphasize that Eq. (3.5) can be brought about without even the periodic orbit condition arising from the trace operation [8,9], that is,

$$\frac{\partial S_1(q,q;t)}{\partial q}=p(t)-p(0)=0. \tag{3.6}$$

Incidentally, the condition of $\varepsilon=E_{\text{cl}}$ is also essential to construct a quantization condition like the EBK condition [1–5], in which only Hamilton's characteristic function [15]

$$\sum \oint p_i dq_i \tag{3.7}$$

remains out of the Hamilton principal function

$$\sum \oint p_i dq_i - E_{\text{cl}} t. \tag{3.8}$$

To obtain the quantization condition, elaborated manipulations including the summation over the infinite cycles along the periodic orbits are necessary [8,9,11]. However, in our context, the condition $\varepsilon=E_{\text{cl}}$ suffices to see that the correlation function can have values only in the positive energy domain of ε.

b. Case of the general ADF. We next proceed to the case of ADF, which is less trivial than the above kernel case. With use of the general form of the decomposition as in Eq. (2.8), the Fourier spectrum based on the correlation function is written as

$$\begin{aligned} P(E)=\int dt \int dq_1 dp_1 \int dq_0 dp_0 \,\delta(q_t(q_0,p_0)-q_1) \\ \times \tilde{G}^*(p_1)\tilde{G}(p_0)F^*(q_1,0)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2} F(q_0,0) \\ \times \exp\left(\frac{i}{\hbar}[S_1(q_t,q_0;t)+q_0p_0-q_1p_1+\varepsilon t]-\frac{i\pi M}{2}\right). \end{aligned} \tag{3.9}$$

Although this function covers the versions ranging from the semiclassical kernel to a SADF depending on the selection of F and G, we first confine ourselves to a case of the kernel limit and its proximity. The case of SADF will be considered separately. It was readily shown in a previous paper [14] that $P(E)$ is dominated by trajectories which satisfy

$$q_t(q_0,p_0)=q_1 \tag{3.10}$$

arising from the δ function in Eq. (3.9), and

$$p_t=p_1 \tag{3.11}$$

that comes from the stationary phase condition to the integral q_0 with fixing (q_1,p_1). Thus trajectories making a dominant contribution to the integral should pass repeatedly through a point, $(q_t(q_0,p_0),p_t(q_0,p_0))=(q_1,p_1)$. This is a periodic orbit. All the possible periodic orbits are to be summed up by integrating in the (q_1,p_1) space.

We now want to consider the stationary phase on the time coordinate in Eq. (3.9). Before applying the stationary phase condition, however, care should be taken as to how the time derivative of the action integral $S_1(q_t,q_0,t)$ should be made. In contrast to the case of Eqs. (3.4) and (3.5), the time integral proceeds with the point q_t along a trajectory, and thus we should take

$$\frac{d}{dt}\{S_{\text{cl}}(q_t,q_0;t)+\varepsilon t\}=L+\varepsilon, \tag{3.12}$$

where $L(=T-V)$ is the classical Lagrangian. Applying the stationary phase argument to Eq. (3.9) under the obvious constraint $q_1=q_t$, we have rather a complicated form

$$\begin{aligned} &\frac{d}{dt}[S_1(q_t,q_0;t)+q_0p_0-q_1p_1+\varepsilon t] \\ &=\frac{d}{dt}[S_1(q_t,q_0;t)-q_tp_1]+\varepsilon \\ &=\frac{1}{2}p_t^2-V(q_t)-\frac{dq_t}{dt}p_1+\varepsilon. \end{aligned} \tag{3.13}$$

It thus turns out that a simple application of the stationary phase condition does not warrant that ε should coincide with the energy of the corresponding classical trajectory. However, we know that the correlation function should be dominated by the trajectories specified by Eqs. (3.10) and (3.11). Let us call these trajectories ''dominant trajectories'' in that they make a stationary phase contribution to the correlation function $C(t)$. All other trajectories should make a very minor contribution due to the Riemann-Lebesgue lemma [19], provided that sampling of classical trajectories to evaluate $C(t)$ is not biased. In other words, if both the dominant trajectories and nondominant trajectories are dealt with appropriately, the correct value of the Fourier transform in Eq. (3.9) must be determined by the dominant trajectories only. We thus insert the periodic orbit condition Eq. (3.11) into Eq. (3.13) and get

$$\begin{aligned} &\frac{d}{dt}[S_1(q_t,q_0;t)+q_0p_0-q_1p_1+\varepsilon t] \\ &=-\frac{1}{2}p_t^2-V(q_t)+\varepsilon=-E_{\text{cl}}+\varepsilon, \end{aligned} \tag{3.14}$$

which is essentially the same as Eq. (3.5). Again, it is stressed that the contribution from the nondominant trajectories, which do not satisfy Eq. (3.11), to the correlation function must be canceled out by their destructive interference beforehand.

c. Case of Single ADF. We next consider the case of SADF separately, since the stationary phase argument for SADF is a little different from that applied to the kernel, and since a SADF tends to have negative spectrum more often than the kernel does. The energy spectrum represented in terms of a SADF is

$$\begin{aligned} P(E)=\int dt \int dq_0 F^*(q_t,0)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2} F(q_0,0) \\ \times \exp\left(\frac{i}{\hbar}[S_1(q_t,q_0;t)+q_0p_0-q_tp_0+\varepsilon t]-\frac{i\pi M}{2}\right). \end{aligned} \tag{3.15}$$

The dominant trajectories to determine the correlation function are those that satisfy

$$\frac{\hbar}{i}\frac{d}{dq_0}\left[-\frac{i}{\hbar}p_0q_t+\frac{i}{\hbar}p_0q_0+\frac{i}{\hbar}S_{\rm cl}(q_t,q_0;t)-i\frac{\pi}{2}M\right]$$
$$=p_0+\frac{\partial}{\partial q_0}S_{\rm cl}(q_t,q_0;t)+\frac{\partial q_t}{\partial q_0}\frac{\partial}{\partial q_t}[S_{\rm cl}(q_t,q_0;t)-p_0q_t]$$
$$=\frac{\partial q_t}{\partial q_0}(p_t-p_0)=0, \tag{3.16}$$

that is,

$$p_t=p_0, \tag{3.17}$$

provided that $F(q_0,0)$ and other preexponential factors in Eq. (3.15) are smooth enough. Note again that the orbits of Eq. (3.17) are not necessarily periodic. The spectrum given as in Eq. (3.14) is to be dominated by the stationary phase condition for the Fourier time integral such that

$$\frac{\hbar}{i}\frac{d}{dt}\left[-\frac{i}{\hbar}p_0q_t+\frac{i}{\hbar}p_0q_0+\frac{i}{\hbar}S_{\rm cl}(q_t,q_0;t)+\varepsilon t\right]$$
$$=-p_tp_0+\frac{1}{2}p_t^2-V+\varepsilon=0. \tag{3.18}$$

Again if the correlation function is really dominated by the trajectories satisfying Eq. (3.17), we have

$$\frac{\hbar}{i}\frac{d}{dt}\left[-\frac{i}{\hbar}p_0q_t+\frac{i}{\hbar}p_0q_0+\frac{i}{\hbar}S_{\rm cl}(q_t,q_0;t)+\varepsilon t\right]$$
$$=\left(\frac{1}{2}p_t^2+V\right)+\varepsilon=-E_{\rm cl}+\varepsilon=0. \tag{3.19}$$

Thus, ε should be positive irrespective of the absolute values of the individual peaks that are eventually extracted. However, negative spectra can arise, if, for instance, trajectories satisfying $-p_0p_t-2V=0$ happen to have a large contribution of order $O(\hbar^0)$ to the correlation function for an accidental reason, thereby leading to

$$\varepsilon=-E_{\rm cl}. \tag{3.20}$$

d. Case of the δ function as a SADF. Another example can be made in a pathological case of the SADF, in which $F(q)=\delta(q-q_c)$, as in Eq. (2.17). Since $F(q)$ is not smooth, the stationary phase condition in Eq. (3.17) is never valid. Hence, there is no mechanism leading to the condition $\varepsilon=E_{\rm cl}$ in the corresponding spectrum

$$P(E)=\int dt\int dq\,\delta(q-q_c)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2}\delta(q-q_t(q_c,p_c))$$
$$\times\exp\left(\frac{i}{\hbar}[S_1(q_t,q_0;t)+q_0p_c-q_cp_c+\varepsilon t]-\frac{i}{\hbar}M\right)$$
$$=\int dt\,\delta(q_t(q_c,p_c)-q_c)\left|\frac{\partial q_t}{\partial q_0}\right|^{1/2}\exp\left(\frac{i}{\hbar}[S_1(q_t,q_0;t)\right.$$
$$\left.+q_0p_c-q_tp_c+\varepsilon t]-\frac{i}{\hbar}M\right). \tag{3.21}$$

Here we find neither $\varepsilon=E_{\rm cl}$ nor other conditions in this expression. It is therefore not surprising to observe that this δ-function representation of a SADF is always associated with negative spectra.

3. Summary from the examples

The equality $\varepsilon=E_{\rm cl}$ has thus been identified as a condition for a negative spectrum in a positive potential not to appear. This is never an unusual equality but rather is seen quite universally in the literature [18]. However, as far as we are aware, it has not been presented before what consequence would occur if this condition is not well fulfilled. Incidentally, we note that Eqs. (3.5), (3.14), and (3.19) are only a necessary condition for a negative spectrum not to appear. Even if they are not fulfilled, the negative spectrum can happen not to appear numerically.

Through the above case studies, we notice that there can be a robustness class to an extent for the equality $\varepsilon=E_{\rm cl}$ to hold or to break down. In the semiclassical integral of the density of states Eq. (3.4), for instance, it is hard to break $\varepsilon=E_{\rm cl}$ unless a very poor set of classical trajectories is employed. As noted there, $\varepsilon=E_{\rm cl}$ holds even without the periodic orbit condition of Eq. (3.6). [The periodic orbit theory itself does not take into account the numerical calculation of Eq. (3.4), since it proceeds to the final expression assuming $\varepsilon=E_{\rm cl}$ is perfectly satisfied.] On the other hand, $\varepsilon=E_{\rm cl}$ in Eqs. (3.14) and (3.19) is not independent of the numerical accuracy of the correlation function. In particular, contributions to the correlation function from trajectories that are not the dominant trajectories should be well canceled out among them. If the cancellation is not well realized due to a poor choice of a set of classical trajectories, a part of the correlation function that should be very small otherwise can survive, thereby rendering itself to the time integral without satisfying $\varepsilon=E_{\rm cl}$. In analogy to the Riemann-Lebesgue lemma that holds for an oscillatory integral [19], one can generally expect that a larger number of trajectories is more favorable to destructive interference of quantum phases. In this sense, the condition $\varepsilon=E_{\rm cl}$ becomes more robust in the order: the kernel [Eq. (3.4)) $>$general ADF [Eq. (3.9)] $>$single ADF [Eq. (3.15)] $>\delta$ function SADF [Eq. (3.21)]. We will show that this is really the case in a different numerical example in the next section.

B. Harmonics and subharmonics arising from quantizing trajectories

We next turn to another kind of example, in which destructive interference among the quantum phases is essential to remove the unnecessary spectral components. Here our focus is placed on the role of anonymous orbits that are not the quantizing trajectories.

1. Role of unquantizing trajectories

The simplest way to examine the role of the anonymous trajectories would be to estimate an energy spectrum without them and see the difference. As a sample system, we adopt a

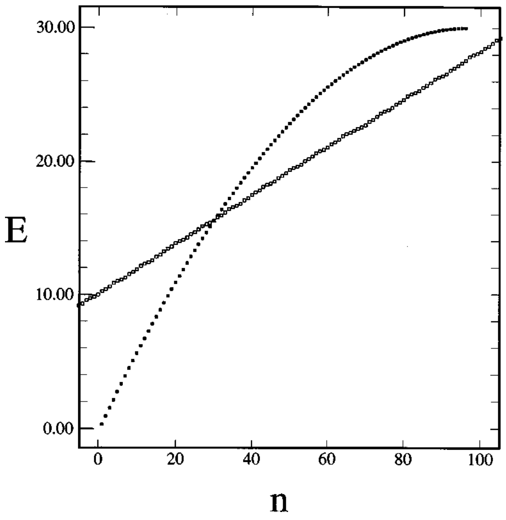

FIG. 2. The energies plotted against the quantum numbers for a one-dimensional anharmonic oscillator. The black squares on the convex curve represent the true eigenvalues. The white squares on the straight line have been given by the δ-function SADF with use of a single classical trajectory that is responsible for quantizing the state of $n=30$.

one-dimensional Morse oscillator retaining the first coordinate in Eq. (3.1) with the parameters $D=30$ and $\lambda=0.08$. The Planck constant is again chosen at $\hbar=1.0$. An initial wave packet takes the form

$$\Psi(q,0)=\left(\frac{\alpha}{\pi}\right)^{1/4}\exp\left[-\frac{\alpha}{2}(q-q_c)^2\right]. \qquad (3.22)$$

The correlation function is now to be evaluated with only one of the quantizing trajectories. We pick a trajectory which is responsible for producing the quantum state of the quantum number $n=30$. The spectrum is calculated with a SADF. To justify that only a single trajectory is used to evaluate the correlation function, it seems natural to set $F(q)=\delta(q-q_c)$, $\tilde{G}(p)=\delta(p-p_c)$, and $G(q)=\exp[(i/\hbar)p_c q]$, see Eq. (2.17) with (q_c,p_c) being placed on the relevant orbit. To mimic this δ function, we choose α in the Gaussian to be 10^7.

The Fourier spectrum obtained from the thus estimated correlation function is depicted in Fig. 2; each white square on the straight line marks an energy in the order of the corresponding quantum numbers. The energy arrangement hence looks as though it came from a harmonic oscillator. For a comparison, a set of the correct energies is displayed in Fig. 2, which forms a convex curve (black squares). The two lines cross each other at $n=30$ as they should. However, the other energy values estimated based on the single trajectory show large deviations from the true values. The Fourier energies other than that of $n=30$ are all spurious and have arisen as harmonics of the fundamental frequency given by this trajectory. It is not surprising that such harmonics are generated through the phase factor of this anharmonic motion, since it consists of many harmonics in itself. The point is, however, that these unnecessary harmonic components must be eliminated, leaving only the true eigenstate in quantum mechanics. Therefore one can conclude that without the anonymous trajectories other than the quantizing orbits these virtual states cannot be canceled away.

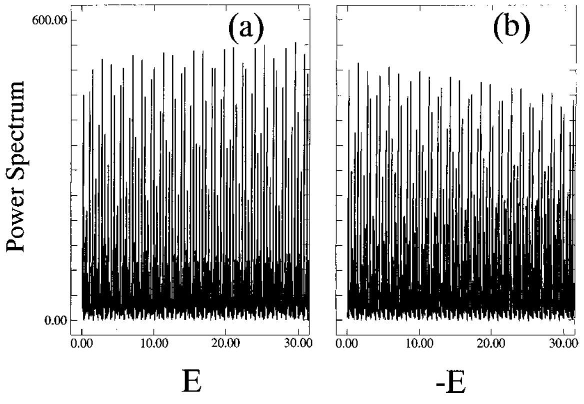

FIG. 3. Power spectrum of the correlation function in terms of the δ-function SADF with use of a single classical trajectory that is responsible for quantizing the state of $n=30$. (a) and (b) are for the positive and negative energies.

2. An effect of the δ function

We further consider what makes the approximation based on a single trajectory so bad. Here again we examine the negative energies, since we have seen above that the spuriously negative spectrum is an indicator of poor quality in the semiclassical approximation. Figure 3 exhibits both positive and negative energies in (a) and (b), respectively. Negative energy components are observed as high as in the positive domain, indicating a very bad quality of the spectrum. This is not only because we have used a single trajectory representation but also because a δ-function-like sharp function has been adopted in the correlation function.

In a previous paper [14], we discussed that there are two general requirements to keep the correlation function good: (i) The phase should satisfy the stationary condition, and (ii) the initial amplitude function $F(q,0)$ must be smooth enough. It is obvious that the pathological case in which $F(q)=\delta(q-q_c)$ and $\tilde{G}(p)=\delta(p-p_c)$ meets none of these requirements. Although the harmonic components cannot be eliminated without the presence of anonymous trajectories, the quality of the approximation is expected to be improved to some extent by relaxing the δ function.

We then relax the effect of relaxing the δ function by reducing the exponent of the Gaussian function, Eq. (3.22) to $\alpha=1.0$. The Gaussian function now becomes much smoother in shape. Nonetheless only a single trajectory that is exactly the same as that used above for the "δ-function" case is adopted to represent the integral. Figure 4 exhibits the energies obtained as a function of the quantum numbers. Here again, the harmonic frequencies, aligning on a line, have been generated as a natural consequence of the use of a single trajectory, and the energy at $n=30$ is set to be exact. However, we notice significant difference between the cases of Figs. 2 and 4. First, the Fourier amplitude arising from the correlation function becomes too small beyond $n=45$ to assign the energies. Second and moreover, the straight line on which the harmonic energies lie seems tangent to the convex curve for the exact energies, thus displaying that the energies nearby $n=30$ are also good approximations to the exact val-

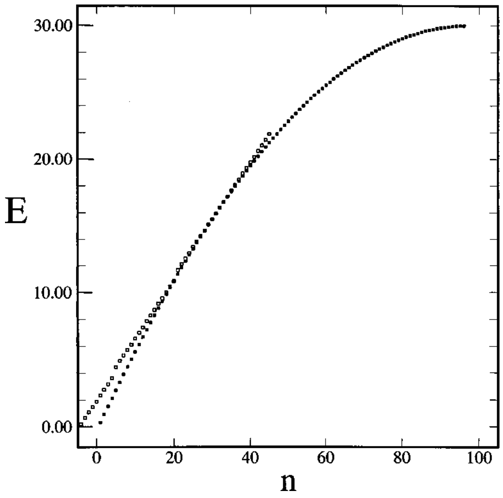

FIG. 4. The same as Fig. 2, except that a smooth initial Gaussian function is adopted in place of the δ function for the SADF calculation.

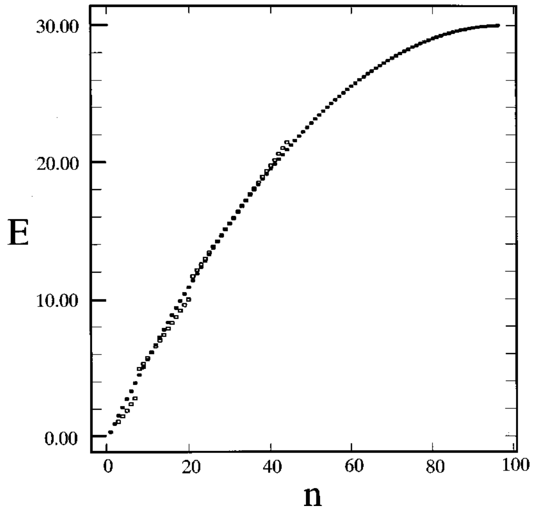

FIG. 6. The same as Fig. 2, except that a smooth initial Gaussian function is adopted and the kernel limit has been taken.

ues. This makes a clear contrast to the δ-function case. Figure 5 shows the positive and negative spectra of the present wide Gaussian wave packet. As anticipated theoretically, the negative component bears only small amplitudes.

We further proceed to the kernel limit of ADF, which is more time consuming but more accurate. As in Eqs. (2.12) and (2.13) we simply set $F(q)=1$ and set $G(q)=\Psi(q)$ as the Gaussian function of $\alpha=1.0$ that was used above in the SADF calculation. Again the trajectory quantizing $n=30$ is examined. In contrast to the previous cases, however, 1000 different points have been prepared on this single periodic orbit in phase space in order to carry out the integration of the correlation function. Figures 6 and 7 are the counterparts corresponding to Figs. 2(4) and 3(5). As discussed in the preceding section, the amplitudes in the negative energy range are the smallest in the kernel version. The global feature of the positive spectrum seems to be divided into three groups as in the case of SADF [Fig. 5(a)]. Unlike the SADF case, the harmonics seen in Fig. 6 are also grouped into three bunches and each has come closer to the true eigenvalues.

Thus, we have shown that although the harmonic appearance of the spectrum cannot be eliminated, the quality of the approximation is improved with use of the smoother initial wave packet. In order to remove the harmonic components and retain the correct spectrum only, an appropriate treatment of the anonymous trajectories which are not the quantizing orbits is unavoidable.

IV. CONCLUDING REMARKS

There can exist in principle two types of phase interference that work in generating quantum eigenstates and their energy spectrum. One is the constructive interference of quantum phases among particular trajectories such as those satisfying the EBK condition and the periodic orbits. These trajectories or paths can support on them appropriate classical actions, together with the Maslov index, that can in turn represent standing waves on manifolds in phase space. This kind of role of the phase interference is well known to date and the most important activity in this regard is directed towards the study of spectrum for classically chaotic systems [5,9–11].

The other one is destructive interference under a random phase situation. We have shown in the present paper two examples of quantum destructive interference that removes undesired components in a discrete energy spectrum and thereby makes it possible for only correct eigenvalues to sur-

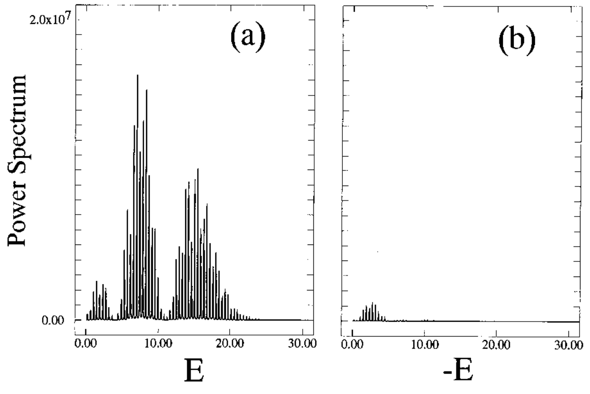

FIG. 5. The same as Fig. 3, except that a smooth initial Gaussian function is adopted in place of the δ function for the SADF calculation.

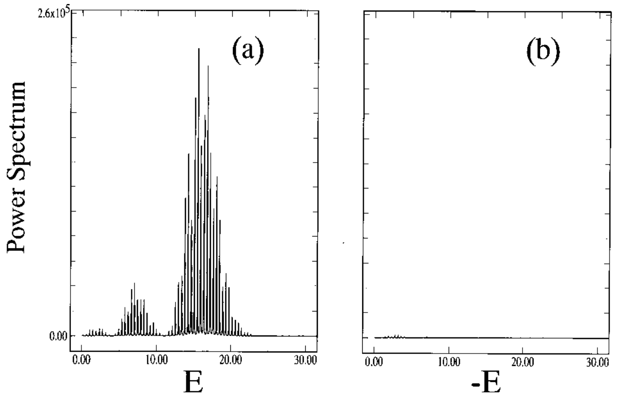

FIG. 7. The same as Fig. 3, except that a smooth initial Gaussian function is adopted and the kernel limit has been taken.

vive in the Fourier transform of the correlation function. It has been shown that the Fourier spectra can suffer from anomalous features without these phase-interference mechanisms. The first one is components that appear in the negative domain of the energy in scanning the Fourier frequencies. This spurious spectrum can arise due to failure in random phase cancellation in the correlation function, which should not remain to the integration at $\varepsilon \neq E_{\mathrm{cl}}$. Therefore the correlation function must be evaluated correctly not only for the part that brings about the energy peaks but also for the portion with which no eigenstate is associated. Hence appearance of the negative energies can be used as a useful indicator to check the quality of a semiclassical wave function. The second example of destructive interference is related to the harmonic spectra which are born from the quantizing orbits that satisfy the quantization condition and are responsible for giving energy peaks at correct locations. While these quantizing orbits support the standing waves on them, they alone should inevitably generate their harmonics and subharmonics too, which are of course spurious in anharmonic systems. These unnecessary (sub)harmonics should be eliminated by the destructive interference among other anonymous trajectories.

The study of the destructive interference is therefore highly vital to distinguishing the mathematical structure of quantum mechanics from that of classical mechanics. The examples we have raised in this paper are rather simple. A much more subtle example of the destructive quantum interference is the so-called quantum smoothing of the infinitely nested structure of classical phase space in a nonintegrable system [10]. This subject is under study in terms of our semiclassical scheme.

ACKNOWLEDGMENT

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