A semiclassical approximation to quantum dynamics

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In this paper we advance a new approximation scheme for the dynamics of an N particle system, which is based on the expansion of the Heisenberg equations of motion in powers of ħ in the coherent state representation. The time evolution of the physical observables is generated classically by a Hamiltonian H_s, which is derived from the original Hamiltonian by adding $2N^2$ virtual particles to the system. These virtual particles are related to the dispersion of the quantum mechanical wave function, and reflect the (time dependent) sensitivity of the instantaneous positions and momenta x_i, p_i to the variation of the initial conditions. The approximate equations of motion preserve the commutation relations between the coordinates and the momenta and the total (quantum) energy. The present approximation may be adequate for the study of the dynamics of coupled anharmonic oscillators in the quasiperiodic regime.

I. INTRODUCTION

The semiclassical approximation,[1] introduced in the early days of quantum mechanics,[2] is an important tool for the study of the properties of microscopic systems in states characterized by high quantum numbers. As such, it continues to attract considerable attention. The semiclassical approach was applied extensively to the theory of molecular collisions utilizing the stationary phase approximation and the superposition principle[3–5] or the classical trajectories method.[6] Recent developments include a comprehensive study of bound states in the semiclassical limit[7] and many other important contributions.[8–10] The main effort in these studies was directed towards the calculations of the energy spectrum and the stationary wave function of the system. While these quantities yield direct information concerning the resonance frequencies and the transition probabilities, they do not provide convenient starting point for the study of the spatial dynamics of the system. The conventional quantum mechanical approach which rests on the expansion in terms of the basis set functions imposes several practical difficulties at high energies.

The dynamics of classical coupled harmonic oscillators attracted much attention in the past two decades. This was mainly due to two aspects of such systems. First, the observation that nonlinear coupling between harmonic oscillators do not necessarily result in statistical equipartition of the energy[11] attracted considerable interest.[12–14] Second, the nature of the soliton[15] and its dynamics are under active study.[16] Recently, there were few attempts to apply the knowledge and the concepts which were acquired in the course of the study of classical systems[17] to quantum systems.[18,19] This is most naturally accomplished in the spirit of the semiclassical approach by adding quantum corrections to the classical equations of motion. As we have already noted, the traditional semiclassical formalism is not directly applicable for this purpose, so that new approximation schemes were advanced. Ichikawa *et al.*[20] established a quantum correction to the classical equations of motion of a linear anharmonic chain by assuming that a coherent state preserves its coherence properties for times which are long relative to the time scale of the relevant dynamic phenomena. Within the framework of this approximation, they demonstrated the existence of solitons in an anharmonic chain with cubic nonlinearity. This method was generalized and applied also to the Morse and Toda lattices,[21] leading to the exhibition of solitons in these systems. It is known, however, that in the presence of nonlinear couplings, an initially coherent state loses its coherence properties.[22] Therefore, it is impossible to estimate, even qualitatively, the error which is introduced by the Ichikawa *et al.* approximation. A different semiclassical approach to the soliton problem based on a generalized WKB theory was devised by Shirajufi.[23] In another recent work, Heller[24] derived the approximate equation of motion for a wave packet characterized by an arbitrary number of parameters by utilizing a variational principle.

The approximation scheme introduced in the present article is based on the expansion of the Heisenberg equations of motion in $\hbar$. This approach differs from the traditional semiclassical methods[1] which rest on expansion of the Schrödinger equation. In this manner, we derive equations of motion which have a classical form with a quantum correction. The same idea was recently used to study the condition of stochasticity in a particular forced nonlinear oscillator.[25] The formalism given here applies to any system of N particles with a velocity independent potential. Our equations of motion have the virtue of preserving, to first order in $\hbar$, the commutation relations between the coordinates and the momenta, and the total (quantum) energy.

II. THE SEMICLASSICAL EQUATIONS OF MOTION

We consider a quantum system of N interacting particles with the Hamiltonian

$$H=\sum_{j=1}^{N}\frac{\hat{p}_j^2}{2m_j}+V(\hat{x}_1,\ \ldots\ ,\hat{x}_N)\,. \tag{1}$$

As a basis to the Hilbert space, we use the Gaussian

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functions

$$|\boldsymbol{\xi},\boldsymbol{\pi}\rangle = \prod_{j=1}^{N} |\xi_j,\pi_j\rangle , \quad (2)$$

where

$$\langle x_j|\xi_j,\pi_j\rangle = (\pi\sigma_j^2)^{-1/4} \exp\left[-\frac{(x_j-\xi_j)^2}{2\sigma_j^2} + \frac{i\pi_j n_j}{\hbar} - \frac{i\pi_j\xi_j}{2\hbar}\right] \quad (3)$$

and σ_j are constants with dimensions of length, which serve as input data for the problem. We introduce the variables

$$\alpha_j = \frac{1}{\sqrt{2}}\left(\frac{\xi_j}{\sigma_j} + \frac{i\sigma_j}{\hbar}\pi_j\right) , \quad (4)$$

so that

$$\xi_j = \frac{\sigma_j}{\sqrt{2}}(\alpha_j+\bar{\alpha}_j) , \quad \pi_j = \frac{\hbar}{i\sqrt{2}\sigma_j}(\alpha_j-\bar{\alpha}_j) . \quad (5)$$

The basis functions (2) can be labeled now in terms of the complex variables $\boldsymbol{\alpha}$. It is readily recognized that $|\boldsymbol{\alpha}\rangle$ is a coherent state,[26] which constitutes an eigenstate of the boson annihilation operator a_j:

$$a_j|\boldsymbol{\alpha}\rangle = \alpha_j|\boldsymbol{\alpha}\rangle , \quad (6)$$

where

$$a_j = \frac{1}{\sqrt{2}}\left(\frac{\hat{x}_j}{\sigma_j} + \frac{i\sigma_j}{\hbar}\hat{p}_j\right) . \quad (7)$$

The Heisenberg equations of motion for the operators $\hat{x}_j$ and $\hat{p}_j$ are

$$\frac{d\hat{x}_j}{dt} = \frac{\partial H}{\partial \hat{p}_j} = \frac{\hat{p}_j}{m_j} , \quad (8)$$

$$\frac{d\hat{p}_j}{dt} = -\frac{\partial H}{\partial \hat{x}_j} = -\frac{\partial V}{\partial \hat{x}_j} . \quad (9)$$

In what follows, we shall use two semiclassical expansions, which are proved in the Appendix: (A) First semiclassical expansion: Let Ω_1 and Ω_2 be any two operators defined in the N particle Hilbert space $\mathcal{H}_N$. Then,

$$\langle\alpha|(\Omega_1\Omega_2|\boldsymbol{\alpha}\rangle = O_1O_2 + (\nabla_\alpha O_1\cdot\nabla_{\bar{\alpha}}O_2) + 0(\hbar^2) , \quad (10)$$

where

$$O_{1,2}(\boldsymbol{\alpha},\bar{\boldsymbol{\alpha}}) \equiv \langle\boldsymbol{\alpha}|\Omega_{1,2}|\boldsymbol{\alpha}\rangle , \quad (11)$$

$$(\nabla_\alpha)_k = \frac{\partial}{\partial\alpha_k} , \quad (\nabla_{\bar{\alpha}})_k = \frac{\partial}{\partial\bar{\alpha}_k} . \quad (12)$$

(B) Second semiclassical expansion: Let $\Omega_1, \ldots, \Omega_M$ be a set of commutative operators defined in $\mathcal{H}_N$, and let f be an analytic function of M arguments. Then,

$$\langle\boldsymbol{\alpha}|f(\Omega_1,\ldots,\Omega_M)|\boldsymbol{\alpha}\rangle = f(O_1,\ldots,O_M) + \frac{1}{2}\sum_{k,l=1}^{M}\frac{\partial^2 f}{\partial O_k\partial O_l}(\nabla_\alpha O_k\cdot\nabla_{\bar{\alpha}}O_l) + 0(\hbar^2) . \quad (13)$$

The nature of the term $0(\hbar^2)$ is discussed in the Appendix. From now on, we shall drop this term for the sake of simplicity. It will be more convenient to use the variables ξ_j and π_j instead of the α_j. To carry out the transformation, we introduce the following definitions:

$$(\nabla_\xi)_k = \frac{\sigma_k}{\sqrt{2}}\frac{\partial}{\partial\xi_k} , \quad (\nabla_\pi)_k = \frac{\hbar}{\sqrt{2}\sigma_k}\frac{\partial}{\partial\pi_k} . \quad (14)$$

It is easily verified that the term appearing in Eq. (13) is

$$(\nabla_\alpha O_k\cdot\nabla_{\bar{\alpha}}O_l) = (\nabla_\xi O_k\cdot\nabla_\xi O_l) + i(\nabla_\xi O_k\cdot\nabla_\pi O_l) - i(\nabla_\pi O_k\cdot\nabla_\xi O_l) + (\nabla_\pi O_k\cdot\nabla_\pi O_l) . \quad (15)$$

This expression can be simplified if Ω_k and Ω_l commute. Using the first semiclassical expansion and Eq. (15), we get

$$\langle\alpha|[\Omega_k,\Omega_l]|\alpha\rangle = (\nabla_\alpha\Omega_k\cdot\nabla_{\bar{\alpha}}\Omega_l) - (\nabla_{\bar{\alpha}}\Omega_k\cdot\nabla_\alpha\Omega_l) = 2i[(\nabla_\xi O_k\cdot\nabla_\pi O_l) - (\nabla_\xi O_l\cdot\nabla_\pi O_k)] . \quad (16)$$

Therefore, if $[\Omega_k,\Omega_l]=0$, we obtain

$$(\nabla_\alpha O_k\cdot\nabla_{\bar{\alpha}}O_l) = (\nabla_\xi O_k\cdot\nabla_\xi O_l) + (\nabla_\pi O_k\cdot\nabla_\pi O_l) . \quad (17)$$

Substitution of Eq. (17) into (13) yields

$$\langle\boldsymbol{\xi},\boldsymbol{\pi}|f(\Omega_1,\ldots,\Omega_M)|\boldsymbol{\xi},\boldsymbol{\pi}\rangle = f(O_1,\ldots,O_M) + \frac{1}{2}\sum_{k,l=1}^{M}\frac{\partial^2 f}{\partial O_k\partial O_l}\cdot[(\nabla_\xi O_k\cdot\nabla_\xi O_l) + (\nabla_\pi O_k\cdot\nabla_\pi O_l)] . \quad (18)$$

We are now in a position to derive the semiclassical equations of motion. For the sake of simplicity, we introduce

$$x_j(\boldsymbol{\xi},\boldsymbol{\pi}) = \langle\boldsymbol{\xi},\boldsymbol{\pi}|\hat{x}_j|\boldsymbol{\xi},\boldsymbol{\pi}\rangle , \quad (19)$$

$$p_j(\boldsymbol{\xi},\boldsymbol{\pi}) = \langle\boldsymbol{\xi},\boldsymbol{\pi}|\hat{p}_j|\boldsymbol{\xi},\boldsymbol{\pi}\rangle . \quad (20)$$

The equation of motion for x_j is obtained by rewriting Eq. (8) as

$$\frac{dx_j}{dt} = \frac{p_j}{m_j} . \quad (21)$$

To get an equation of motion for p_j, we apply Eq. (18) to (9) and choose $\Omega_1 = x_1, \ldots, \Omega_N = x_N$, which results in

$$\frac{dp_j}{dt} = -\frac{\partial}{\partial x_j} \times \left\{V + \frac{1}{2}\sum_{k,l=1}^{M}\frac{\partial^2 V}{\partial x_k\partial x_l}[(\nabla_\xi x_k\cdot\nabla_\xi x_l) + (\nabla_\pi x_k\cdot\nabla_\pi x_l)]\right\} . \quad (22)$$

Equations (21) and (22) have to be augmented by the equations of motion for the gradients $\nabla_\xi x_k$ and $\nabla_\pi x_k$. These can be derived by differentiation of the primary equations of motion (21) and (22):

$$\frac{d}{dt}\nabla_{\xi,\pi}x_j = \frac{\nabla_{\xi,\pi}p_j}{m_j} , \quad (23)$$

$$\frac{d}{dt}\nabla_{\xi,\pi}p_j = -\frac{\partial}{\partial x_j}\sum_{k=1}^{M}\frac{\partial V}{\partial x_k}\nabla_{\xi,\pi}x_k . \quad (24)$$

In deriving Eq. (24), we neglected terms of the order of $\hbar$ in the rhs, since these terms will contribute terms of order $\hbar^2$ to the primary equations of motion (21)–(22), and such terms are discarded anyway. It should be noted that this is a crucial step in the present approximation scheme, which enabled us to derive a closed set of equations of motion for x_j and p_j.

In order to solve Eqs. (21)–(24), we have to supply the initial conditions. These are derived from the requirement that, at $t=0$, the Heisenberg and the Schrödinger pictures coincide. From this requirement, it follows that, at $t=0$,

$$x_j = \xi_j \ , \tag{25}$$

$$p_j = \pi_j \ , \tag{26}$$

$$\nabla_\xi x_j = \frac{\sigma_j}{\sqrt{2}} \mathbf{v}_j, \ \nabla_\pi p_j = \frac{\hbar}{\sqrt{2}\sigma_j} \mathbf{v}_j \ , \tag{27}$$

$$\nabla_\pi x_j = 0 \ , \quad \nabla_\xi p_j = 0 \ , \tag{28}$$

where $\mathbf{v}_j$ is a unit vector in the N dimensional space in the direction of the jth coordinate. Equations (21)–(28) constitute a complete dynamic theory. It is important to note that Eqs. (21)–(24) are isomorphous to the classical equations of motion for a system of $N+2N^2$ particles, which are generated by the (classical) Hamiltonian

$$H_s = \sum_{j=1}^{N} \left[\frac{p_j^2}{2m_j} + \frac{(\nabla_\xi p_j)^2}{2m_j} + \frac{(\nabla_\pi p_j)^2}{2m_j} \right] + V + \frac{1}{2} \sum_{k,l=1}^{N} \frac{\partial^2 V}{\partial x_k \partial x_l} \left[(\nabla_\xi x_k \cdot \nabla_\xi x_l) + (\nabla_\pi x_k \cdot \nabla_\pi x_l) \right] . \tag{29}$$

The components of the vectors $\nabla_\xi x_k$, $\nabla_\pi x_k$ and $\nabla_\xi p_k$, $\nabla_\pi p_k$ in Eq. (29) are interpreted as the coordinates and the momenta, respectively, of $2N^2$ additional "virtual particles." Thus, in the present approximation, all the information about the quantum system characterized by H can be derived from a purely classical study of H_s. Note that the only traces of quantum mechanics which survived in the present treatment are the quantities $\hbar$ and σ_j which appear in the initial conditions.

III. CONSERVATION RELATIONS

Consider first energy conservation. Using the second semiclassical expansion [Eq. (18)], it is easily verified that

$$\langle \boldsymbol{\xi}, \boldsymbol{\pi} | H | \boldsymbol{\xi}, \boldsymbol{\pi} \rangle = H_s \tag{30}$$

and therefore our equations of motion conserve the total (quantum) energy.

Next, we demonstrate the conservation of the commutation relations of the dynamic variables. As a matter of fact, in the derivation of Eq. (22), we used the commutation of the operators $\hat{x}_j$. In what follows, we show that our equations (21)–(24) do indeed preserve the commutation relations of the various coordinate and momenta operators in such a manner that

$$\langle [\hat{x}_j, \hat{x}_k] \rangle = \langle [p_j, p_k] \rangle = 0 \ , \tag{31}$$

$$\langle [\hat{x}_j, \hat{p}_k] \rangle = i\hbar \delta_{jk} \ , \tag{32}$$

where we introduced the shortened notation

$$\langle \Omega \rangle = \langle \boldsymbol{\xi}, \boldsymbol{\pi} | \Omega | \boldsymbol{\xi}, \boldsymbol{\pi} \rangle \ .$$

Using Eq. (16), we get

$$\langle [\hat{x}_j, \hat{x}_k] \rangle = 2i[(\nabla_\xi x_j \cdot \nabla_\pi x_k) - (\nabla_\pi x_j \cdot \nabla_\xi x_k)] \ , \tag{33}$$

$$\langle [\hat{p}_j, \hat{p}_k] \rangle = 2i[(\nabla_\xi p_j \cdot \nabla_\pi p_k) - (\nabla_\pi p_j \cdot \nabla_\xi p_k)] \ , \tag{34}$$

$$\langle [\hat{x}_j, \hat{p}_k] \rangle = 2i[(\nabla_\xi x_j \cdot \nabla_\pi p_k) - (\nabla_\pi x_j \cdot \nabla_\xi p_k)] \ . \tag{35}$$

Differentiating Eqs. (33)–(35) with respect to time, and using Eqs. (23) and (24), we obtain

$$\frac{d}{dt} \langle [\hat{x}_j, \hat{x}_k] \rangle = \frac{1}{m_k} \langle [\hat{x}_j, \hat{p}_k] \rangle - \frac{1}{m_j} \langle [\hat{x}_k, \hat{p}_j] \rangle \ , \tag{36}$$

$$\frac{d}{dt} \langle [\hat{p}_j, \hat{p}_k] \rangle = \frac{\partial}{\partial x_j} \sum_{l=1}^{N} \frac{\partial V}{\partial x_l} \langle [\hat{p}_k, \hat{x}_l] \rangle - \frac{\partial}{\partial x_k} \sum_{l=1}^{N} \frac{\partial V}{\partial x_l} \langle [\hat{p}_j, \hat{x}_l] \rangle \ , \tag{37}$$

$$\frac{d}{dt} \langle [\hat{x}_j, \hat{p}_k] \rangle = \frac{1}{m_j} \langle [\hat{p}_j, \hat{p}_l] \rangle - \frac{\partial}{\partial x_k} \sum_{l=1}^{N} \frac{\partial V}{\partial x_l} \langle [x_j, x_l] \rangle \ . \tag{38}$$

Equations (36)–(38) determine the various commutation relations in a unique manner once the initial conditions are specified. From Eqs. (27) and (28), we see that the initial conditions are

$$\langle [\hat{x}_j, \hat{x}_k] \rangle |_{t=0} = \langle [\hat{p}_j, \hat{p}_k] \rangle |_{t=0} = 0 \ , \tag{39}$$

$$\langle [\hat{x}_j, \hat{p}_k] \rangle |_{t=0} = i\hbar \delta_{jk} \ . \tag{40}$$

It is easily verified that Eqs. (31) and (32) provide the solution of Eqs. (36)–(38) with the initial conditions (39) and (40). Therefore, the commutation relations conserve their correct values, and our previous assumption about the commutativity of the coordinate operators is justified.

IV. PHYSICAL SIGNIFICANCE OF THE VIRTUAL PARTICLES

The additional virtual particles resulting from the present semiclassical treatment can be assigned both a classical and a quantum interpretation. From the classical point of view, ξ_j and π_j are the initial coordinates and momenta, respectively. The virtual coordinate $(\nabla_\xi x_k)_j$ represents the change in the instantaneous value of x_k due to an addition of the quantity $\sigma_j/\sqrt{2}$ to the initial condition ξ_j, the virtual momentum $(\nabla_\xi p_k)_j$ represents the change in the instantaneous value of p_k due to an addition of the quantity $\hbar/\sqrt{2}\sigma_j$ to the initial condition π_j, etc. From the quantum mechanical point of view, the additional virtual particles are related to the dispersion of the operators $\hat{x}_k$ and $\hat{p}_k$. Indeed, using Eq. (18), we obtain

$$\langle x_k^2 \rangle - \langle x_k \rangle^2 = (\nabla_\xi x_k)^2 + (\nabla_\pi x_k)^2 \ , \tag{41}$$

$$\langle p_k^2 \rangle - \langle p_k \rangle^2 = (\nabla_\xi p_k)^2 + (\nabla_\pi p_k)^2 \ . \tag{42}$$

An important conclusion from the above considerations is that the evolution of the dispersion of the coordinate and of the momentum operators in a quantum system is closely related to the sensitivity of the trajectories of the corresponding classical system to the initial conditions.

V. DISCUSSION

The time has come to consider the limitations of our semiclassical scheme for the dynamics of an N particle system. We shall be somewhat more specific in the discussion of the validity of this approximation than just merely invoking the usual correspondence principle requirement of high quantum numbers.

We consider first the potential. It is important that the motion of the system will occur in a region where the potential is a smooth analytic function of the coordinates. As the present derivation involves an expansion of the potential in Taylor series, the smoothness of the potential is obviously necessary. Higher quantum corrections will probably contain higher derivatives of the potential with respect to the coordinates. Therefore, whenever the system approaches a singularity of the potential, our approximation will break down.

Second, consider the validity condition for the expansion which leads to the present scheme. A general necessary condition for the validity of a perturbation treatment is that the corrective terms will be small relative to the leading terms. In our case, the correction is the second term in the rhs of Eq. (22), and therefore a necessary condition for the validity of our semiclassical approximation is

$$\left|\frac{\partial V}{\partial x_j}\right| \gg \frac{1}{2}\left|\frac{\partial}{\partial x_j}\sum_{k,l=1}^{N}\frac{\partial^2 V}{\partial x_k \partial x_l}\left[(\nabla_\xi x_k\cdot\nabla_\xi x_l)+(\nabla_\pi x_k\cdot\nabla_\pi x_l)\right]\right|. \tag{43}$$

For a harmonic potential, the rhs of the inequality (43) vanishes altogether and, indeed, for a harmonic potential our scheme is exact.

One of the contributions to the inequality (43) is the spatial dispersion of the coordinate operator (or, in the Schrödinger picture, the spatial dispersion of the wave function). This quantity is expected, in general, to increase with time. Therefore, the range of times for which our scheme is adequate is determined by the rate by which the spatial dispersion expands. As demonstrated in Sec. IV, the dispersion is related to the sensitivity of the classical trajectories to the initial conditions, which in turn are determined by the nature of the classical motion. In a quasiperiodic motion regime, the separation between two trajectories emerging from two adjacent points in the phase space increases linearly with time, while in a stochastic motion regime, this separation increases exponentially with time.[27] Therefore, we do not recommend interpreting the virtual particles resulting from our treatment as additional degrees of freedom in the statistical sense. We suggest that the most effective application of the present new method will involve the study of the dynamics of coupled anharmonic oscillators in the quasiperiodic regime.

APPENDIX: THE SEMICLASSICAL EXPANSIONS OF OPERATORS

Before elaborating on the semiclassical expansions of operators in the coherent state representation, we would like to clarify what we mean here by such an expansion. The quantum parameters that appear in our scheme are σ_j and $\hbar$. Since all the physical quantities can be expressed in terms of the coordinates and of the momenta, the quantities $\sigma_j/\Delta x$ and $\hbar/\sigma_j\Delta p$ can be regarded as the small parameters of the expansion, where Δx and Δp are characteristic ranges of the spatial and of the momentum coordinates, respectively. If the σ_j contain a factor of $\sqrt{\hbar}$, as we shall assume from now on to be the case [recall that for coherent states of a harmonic oscillator $\sigma=(\hbar/m\omega)^{1/2}$], all those small parameters contain a factor $\hbar^{1/2}$. In this sense, the semiclassical expansion can be regarded as an expansion in $\hbar$.

The factor $\hbar$ will not appear explicitly in the expansion. Its presence is implied by the operators $\partial/\partial a^+$ and $\partial/\partial a$ (throughout this Appendix, all operators are the usual Schrödinger operators). Indeed, from Eq. (7), we obtain

$$\frac{\partial}{\partial a^+}=\frac{\sigma_j}{\sqrt{2}}\frac{\partial}{\partial \hat{x}_j}-\frac{\hbar}{i\sqrt{2}\sigma_j}\frac{\partial}{\partial \hat{p}_j}, \tag{A1}$$

$$\frac{\partial}{\partial a_j}=\frac{\sigma_j}{\sqrt{2}}\frac{\partial}{\partial \hat{x}_j}+\frac{\hbar}{i\sqrt{2}\sigma_j}\frac{\partial}{\partial \hat{p}_j}. \tag{A2}$$

Therefore, each of the operators $\partial/\partial a_j^+$ and $\partial/\partial a_j$ implies a factor $\hbar^{1/2}$.

We turn now to the proof of the first semiclassical expansion. Let us represent the operators Ω_1 and Ω_2 as a normally ordered power series in the operators a_k and a_k^+:

$$\Omega_1=\sum_{\mathbf{n}_1,\mathbf{m}_1} b^{(1)}_{\mathbf{n}_1,\mathbf{m}_1}\prod_{k=1}^{N}(a_k^+)^{n_{1k}}a_k^{m_{1k}}, \tag{A3}$$

$$\Omega_2=\sum_{\mathbf{n}_2,\mathbf{m}_2} b^{(2)}_{\mathbf{n}_2,\mathbf{m}_2}\prod_{k=1}^{N}(a_k^+)^{n_{2k}}a_k^{m_{2k}}. \tag{A4}$$

The vector indices have N components, and the summation is performed over each component independently. In order to find the normally ordered presentation of the product $\Omega_1\Omega_2$, we shall use the following identity,[28] which is satisfied by the boson creation and annihilation operators a^+ and a:

$$a^j(a^+)^k=\hat{N}\left[\left(a+\frac{\partial}{\partial a^+}\right)^j(a^+)^k\right]$$
$$=(a^+)^k a^j+\frac{\partial^2}{\partial a\partial a^+}\left[(a^+)^k a^j\right]+0(\hbar^2), \tag{A5}$$

where $\hat{N}$ is the normal ordering operator. All the other terms contain higher order derivatives which imply the presence of $\hbar$ to second power or higher, and this is the meaning of $0(\hbar^2)$. We proceed now with the product $\Omega_1\Omega_2$:

$$\Omega_1\Omega_2=\sum_{\mathbf{n}_1,\mathbf{m}_1}\sum_{\mathbf{n}_2,\mathbf{m}_2} b^{(1)}_{\mathbf{n}_1,\mathbf{m}_1}b^{(2)}_{\mathbf{n}_2,\mathbf{m}_2}\prod_{k=1}^{N}(a_k^+)^{n_{1k}}a_k^{m_{1k}}\prod_{k=1}^{N}(a_k^+)^{n_{2k}}a_k^{m_{2k}}=\sum_{\mathbf{n}_1,\mathbf{m}_1}\sum_{\mathbf{n}_2,\mathbf{m}_2} b^{(1)}_{\mathbf{n}_1,\mathbf{m}_1}b^{(2)}_{\mathbf{n}_2,\mathbf{m}_2}\prod_{k=1}^{N}(a_k^+)^{n_{1k}}\prod_{k=1}^{N}a_k^{m_{1k}}(a_k^+)^{n_{2k}}\prod_{k=1}^{N}a_k^{m_{2k}}$$
$$=\sum_{\mathbf{n}_1,\mathbf{m}_1}\sum_{\mathbf{n}_2,\mathbf{m}_2} b^{(1)}_{\mathbf{n}_1,\mathbf{m}_1}b^{(2)}_{\mathbf{n}_2,\mathbf{m}_2}\prod_{k=1}^{N}(a_k^+)^{n_{1k}}\prod_{k=1}^{N}\left\{(a_k^+)^{n_{2k}}a_k^{m_{1k}}+\frac{\partial^2}{\partial a_k\partial a_k^+}\left[(a_k^+)^{n_{2k}}a_k^{m_{1k}}\right]\right\}\prod_{k=1}^{N}a_k^{m_{2k}}+0(\hbar^2)=\hat{N}\left(\Omega_1\Omega_2+\sum_{k=1}^{N}\frac{\partial\Omega_1}{\partial a_k}\frac{\partial\Omega_2}{\partial a_k^+}\right)+0(\hbar^2) \tag{A6}$$

Taking the expectation value of $\Omega_1\Omega_2$ in the state $|\boldsymbol{\alpha}\rangle$, we get

$$\langle\boldsymbol{\alpha}|\Omega_1\Omega_2|\boldsymbol{\alpha}\rangle=O_1O_2+(\nabla_\alpha O_1\cdot\nabla_{\bar{\alpha}}O_2)+0(\hbar^2), \tag{A7}$$

where we used Eqs. (11) and (12). This is the first semiclassical expansion. For a single particle space ($N=1$), this result was derived by Berman and Zaslavsky.[13] Note that if Ω_1 and Ω_2 commute, then Eq. (A7) implies that

$$(\nabla_\alpha O_1 \cdot \nabla_{\bar{\alpha}} O_2) = (\nabla_{\bar{\alpha}} O_1 \cdot \nabla_\alpha O_2) + 0(\hbar^2)\ . \tag{A8}$$

We turn now to the proof of the second semiclassical expansion. This will be done in two stages. At the first stage, we prove the relation

$$\langle \boldsymbol{\alpha} | \Omega^n | \boldsymbol{\alpha} \rangle = O^n + \tfrac{1}{2} n(n-1) O^{n-2} (\nabla_\alpha O \cdot \nabla_{\bar{\alpha}} O) + 0(\hbar^2)\ . \tag{A9}$$

The proof will be presented by the method of mathematical induction. Equation (A9) is obviously valid for $n=1$; we assume now that it is valid for n and calculate $\langle \boldsymbol{\alpha} | \Omega^{n+1} | \boldsymbol{\alpha} \rangle$. Using Eq. (A7), we get

$$\begin{aligned}\langle \boldsymbol{\alpha} | \Omega^{n+1} | \boldsymbol{\alpha} \rangle &= \langle \boldsymbol{\alpha} | \Omega^n \Omega | \boldsymbol{\alpha} \rangle = \langle \boldsymbol{\alpha} | \Omega^n | \boldsymbol{\alpha} \rangle O + (\nabla_\alpha \langle \boldsymbol{\alpha} | \Omega^n | \boldsymbol{\alpha} \rangle \cdot \nabla_{\bar{\alpha}} O) + 0(\hbar^2) \\ &= [O^n + \tfrac{1}{2} n(n-1) O^{n-2} (\nabla_\alpha O \cdot \nabla_{\bar{\alpha}} O)] \cdot O + n O^{n-1} (\nabla_\alpha O \cdot \nabla_{\bar{\alpha}} O) + 0(\hbar^2) = O^{n+1} + \tfrac{1}{2} n(n+1) O^{n-1} (\nabla_\alpha O \cdot \nabla_{\bar{\alpha}} O) + 0(\hbar^2)\ ,\end{aligned}$$

which completes the proof. The next stage is a generalization of this result to a product of powers of operators:

$$\langle \boldsymbol{\alpha} | \prod_{k=1}^{M} \Omega_k^{n_k} | \boldsymbol{\alpha} \rangle = P_M + \frac{1}{2} \sum_{k,l=1}^{M} \frac{\partial^2 P_M}{\partial O_k \partial O_l} (\nabla_\alpha O_{(k,l)} \cdot \nabla_{\bar{\alpha}} O_{[k,l]}) + 0(\hbar^2)\ , \tag{A10}$$

where

$$P_M = \prod_{k=1}^{M} O_k^{n_k}\ ,$$

$$(k,l) = \min(k,l)\ ,$$

$$[k,l] = \max(k,l)\ ,$$

and $\Omega_1, \ldots, \Omega_M$ are any operators (not necessarily commutative) defined in the N particle Hilbert space. Both Eqs. (A7) and (A9) are special cases of Eq. (A10). We shall prove Eq. (A10) again using the method of mathematical induction. The validity of Eq. (A10) for $M=1$ follows immediately from Eq. (A9). We assume now that Eq. (A10) is valid for M and calculate $\langle \boldsymbol{\alpha} | \Pi_{k=1}^{M+1} \Omega_k^{n_k} | \boldsymbol{\alpha} \rangle$. Using Eq. (A7), we get

$$\begin{aligned}\langle \boldsymbol{\alpha} | \prod_{k=1}^{M+1} \Omega_k^{n_k} | \boldsymbol{\alpha} \rangle &= \langle \boldsymbol{\alpha} | \prod_{k=1}^{M} \Omega_k^{n_k} \cdot \Omega_{M+1}^{n_{M+1}} | \boldsymbol{\alpha} \rangle = \left[P_M + \frac{1}{2} \sum_{k,l=1}^{M} \frac{\partial^2 P_M}{\partial O_k \partial O_l} (\nabla_\alpha O_{(k,l)} \cdot \nabla_{\bar{\alpha}} O_{[k,l]}) \right] \left[O_{M+1}^{n_{M+1}} + \frac{1}{2} \frac{\partial^2 O_{M+1}^{n_{M+1}}}{\partial O_{M+1}^2} (\nabla_\alpha O_{M+1} \cdot \nabla_{\bar{\alpha}} O_{M+1}) \right] \\ &\quad + (\nabla_\alpha P_M \cdot \nabla_{\bar{\alpha}} O_{M+1}^{n_{M+1}}) + 0(\hbar^2) = P_{M+1} + \frac{1}{2} \sum_{k,l=1}^{M} \frac{\partial^2 P_{M+1}}{\partial O_k \partial O_l} (\nabla_\alpha O_{(k,l)} \cdot \nabla_{\bar{\alpha}} O_{[k,l]}) + \frac{1}{2} \frac{\partial^2 P_{M+1}}{\partial O_{M+1}^2} (\nabla_\alpha O_{M+1} \cdot \nabla_{\bar{\alpha}} O_{M+1}) \\ &\quad + \sum_{k=1}^{M} \frac{\partial P_M}{\partial O_k} \frac{\partial O_{M+1}^{n_{M+1}}}{\partial O_{M+1}} (\nabla_\alpha O_k \cdot \nabla_{\bar{\alpha}} O_{M+1}) + 0(\hbar^2) = P_{M+1} + \frac{1}{2} \sum_{k,l=1}^{M+1} \frac{\partial^2 P_{M+1}}{\partial O_k \partial O_l} (\nabla_\alpha O_{(k,l)} \cdot \nabla_{\bar{\alpha}} O_{[k,l]}) + 0(\hbar^2)\ ,\end{aligned}$$

which completes the proof. When the operators $\Omega_1, \ldots, \Omega_M$ commute, their order in the product is immaterial, and in view of Eq. (A8), we get a simplified version of Eq. (A10):

$$\langle \boldsymbol{\alpha} | \prod_{k=1}^{M} \Omega_k^{n_k} | \boldsymbol{\alpha} \rangle = P_M + \frac{1}{2} \sum_{k,l=1}^{M} \frac{\partial^2 P_M}{\partial O_k \partial O_l} (\nabla_\alpha O_k \cdot \nabla_{\bar{\alpha}} O_l) + 0(\hbar^2)\ . \tag{A11}$$

The proof of the second semiclassical expansion is now straightforward. Let us expand the function f in power series

$$f(\Omega_1, \ldots, \Omega_M) = \sum_{\mathbf{n}} f_{\mathbf{n}} \prod_{k=1}^{M} \Omega_k^{n_k}\ , \tag{A12}$$

where $\mathbf{n}$ stands for $(n_1, \ldots, n_M)$ and the operators $\Omega_1, \ldots, \Omega_M$ commute. Applying Eq. (A11) to (A12) term by term and then performing the summation, we obtain

$$\langle \boldsymbol{\alpha} | f(\Omega_1, \ldots, \Omega_M) | \boldsymbol{\alpha} \rangle = f(O_1, \ldots, O_M) + \frac{1}{2} \sum_{k,l=1}^{M} \frac{\partial^2 f}{\partial O_k \partial O_l} (\nabla_\alpha O_k \cdot \nabla_{\bar{\alpha}} O_l) + 0(\hbar^2)\ . \tag{A12}$$

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