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An $\hbar$-Expansion of a Unitary Transformation and Quantum Corrections to a Canonical Transformation

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A relation between classical canonical transformations and quantal unitary transformations is investigated with the use of the phase space method. A unitary transformed operator expressed in the phase space is expanded into a power series of $\hbar$, which shows that a canonical transformation can be regarded as a classical approximation (the limit $\hbar \to 0$) to the unitary transformation. The expansion provides us with a procedure to successively evaluate quantum corrections starting with the classical limit. As an illustrative example, the lowest-order quantum correction to the Birkhoff-Gustavson transformation for a one-dimensional anharmonic oscillator is calculated in the case of Weyl correspondence rule.

§1. Introduction

Many attempts based on a classical approximation have been made for complicated quantum systems for which exact solutions cannot be obtained and furthermore the ordinary perturbative methods are difficult to apply.[1)~3)] In the classical approximation, we treat c-number functions in the phase-space instead of operators or state vectors,[4),5)] and use canonical transformations as approximations to unitary transformations.[3),6),7)]

However, the classical description itself does not tell us the extent to which the classical treatment approximates the exact quantal treatment and it is difficult to evaluate its validity. Therefore, it is to be desired to formulate quantum mechanics such that the zero-th order term of a certain approximate series coincides with the classical treatment and we can systematically evaluate higher order terms (quantum corrections). This subject is important in order to increase the accuracy of the approximation and to give the perspective about its validity, and further to grasp what kind of information is meaningful as an approximation to quantum mechanics. Towards the above goal, we investigate in this paper a relationship between quantal unitary transformations and classical canonical transformations. Within the work along this line, we can see a semiclassical expression of a unitary operator[3),7)] and a study of the action of a unitary transformation on a classical-quantal correspondence rule by using a phase-space method.[6)] Here, we consider a unitary transformed operator rather than a unitary operator itself and investigate the quantum corrections to the classical description based on the above-mentioned phase-space method. In this method, relations of operators are represented by c-number expressions and we can formulate a quantum mechanics in the phase space[*)] such that it is equivalent to the conventional operator formalism.[8),9)] As will be seen in §2, we can treat both a quantal and a classical mechanics on the same footing by changing the "parameter" $\hbar$ and we can get a good perspective of the relation between a classical and a quantal description.

The consequence is as follows: The unitary transformed operator expressed in the

*) It should be noted that this space has a structure different from the ordinary classical phase space, as we see in §2.

phase space is expanded into a power series of $\hbar$, which clearly shows that the canonical transformation is the lowest-order approximation (the classical limit) to the exact quantum mechanical treatment.[3),6),7)] This expansion is useful to evaluate higher-order terms (quantum corrections) successively from the classical limit.

In §2, we recapitulate the classical-quantal correspondence rule and the formulation of quantum mechanics in the phase space. In §3, the unitary transformation is expressed in the phase space and its $\hbar$-expanded form is given. In §4, as an illustrative example, we calculate the lowest-order quantum corrections to the Birkhoff-Gustavson transformation[10),11)] for a one-dimensional anharmonic oscillator in the case of the Weyl correspondence rule.[8)] In §5, we summarize the results and point out future problems.

§ 2. Phase-space formulation of quantum mechanics and classical-quantal correspondence

In this section, following Ref. 8), we recapitulate the phase-space formulation of quantum mechanics and introduce some notations which will be used later. In this formulation, any operator $\hat{O}(\hat{q}, \hat{p})$ is associated with a c-number function $\mathcal{O}(q, p)$ in the q-p space by a mapping $\Omega^{(f)}$,

$$\hat{O}_f(\hat{q}, \hat{p}) = \Omega^{(f)}(\mathcal{O}_f) \equiv \frac{1}{(2\pi)^2}\int d\tau d\theta dq dp e^{i\tau(\hat{p}-p)+i\theta(\hat{q}-q)} \cdot \mathcal{O}_f(q, p) \cdot f(\tau, \theta), \qquad (2\cdot1)$$

where $\hat{q}$ and $\hat{p}$ are the canonical coordinate and momentum operators satisfying $[\hat{q}, \hat{p}] = i\hbar$ and $f(\tau, \theta)$ is called a filter function. For simplicity, we consider the case of one degree of freedom. The inverse mapping of $\Omega^{(f)}$, $\Theta^{(f)} \equiv (\Omega^{(f)})^{-1}$, which maps the operator $\hat{O}_f$ to the c-number function $\mathcal{O}_f$ is given by

$$\mathcal{O}_f(q, p) = \Theta^{(f)}(\hat{O}_f)(q, p) \equiv \frac{\hbar}{2\pi}\int d\tau d\theta (f(\tau, \theta))^{-1} \cdot \mathrm{Tr}[\hat{O}_f e^{-i\theta(\hat{q}-q)-i\tau(\hat{p}-p)}]. \qquad (2\cdot2)$$

For a given filter function $f(\tau, \theta)$ satisfying certain conditions (e.g., $f(0, 0) = 1$), the above relations, Eqs. (2·1) and (2·2), give a one-to-one correspondence between the operators and the c-number functions. Familiar rules of association are obtained by specifying the filter function $f(\tau, \theta)$. For example, the Weyl and the normal rules are obtained by choosing $f = 1$ and $f = e^{4/\hbar(\theta^2/\alpha^2+\alpha^2\tau^2)}$, respectively. Here, the relation between the $(\hat{q}, \hat{p})$ and the boson operators $(\hat{a}, \hat{a}^\dagger)$ is given by

$$\hat{a} = (\alpha\hat{q} + i\hat{p}/\alpha)/\sqrt{2\hbar}, \qquad (2\cdot3a)$$

$$\hat{a}^\dagger = (\alpha\hat{q} - i\hat{p}/\alpha)/\sqrt{2\hbar}. \qquad (2\cdot3b)$$

In the following, we omit the subscript (f) except when a specific correspondence rule is considered. Although the q-p space is analogous to the classical phase-space, it has a structure different from the classical phase space in the case $\hbar \neq 0$. Therefore, we call the q-p space the W-space according to Ref. 5).

As was shown in Ref. 8), the mapping Θ naturally introduces, in the W-space, the $*$-product[12)] $A * B$ which corresponds to the product of operators $\hat{A} \cdot \hat{B}$:

$$(A * B)(q, p) \equiv \Theta(\hat{A} \cdot \hat{B})(q, p)$$

$$=\mathscr{S}\left(\frac{1}{i}\frac{\partial}{\partial p_1},\frac{1}{i}\frac{\partial}{\partial q_1},\frac{1}{i}\frac{\partial}{\partial p_2},\frac{1}{i}\frac{\partial}{\partial q_2}\right)A(q_1,p_1)B(q_2,p_2)\Big|_{\substack{q_1=q_2=q\\ p_1=p_2=p}}, \tag{2·4a}$$

$$\mathscr{S}(\tau_1,\theta_1,\tau_2,\theta_2)=\frac{f(\tau_1,\theta_1)f(\tau_2,\theta_2)}{f(\tau_1+\tau_2,\theta_1+\theta_2)}\cdot e^{i\hbar/2(\tau_1\theta_2-\tau_2\theta_1)}. \tag{2·4b}$$

Corresponding to the commutator of operators $[\hat{A},\hat{B}]$, the quantity $[A*B]$ is defined in the W-space as

$$[A*B](q,p)\equiv\Theta([\hat{A},\hat{B}]/i\hbar)(q,p)=\frac{1}{i\hbar}\cdot(A*B-B*A)(q,p). \tag{2·5}$$

For appropriate functions $A(q,p)$ and $B(q,p)$ in the W-space, the $[A*B]$ can be expanded into a power series of $\hbar$. We denote the coefficient of $\hbar^n$ in $[A*B](q,p)$ as $F^{(n)}(\partial/\partial q, \partial/\partial p;\ A(q,p),B(q,p))$, i.e., we write

$$[A*B](q,p)\equiv\sum_{n=0}^{\infty}\hbar^n F^{(n)}\left(\frac{\partial}{\partial q},\frac{\partial}{\partial p};\ A(q,p),B(q,p)\right). \tag{2·6}$$

For example, for the Weyl rule of association ($f=1$), $[A*B]_{\mathrm{Weyl}}$ is just a well-known Moyal bracket:[13]

$$[A*B]_{\mathrm{W}}(q,p)=\frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\left(\frac{\partial^2}{\partial q_1\partial p_2}-\frac{\partial^2}{\partial p_1\partial q_2}\right)\right]A_{\mathrm{W}}(q_1,p_1)B_{\mathrm{W}}(q_2,p_2)\Big|_{\substack{q_1=q_2=q\\ p_1=p_2=p}}$$

$$=\sum_{n=0}^{\infty}\hbar^{2n}F_{\mathrm{W}}^{(2n)}\left(\frac{\partial}{\partial q},\frac{\partial}{\partial p};\ A_{\mathrm{W}}(q,p),B_{\mathrm{W}}(q,p)\right), \tag{2·7a}$$

$$F_{\mathrm{W}}^{(0)}=\{A,B\}_{\mathrm{PB}}\equiv\frac{\partial A_{\mathrm{W}}}{\partial q}\frac{\partial B_{\mathrm{W}}}{\partial p}-\frac{\partial A_{\mathrm{W}}}{\partial p}\frac{\partial B_{\mathrm{W}}}{\partial q}, \tag{2·7b}$$

$$F_{\mathrm{W}}^{(2n)}=\frac{(-)^{n+1}}{2^{2n}}\sum_{l=0}^{2n+1}\frac{(-)^l}{l!(2n+1-l)!}\cdot\frac{\partial^{2n+1}A_{\mathrm{W}}}{\partial q^l\partial p^{2n+1-l}}\cdot\frac{\partial^{2n+1}B_{\mathrm{W}}}{\partial p^l\partial q^{2n+1-l}}. \tag{2·7c}$$

The $\hbar^0$-term in $[A*B]_{\mathrm{W}}$, $F_{\mathrm{W}}^{(0)}$, is nothing but the familiar Poisson bracket;[14] this is a common feature of general linear mappings $\Theta^{(f)}$. Let us introduce the operators in the W-space, L_G^* and $L_G^{(n)}$, which depend on a function $G(q,p)$ as follows:

$$L_G^*(\mathcal{O})(q,p)=[G*\mathcal{O}](q,p)\equiv\sum_{n=0}^{\infty}\hbar^n L_G^{(n)}(\mathcal{O})(q,p), \tag{2·8a}$$

i.e.,

$$L_G^{(n)}(\mathcal{O})(q,p)=F^{(n)}\left(\frac{\partial}{\partial q},\frac{\partial}{\partial p};\ G(q,p),\ \mathcal{O}(q,p)\right). \tag{2·8b}$$

Various quantal problems can be equivalently treated in the W-space. From Eqs. (2·4) and (2·6), we see that in the limit $\hbar\to 0$ (the classical limit), the $[A*B]$ becomes the Poisson bracket, and the $A*B$ the ordinary c-number product of two functions $A(q,p)\cdot B(q,p)$. Namely, in this limit the W-space reduces to the classical phase space.[5),6),12)]

§ 3. The $\hbar$-expanded form of unitary transformations in the W-space

In this section, we give the $\hbar$-expanded form of the unitary transformation which is generated by $\hat{U}=e^{i/\hbar\hat{G}}$ where $\hat{G}$ is hermite. For this aim, let us consider a one-parameter (t) family of unitary transformations $\hat{U}(t)=e^{i/\hbar\hat{G}t}$. If we set $t=1$, $\hat{U}(t=1)$ becomes a given unitary operator $\hat{U}$. By $\hat{U}(t)$, an operator $\hat{O}(0)$ is transformed into $\hat{O}(t)\equiv e^{i/\hbar\hat{G}t}\hat{O}(0)e^{-i/\hbar\hat{G}t}$. In quantum mechanics, our problem is to obtain $\hat{O}(t)$ with a given initial condition $\hat{O}(0)$. With the use of a mapping Θ, this problem is transformed into the equivalent problem in the W-space; namely, $\mathcal{O}(q,p;t)\equiv\Theta(\hat{O}(t))(q,p)$ is to be obtained with an initial distribution $\mathcal{O}(q,p;0)=\mathcal{O}_0(q,p)=\Theta(\hat{O}(0))(q,p)$. The operator $\hat{O}(t)$ satisfies a differential equation for t (Heisenberg equations of motion), $i\hbar\, d\hat{O}/dt(t)=[\hat{O}(t),\hat{G}]$. This equation is mapped into the W-space as:

$$\frac{\partial}{\partial t}\mathcal{O}(q,p;t)=[\mathcal{O}(t)*G](q,p)=-L_G{}^*(\mathcal{O}(t))(q,p)\,. \tag{3·1}$$

By direct calculations, we obtain the formal solution of Eq. (3·1):

$$\mathcal{O}(q,p;t)=[e^{-tL_G{}^*}\cdot\mathcal{O}_0](q,p)\,, \tag{3·2}$$

where $e^{-tL_G{}^*}$ is defined in terms of its Taylor expansion.[8] We now consider a deviation of $\mathcal{O}(q,p;t)$ from its classical approximation. For this aim, let us adopt an analogue of interaction picture. From Eqs. (2·6) and (2·8), we can put that $L_G{}^*=L_G{}^{(0)}+\Delta L_G$ where $L_G{}^{(0)}(\mathcal{O})$ is the ordinary Poisson bracket and $\Delta L_G=O(\hbar)$. Thus, we can regard $L_G{}^{(0)}$ as the free part and ΔL_G as the perturbation part. Following the conventional treatment of the interaction picture, let us define $\mathcal{O}_I(t)$ as

$$\mathcal{O}_I(t)\equiv e^{tL_G{}^{(0)}}\cdot\mathcal{O}(t)\,. \tag{3·3}$$

Then, we see from Eq. (3·1) that the t-evolution of $\mathcal{O}_I(t)$ is determined by

$$\frac{d}{dt}\mathcal{O}_I(t)=-\widetilde{\Delta L}_G(t)\cdot\mathcal{O}_I(t), \tag{3·4a}$$

$$\widetilde{\Delta L}_G(t)\equiv e^{tL_G{}^{(0)}}\cdot\Delta L_G\cdot e^{-tL_G{}^{(0)}}\,. \tag{3·4b}$$

Integrating the above equation, we obtain $\mathcal{O}_I(t)$. From $\mathcal{O}_I(t)$, we finally get $\mathcal{O}(t)$ as follows:

$$\mathcal{O}(t)=e^{-tL_G{}^{(0)}}\cdot\mathcal{O}_0-\sum_{n=1}^{\infty}\hbar^n\int_0^t ds\, e^{-(t-s)L_G{}^{(0)}}\cdot L_G{}^{(n)}\cdot\mathcal{O}(s). \tag{3·5}$$

With the use of $F^{(n)}$ defined in Eq. (2·6), let us explicitly express the above equation in terms of the (q,p)-component as

$$\begin{aligned}\mathcal{O}(q,p;t)=&\,\mathcal{O}_0(u(t;q,p),\ v(t;q,p))\\&+\sum_{n=1}^{\infty}\hbar^n\int_0^t ds\left[F^{(n)}\left(\frac{\partial}{\partial Q},\frac{\partial}{\partial P};\mathcal{O}(Q,P;s),\ G(Q,P)\right)\right]\Bigg|_{\substack{Q=u(t-s\,;\,q,p)\\P=v(t-s\,;\,q,p)}},\end{aligned} \tag{3·6}$$

where (u,v) is the classical orbit generated by G, which starts from the point (q,p); namely it is the solution of the following equations of motion:

$$\frac{d}{ds}u(s;q,p)=\frac{\partial}{\partial P}G(Q,P)\Bigg|_{\substack{Q=u(s\,;\,q,p)\\P=v(s\,;\,q,p)}}, \tag{3·7a}$$

$$\frac{d}{ds}v(s;q,p)=-\frac{\partial}{\partial Q}G(Q,P)\Big|_{\substack{Q=u(s;q,p)\\P=v(s;q,p)}}, \tag{3·7b}$$

with the initial condition

$$u(0;q,p)=q\,, \tag{3·8a}$$

$$v(0;q,p)=p\,. \tag{3·8b}$$

With the use of $L_G{}^{(0)}$, u and v are formally expressed as

$$u(t;q,p)=[e^{-tL_G{}^{(0)}}\cdot q](q,p)\,, \tag{3·9a}$$

$$v(t;q,p)=[e^{-tL_G{}^{(0)}}\cdot p](q,p)\,. \tag{3·9b}$$

Equations (3·6) and (3·9) are nothing but the transformed form of the partial differential equations (3·1) into the linear integro-differential equations. However, since Eq. (3·6) has the classical-limit solution $\mathcal{O}_0(u(t;q,p),\,v(t;q,p))$ as an inhomogeneous term, we can get the following solution of $\mathcal{O}(t)$ in a formal power series of $\hbar$*) as:

$$\mathcal{O}(q,p;t)=\sum_{n=0}^{\infty}\hbar^n\mathcal{O}^{(n)}(q,p;t), \tag{3·10a}$$

$$\begin{aligned}\mathcal{O}^{(0)}(q,p;t)&=\mathcal{O}_0(u(t;q,p),v(t;q,p))\\&=[e^{-tL_G{}^{(0)}}\cdot\mathcal{O}_0](q,p)\ ;\ \text{classical approximation}\,,\end{aligned} \tag{3·10b}$$

$$\mathcal{O}^{(n)}(q,p;t)=\sum_{\substack{l+m=n\\l\ge1}}\int_0^t ds\Big[F^{(l)}\Big(\frac{\partial}{\partial Q},\frac{\partial}{\partial P};\mathcal{O}^{(m)}(Q,P;s),\ G(Q,P)\Big)\Big]_{\substack{Q=u(t-s;q,p)\\P=v(t-s;q,p)}}\ ;n\ge1\,. \tag{3·10c}$$

Some remarks on the above expressions are in order.**) Since $\hat{U}(1)$ is equal to the given unitary operator $\hat{U}$, Eqs. (3·10) with $t=1$***) give us an $\hbar$-expansion of the unitary transformed operator $\hat{U}\hat{O}(0)\hat{U}^{-1}$ in the W-space for any $\hat{O}(0)$. Furthermore, we see from Eqs. (3·7)~(3·9) that $(Q=u(t=1;q,p),\ P=v(t=1;\ q,p))$ gives the canonical transformation whose infinitesimal generator is $G(q,p)=\Theta(\hat{G})(q,p)$.[14] Therefore the zeroth-order term in Eq. (3·10a) gives the canonical transformed form of the function $\mathcal{O}_0(q,p)$. In the limit $\hbar\to0$ (the classical limit), only the zeroth-order term remains. In this sense, we can say that the canonical transformation is a classical approximation to the unitary transformation expressed in the W-space. Equation (3·10c) provides us with a method to successively evaluate the higher-order terms (quantum corrections) of $\mathcal{O}(q,p;t=1)$ starting from $\mathcal{O}^{(0)}$ (classical approximation) in accordance with the mapping Θ given (i.e.,

*) In some cases, $\mathcal{O}_0(q,p)=\Theta(\hat{O}(0))(q,p)$ has $\hbar^n$-dependent terms where n is a positive integer (e.g., $\Theta^{(W)}(\hat{p}\hat{q}^4\hat{p})=p^2q^4+3\hbar^2q^2$). In the $\hbar$-expansion of $\mathcal{O}(q,p;t)$, we do not take into account this $\hbar$-dependence which comes from a quantal-classical mapping Θ and does not come from a unitary transformation.

**) The W-space with Weyl rule is known to have an invariant structure under linear inhomogeneous canonical transformation.[5] We can explicitly verify that each order term $\mathcal{O}^{(n)}$ in Eqs. (3·10) is invariant under this transformation when Weyl rule is adopted.

***) It is not essential to fix t to a specific value 1. We obtain the same result by replacing $t=1$ with $t=t_0$ and G with G/t_0.

$F^{(l)}$). It should be emphasized that even when we do not know the quantal unitary transformation, we can construct it by means of Eqs. (3·10) if we can find the generator G of the canonical transformation given. It is therefore an interesting problem to investigate the existence and the uniqueness of the generator G. We give in the Appendix a possible procedure to construct the generator G of the given canonical transformation which can be expanded into a Taylor series.

§ 4. Evaluation of quantum corrections for the Birkhoff-Gustavson transformation

In this section, as an example to illustrate the procedure of evaluating the quantum corrections, we calculate, for the case of the Weyl rule of association, the lowest-order quantum correction to the Birkhoff-Gustavson (B-G) transformation[10),11)] for a one-dimensional anharmonic oscillator. This transformation was first proposed by Birkhoff[10)] and generalized by Gustavson.[11)] We consider a given n-dimensional classical Hamiltonian which can be expanded around an equilibrium point, into a Taylor series as follows:

$$\mathcal{H}=\sum_{s=2}^{\infty}\mathcal{H}(s) \qquad s\text{:degree of polynomials}\,, \tag{4·1a}$$

$$\mathcal{H}(2)=\sum_{a=1}^{n}(p_a{}^2+\omega_a{}^2 q_a{}^2)/2\,, \tag{4·1b}$$

where the degree-2 term $\mathcal{H}(2)$ is assumed to be in a standard form. The basic idea of this method is to transform $\mathcal{H}$ into a normal form Γ by successive canonical transformations. Here Γ is called a normal form when it satisfies $\{\Gamma, \mathcal{H}(2)\}_{\mathrm{PB}}=0$. For non-resonant cases, Γ is normal when it is a function of number variables $\hbar n_a \equiv \frac{1}{2}(p_a{}^2+\omega_a{}^2 q_a{}^2)/\omega_a$ alone. In the following, we consider only the non-resonant cases. This transformation was used initially to investigate classical non-linear systems. But it has also been used as a (semi-) classical approximation to obtain energy eigenvalues of these systems by replacing the number variables n_a with the operators $\hat{n}_a$ (or $\hat{n}_a+1/2$, etc.).[15)~18)] Here, it should be noted that the quantum Hamiltonian obtained from $\Gamma(n_a)$ by a certain mapping (e.g., the Weyl and the normal rules) is also a function of only the number operators although its form is different from $\Gamma(\hat{n}_a)$.[18)] Namely, the B-G transformation should be regarded as a classical approximation to the unitary transformation which diagonalizes the corresponding quantal system. Here, we investigate a deviation from the classical result by calculating the quantum corrections to the B-G transformation according to the procedure of §3.

In order to apply the method given in §3, we modify the original formulation of the B-G transformation in the following two points. First, instead of considering the canonical transformation of the type $Q=(\partial/\partial P)F(P,q)$ and $p=(\partial/\partial q)F(P,q)$, and determining the function $F(P,q)$, we try to determine $G(q,p)$ in the transformation (3·9) (Lie transforms[19)]). Second, instead of considering successive canonical transformations, we consider a single transformation generated by G, and determine G iteratively according to the degree of polynomials in G. The practical procedure is as follows. For the convenience of expressions, we use the variables z_a and $z_a{}^*$ which are related to q_a and p_a by

$$z_a = (\omega_a q_a + i p_a)/\sqrt{2\omega_a}\ ; a=1,\cdots,n\,, \tag{4·2a}$$

$$z_a^* = (\omega_a q_a - i p_a)/\sqrt{2\omega_a}\,. \tag{4·2b}$$

The generator G of the canonical transformation is expanded into a Taylor series:

$$G = \sum_{s=3}^{\infty} G(s)\,, \tag{4·3a}$$

$$G(s) = \sum_{|k|+|\bar{k}|=s} g(k=(k_1,\cdots,k_n), \bar{k}=(\bar{k}_1,\cdots,\bar{k}_n))\cdot(z)^k\cdot(z^*)^{\bar{k}}\,, \tag{4·3b}$$

where

$$|k| \equiv k_1+\cdots+k_n,\quad |\bar{k}| \equiv \bar{k}_1+\cdots+\bar{k}_n\,, \tag{4·3c}$$

$$(z)^k \equiv z_1^{k_1}\cdots z_n^{k_n}\,,\ (z^*)^{\bar{k}} \equiv (z_1^*)^{\bar{k}_1}\cdots(z_n^*)^{\bar{k}_n}\,. \tag{4·3d}$$

It should be noted that the expansion begins with the third-degree term. The transformed Hamiltonian $\Gamma = e^{-L_{G^{(0)}}}\cdot\mathcal{H}$ can also be expanded as

$$\Gamma = \sum_{s=2}^{\infty} \Gamma(s)\,, \tag{4·4a}$$

$$\Gamma(s) = \mathcal{H}(s) + \{\mathcal{H}(2),\ G(s)\}_{\rm PB} + \Delta\Gamma(s)\,, \tag{4·4b}$$

$$\Delta\Gamma(s) \equiv \sum_{l=3}^{s-1} \{\mathcal{H}(l),\ G(s-l+2)\}_{\rm PB}$$

$$+\sum_{k=2}^{s-2}\frac{1}{k!}\sum_{l+j_1+\cdots+j_k=s+2k}\{\{\cdots\{\mathcal{H}(l),\ G(j_1)\},\cdots\},G(j_k)\}_{\rm PB}\,. \tag{4·4c}$$

For the coefficients $h(k,\bar{k})$, $\gamma(k,\bar{k})$ and $\Delta\gamma(s;k,\bar{k})$ of $(z)^k\cdot(z^*)^{\bar{k}}$ in $\mathcal{H}(s)$, $\Gamma(s)$ and $\Delta\Gamma(s)$, we obtain from Eq. (4·4b)

$$i(\omega\cdot\bar{k}-k)g(k,\bar{k}) = h(k,\bar{k}) - \gamma(k,\bar{k}) + \Delta\gamma(s;k,\bar{k}),$$

$$\omega = (\omega_1,\cdots,\omega_n),\quad |k|+|\bar{k}|=s\,, \tag{4·5}$$

where $(\cdot)$ denotes an inner-product of vectors. Since $\Delta\Gamma(s)$ does not contain $G(r)$ with $r\geq s$, we can, aside from the convergence problem, iteratively determine the $(k\neq\bar{k})$-components $g(k,\bar{k})$ of $G(s)$ so as to eliminate the $(k\neq\bar{k})$-components of $\Gamma(s)$, provided ω is non-resonant. Then, the transformed Hamiltonian Γ is a function of only the number variables $n_a = z_a^* z_a$. Here it should be mentioned that the $(k=\bar{k})$-components of G cannot be determined in the above procedure. This arbitrariness is inherent in the B-G transformation, and these $(k=\bar{k})$ components are usually set to 0.[15)~18)] Let us now consider the following one-dimensional anharmonic oscillator (the generalization to multi-dimensional cases is complicated but straightforward):

$$\hat{H} = \frac{1}{2}(\hat{p}^2 + \omega^2\hat{q}^2) + \frac{\varepsilon}{4}\omega^2\hat{q}^4\,. \tag{4·6a}$$

For the classical-quantal mapping, we adopt the Weyl rule. Then the classical equivalent of $\hat{H}$ is given by

$$\mathcal{H}=\Theta^{(\mathrm{W})}(\hat{H})=\frac{1}{2}(p^2+\omega^2 q^2)+\frac{\varepsilon}{4}\omega^2 q^4 . \tag{4·6b}$$

By means of the above procedure, we obtain the low-degree terms of G as

$$G(3)=0 , \tag{4·7a}$$

$$G(4)=\frac{i\varepsilon}{64\omega}(z^4+8z^3z^*-8zz^{*3}-z^{*4})+g(2,2)z^2z^{*2} . \tag{4·7b}$$

As was mentioned above, $g(2,2)$ is undetermined except that it is real to guarantee the hermiticity of G. The canonical transformation $Z^{(0)}(z,z^*)$ and the transformed Hamiltonian $\Gamma^{(0)}$ are calculated to be

$$Z^{(0)}(t;z,z^*)=e^{-tL_{G^{(0)}}}\cdot z$$
$$=z+t\cdot\left[\frac{\varepsilon}{16\omega}(2z^3-6zz^{*2}-z^{*3})-2ig(2,2)z^2z^*\right]+\cdots , \tag{4·8a}$$

$$Z^{*(0)}(t;z,z^*)=e^{-tL_{G^{(0)}}}\cdot z^*$$
$$=z^*+t\left[\frac{\varepsilon}{16\omega}(2z^{*3}-6z^2z^*-z^3)+2ig(2,2)zz^{*2}\right]+\cdots , \tag{4·8b}$$

$$\Gamma^{(0)}(t;z,z^*)=\omega z^*z+\frac{3}{8}\varepsilon\cdot z^2z^{*2}$$
$$+\frac{\varepsilon}{16}(1-t)\cdot(z^4+4z^3z^*+4zz^{*3}+z^{*4})+\cdots . \tag{4·9}$$

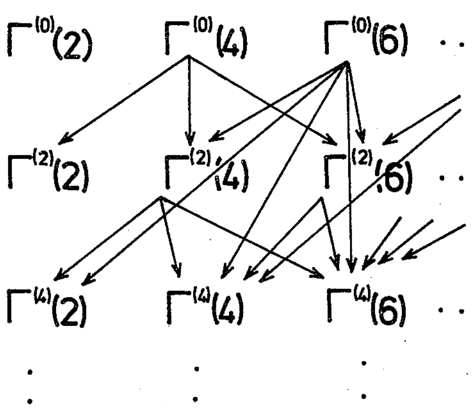

Fig. 1. The schematic figure of the B-G series and its quantum corrections. The terms at the start points of arrows produce the terms at the end points.

If we set $t=1$ in the above expressions we obtain the B-G transformation.

Before evaluating the quantum corrections, we should note the following point: The B-G transformation gives the series whose expansion parameter is the degree of polynomials, whereas the procedure in §3 gives the series whose expansion parameter is $\hbar$ ($\hbar^2$ in the case of the Weyl rule of association). Thus, we obtain a double series with respect to $\hbar$ and the degree of polynomials. Equations (2·7) and (3·10) indicate that the term $\Gamma^{(0)}(n)$ with $n\geq 4$ $(=O(\hbar^0))$ produces $\Gamma^{(2)}(n-2)$, $\Gamma^{(2)}(n)$, $\Gamma^{(2)}(n+2),\cdots$ etc. in the $\hbar^2$-order and $\Gamma^{(4)}(n-4)$, $\Gamma^{(4)}(n-2),\cdots$etc. in the $\hbar^4$-order for the case $n\geq 6$. This is illustrated in Fig. 1 where the terms at the start points of arrows produce the terms at the end points. Therefore as the lowest-order term of this double series, we evaluate $\Gamma^{(2)}(2)$. From Eq. (3·10), $\Gamma^{(2)}(2)$ is calculated to be

$$\Gamma^{(2)}(2;z,z^*)=\int_0^t ds\left[F_{\mathrm{W}}^{(2)}\left(\frac{\partial}{\partial Z},\frac{\partial}{\partial Z^*};\ \Gamma^{(0)}(4),\ G\right)\right]_{\substack{Z=Z^{(0)}(t-s\,;\,z,z^*)\\ Z^*=Z^{*(0)}(t-s\,;\,z,z^*)}}. \tag{4·10}$$

With the use of Eqs. (2·7) and (4·7) ~ (4·9), we obtain

$$F_{\mathrm{W}}^{(2)}\left(\frac{\partial}{\partial Z},\frac{\partial}{\partial Z^*};\Gamma^{(0)}(4;Z,Z^*),G(Z,Z^*)\right)\Bigg|_{\substack{Z=Z^{(0)}(t-s\,;\,z,z^*)\\ Z^*=Z^{*(0)}(t-s\,;\,z,z^*)}}$$

$$=i\frac{3}{8}\left[i\frac{3\varepsilon^2}{16\omega}\cdot(1-s)\cdot(z+z^*)^2-\frac{\varepsilon}{2}\cdot\left(i\frac{3\varepsilon}{4\omega}\cdot z+4g(2,2)\cdot z^*\right)\cdot((1-s)z^*+z)\right.$$
$$\left.+\frac{\varepsilon}{2}\cdot\left(-i\frac{3\varepsilon}{4\omega}\cdot z^*+4g(2,2)\cdot z\right)\cdot((1-s)z+z^*)\right]+\cdots. \tag{4·11}$$

Integrating over s, we finally obtain

$$\Gamma^{(2)}(2;z,z^*;t)=i\frac{3}{8}\left[i\frac{3\varepsilon^2}{16\omega}\cdot\left\{-t\left(1+\frac{t}{2}\right)\cdot(z^2+z^{*2})-2t\cdot\left(1-\frac{t}{2}\right)\cdot zz^*\right\}\right.$$
$$\left.+2\varepsilon g(2,2)\cdot t\left(1-\frac{t}{2}\right)\cdot(z^2-z^{*2})\right]. \tag{4·12}$$

By setting $t=1$ in the above expression, we obtain the lowest-order quantum correction to the B-G series. It is straightforward to map $\Gamma^{(2)}(2)$ into an operator form; each term in Eq. (4·12) is mapped by $\Omega^{(\mathrm{W})}$ as follows: $\Omega^{(\mathrm{W})}(z^2+z^{*2})=\omega\hat{q}^2-\hat{p}^2/\omega$, $\Omega^{(\mathrm{W})}(zz^*)=(\hat{p}^2+\omega^2\hat{q}^2)/2\omega$ and $\Omega^{(\mathrm{W})}(z^2-z^{*2})=i(\hat{q}\hat{p}+\hat{p}\hat{q})$.

Here, we give a few comments concerning the above. First, as is expected, Eq. (4·12) shows that although $\Gamma^{(0)}$ is a function of $n=z^*z$ alone, the quantum correction $\Gamma^{(2)}(2)$ brings about the z^2 and z^{*2} terms which are not diagonal within the treatment of the B-G approximation. Then, it is an interesting problem to seek a systematic procedure to get higher order approximation starting from the B-G series. One possibility is to include $\hbar^2$-(and higher order) terms in G. Next, the generator G has some undetermined components (e.g., $g(2,2)$) which, in effect, cause a transformation adding phase factors: $z_a\to z_a e^{i\theta_a(n)}$. Then, this arbitrariness in the B-G transformation does not change the number variables $n_a=z_a{}^*z_a$ and the form of $\Gamma^{(0)}$ at $t=1$ (see Eq. (4·9)). Therefore, we can say that all these B-G transformations are equivalent within the classical theory apart from the truncation of the series. However, Eq. (4·12) suggests that they are different as a classical approximation to the quantal theory, i.e., the accuracy of the approximation depends on the values of these arbitrary components. The above problems are beyond the scope of this paper, and require further investigations.

§ 5. Concluding remarks

With the use of the W-space formulation of quantum mechanics, we have investigated the relation between classical canonical transformations and quantal unitary transformations. By expanding unitary transformed operators expressed in the W-space into a power series of $\hbar$, canonical transformations are shown to be regarded as the classical approximation (the limit $\hbar\to 0$) to the unitary transformations. Furthermore, we have given the procedure to successively evaluate the quantum corrections starting with the classical approximation. As an illustrative example, we have evaluated the lowest-order quantum correction to the B-G transformation for a one-dimensional anharmonic oscillator.

In this paper, we have considered the quantum system made of bosons or distinguishable particles whose classical-quantal correspondence has been rather well known.[4)~9)] For fermion systems, such direct c-number classical versions do not exist.[20)] However, in many cases, the approach based on the time-dependent variational principle (e.g., the time-dependent Hartree-Fock method) can be regarded as a kind of classical approximation. In this approach, the classical image is obtained as expectation values of fermion operators with respect to the so-called generalized coherent states.[21)~24)] Then, we can see an analogy to the case of a boson system with a normal rule where a classical image is an expectation value with respect to a usual boson coherent state. Therefore, it seems very interesting to investigate the classical-quantal correspondence of fermion systems along the discussion of this paper by paying special attention to the structure of the quantum corrections.

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Appendix

We give a possible method to construct G for a given n-dimensional canonical transformation. We assume that the canonical transformation can be expanded into a Taylor series as follows:

$$X_\sigma(x)=x_\sigma+\sum_{s=2}^{\infty}X_\sigma(s, x), \quad s\text{: degree of polynomials,} \tag{A·1}$$

where X_σ and x_σ with $\sigma=1,\cdots,2n$ denote (Q_a,P_a) and (q_a,p_a) with $a=1,\cdots,n$, respectively. Although $X_\sigma(x)$ begins with x_σ in (A·1), we can relax this restriction with the use of linear symplectic transformations (whose generator are easily constructed in quadratic form). Let us first consider the vector field $\sum_{\sigma=1}^{2n}y_\sigma(x)\partial/\partial x_\sigma$ which generates this transformation:

$$X_\sigma(x)=\exp\left[\sum_\rho y_\rho(x)\frac{\partial}{\partial x_\rho}\right]\cdot x_\sigma\,;\quad \sigma=1,\cdots,2n\,. \tag{A·2}$$

By expanding both the sides into Taylor series, we obtain

$$X_\sigma(s)=y_\sigma(s)$$
$$+\sum_{k=2}^{s-1}\frac{1}{k!}\sum_{i_1+\cdots+i_k=s+k-1} y_{\rho_1}(i_1)\frac{\partial}{\partial x_{\rho_1}}\cdots y_{\rho_{k-1}}(i_{k-1})\frac{\partial}{\partial x_{\rho_{k-1}}}\cdot y_\sigma(i_k). \qquad \text{(A·3)}$$

Here we have assumed that y_σ begins with $y_\sigma(2)$. Since the second term in Eq. (A·3) does not contain $y_\rho(r)$ with $r\geq s$, we can iteratively determine y_σ starting from X_σ according to the degree of polynomials. Then, assuming the convergence of the series, we can obtain the vector field $\sum_\sigma y_\sigma\cdot\partial/\partial x_\sigma$ from a given transformation (A·1). If this vector field y_σ satisfies the following integrability conditions:

$$\frac{\partial y_{q_a}}{\partial q_b}=-\frac{\partial y_{p_b}}{\partial p_a}\ ;\ a,b=1,\ \cdots,\ n\ , \qquad \text{(A·4a)}$$

$$\frac{\partial y_{p_a}}{\partial q_b}=\frac{\partial y_{p_b}}{\partial q_a},\quad \frac{\partial y_{q_a}}{\partial p_b}=\frac{\partial y_{q_b}}{\partial p_a}, \qquad \text{(A·4b)}$$

we can get $G(x)$ by integrating $\partial G/\partial p_\sigma=y_{q_\sigma}$ and $\partial G/\partial q_\sigma=-y_{p_\sigma}$. This function G is nothing but the generator of the given canonical transformation (A·1). Below, we show the conditions (A·4) to hold for a one dimensional case. Since $X_\sigma(x)$ is a canonical transformation, we obtain, with the use of Eq. (A·2),

$$y_q(X)\,dP-y_p(X)\,dQ=y_q(x)\,dp-y_p(x)\,dq\ . \qquad \text{(A·5)}$$

From this, we can derive the following relations:

$$\Delta(Q,P)=\frac{\partial y_q}{\partial q}(X)+\frac{\partial y_p}{\partial p}(X)$$
$$=\exp\left[y_q(x)\frac{\partial}{\partial q}+y_p(x)\frac{\partial}{\partial p}\right]\cdot\Delta(q,p)=\Delta(q,p), \qquad \text{(A·6a)}$$

where

$$\Delta(q,p)\equiv\frac{\partial y_q}{\partial q}(x)+\frac{\partial y_p}{\partial p}(x)\ . \qquad \text{(A·6b)}$$

By expanding both the sides of the third equation in Eq. (A·6a), we obtain

$$\left(y_q(x)\frac{\partial}{\partial q}+y_p(x)\frac{\partial}{\partial p}\right)\cdot\Delta(q,p)=0\ . \qquad \text{(A·7)}$$

Then, defining the parameter (t) dependent transformation as

$$X_\sigma(t;x)\equiv\exp\left[t\cdot\left(y_q(x)\frac{\partial}{\partial q}+y_p(x)\frac{\partial}{\partial p}\right)\right]\cdot x_\sigma\ , \qquad \text{(A·8)}$$

we obtain

$$\Delta(X(t;x))=\Delta(X(0;x)=x)\qquad \text{for any } t. \qquad \text{(A·9)}$$

Next, we define a t-dependent function as

$$\Lambda(t;x)\equiv\frac{\partial Q(t)}{\partial q}\cdot\frac{\partial P(t)}{\partial p}-\frac{\partial Q(t)}{\partial p}\cdot\frac{\partial P(t)}{\partial q}\ . \qquad \text{(A·10)}$$

Calculating t-derivative of $\Lambda(t;x)$, we obtain

$$\frac{d\Lambda(t)}{dt}=\Delta(X(t))\cdot\Lambda(t)\,. \tag{A·11}$$

From Eqs. (A·9) and (A·11), it follows that

$$\Lambda(t;\,x)=e^{\Delta(x)t}\Lambda(0;\,x)\,. \tag{A·12}$$

On the other hand, $\Lambda(1,x)=\Lambda(0,x)=1$ since $X(x)$ is a canonical transformation. Therefore we obtain $\Delta(X(t))=\Delta(x)=0$ which ensures the integrability condition Eq. (A·4) to hold. For multidimensional cases, we could not get the proof as the one-dimensional case. But the direct calculation of Eqs. (A·4) up to the 4th-order terms indicates that the condition that $X(x)$ is a canonical transformation certainly ensures the integrability condition to hold.

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