Diagrams in classical and semiclassical perturbation theory

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We describe a diagrammatic method for the Poincare–Birkhoff normal forms algorithm of classical mechanics, and indicate the use of the diagrams with an example from hydrodynamics. We also present a generalization of the diagrammatic method to quantum mechanics. The quantum diagrams can be used in the semiclassical version of normal forms developed by Graffi, Paul, and others. © *1998 American Institute of Physics.* [S0022-2488(98)02503-1]

I. INTRODUCTION

The dynamics of a Hamiltonian system near an elliptic fixed point is one of the basic problems of classical physics, arising in the stability of motion in mechanics, in weakly nonlinear waves in fluids, plasmas, and other media, and in many other situations. A powerful tool to analyze such dynamical systems is the Poincare–Birkhoff normal forms method of eliminating nonresonant terms in the Hamiltonian via canonical transformations (see, e.g., Ref. 1). Normal forms also appear in generalizations of the Bohr–Sommerfeld quantization condition to near-integrable systems. A recent approach to this question, developed by in Refs. 2–4 and others, led to a theory of semi-classical Poincare–Birkhoff normal forms that can be applied to many problems of quantum perturbation theory.

In most recent applications of classical normal forms, canonical transformations are constructed by the so-called Lie series method (see, e.g., Refs. 5–7). An analog of the Lie series is also used in semiclassical normal forms to construct unitary transformations (see, e.g., Refs. 3 and 8). A computational issue in using Lie series and its semiclassical analog is the efficient evaluation of repeated Poisson brackets (see, e.g., Ref. 9). In this note we point out that these operations have an elementary diagrammatic interpretation and that using the diagrams speeds up the calculations significantly. We indicate the use of the diagrams with an example of a normal form for an infinite-dimensional Hamiltonian system arising in hydrodynamics. We also show that diagrams and the operations between them have a natural "quantization," and that in the $\hbar \to 0$ limit we obtain the classical diagrams. Quantum diagrams can be applied to semi-classical normal forms calculations, very much along the lines of the classical case.

II. CLASSICAL DIAGRAMS

The classical diagrammatic method consists of a correspondence between diagrams and functions on the phase space M, and a rule for assigning a new graph to the Poisson bracket of two graphs.

The classical phase space M will be $\mathbf{R}^{2d}$ with the canonical symplectic structure and corresponding Poisson bracket. Given a harmonic oscillator Hamiltonian with frequencies $\omega = [\omega_1,\ldots,\omega_d]$ we define the complex variables a_i, a_i^* by

$$a_i = \frac{1}{\sqrt{2}}\left(\sqrt{\omega_i} q_i + i\,\frac{p_i}{\sqrt{\omega_i}}\right), \quad a_i^* = \frac{1}{\sqrt{2}}\left(n\sqrt{\omega_i} q_i - i\,\frac{p_i}{\sqrt{\omega_i}}\right). \tag{2.1}$$

The map $a(q,p)$ embeds M canonically to $\mathbf{C}^{2d}$ with the Poisson bracket J given by

$$J(f,g) = \{f,g\} = i\sum_{i=1}^{d}\left(\frac{\partial f}{\partial a_i}\frac{\partial g}{\partial a_i^*} - \frac{\partial g}{\partial a_i}\frac{\partial f}{\partial a_i^*}\right). \tag{2.2}$$

We may also consider infinite-dimensional analogs of the above phase space, e.g., with the index i running over $\mathbf{Z}^n$. What follows applies to the infinite-dimensional case as well. Observables will be assumed to be real analytic (i.e., polynomials in a_i, a_j^* for the purposes of formal calculations), vanishing at the origin. We now describe the diagrammatic rules.

(1) The set of graphs will be the set D of simply connected directed trees with indices at each leg (branch). (Legs will meet at vertices.) Legs connecting two vertices will be referred to as internal legs, while legs with a free end will be referred to as external legs. The one-vertex trees obtained by cutting the internal legs of a multi-vertex tree t will be called the one-vertex subtrees of t. External legs will carry one index. Internal legs will carry two indices, one for each vertex being connected, so that the one-vertex subtrees will be in D.

(2) To describe the correspondence between trees and polynomials, we start with one-vertex trees. We assign to each homogeneous polynomial term

$$\sum_{\kappa_1,\ldots,\kappa_n,\lambda_1,\ldots,\lambda_m} I_{\kappa_1\ldots\kappa_n\lambda_1\ldots\lambda_m} a_{\kappa_1}\cdots a_{\kappa_r} a^*_{\lambda_1}\cdots a^*_{\lambda_m}$$

a vertex with $n+m$ legs (branches), one leg corresponding to each of the a_{κ_i} and $a^*_{\lambda_j}$. On each leg there will be an arrow, pointing into the vertex for legs representing the $a^*_{\lambda_j}$ and outwards from the vertex for legs representing the a_{κ_i}. Also, each leg will carry the index of the a_{κ_i} or $a^*_{\lambda_j}$ it represents. The dots in the vertices represent the coefficients $\omega_{\kappa\lambda}$, $A_{\kappa\lambda\mu}$, etc., and the summation over the indices. The dots in the vertices should be represented by different symbols, e.g., boxes, triangles letters, so that we can distinguish between graphs with the same number of in-going and out-going legs but different coefficients.

(3) A multi-vertex tree represents a homogeneous polynomial in the variables indexed by the external legs of the tree. The out-going and in-going arrows represent the a_{κ_i} and $a^*_{\lambda_j}$, respectively. The coefficient of this polynomial will be the product of the coefficients of all the one-vertex subtrees of the multi-vertex tree, summed over all the indices appearing in external legs and contracted over the pairs of indices representing legs that connect vertices. Also, the polynomial represented by multi-vertex tree may be alternatively represented by a one-vertex tree with an appropriate coefficient.

Proposition 2.1: With the above conventions, the Poisson bracket $\{f,g\}$ of two trees $f,g \in D$ is the sum of the graphs obtained by joining an out-going arrow of f to an in-going arrow of g and the trees obtained by joining an in-going arrow of f to an out-going arrow of g. The trees obtained this way will also have signs: $(-i)$ for trees obtained by joining an out-going arrow of f to an in-going arrow of g, and $(+i)$ for trees formed by joining an in-going arrow of f to an out-going arrow of g.

Proof: Let

$$F=\sum_{c_1,\ldots,c_n,c_{n+1},\ldots,c_{n+m}} I_{c_1\ldots c_n c_{n+1}\ldots c_{n+m}} a_{c_1}\cdots a_{c_n} a^*_{c_{n+1}}\cdots a^*_{c_{n+m}}$$

and F' same as F with the I, n, and m primed. Using the bilinearity and the derivation property of the bracket we have

$$\{F,F'\}=\sum_{i,j}\sum_{\substack{c_1,\ldots,c_n,c_{n+1},\cdots,c_{n+m}\\ c_1',\ldots,c_{n'},c_{n'+1},\ldots,c_{n'+m'}}} I_{c_1\ldots c_n c_{n+1}\ldots c_{n+m}} I'_{c_1'\ldots c_n' c_{n'+1}\ldots c_{n'+m'}}$$
$$\times\{f_{c_i},f_{c_j}\}\prod_{\alpha=1,\alpha\neq i}^{n+m} f_{c_\alpha}\prod_{\beta=1,\beta\neq j}^{n'+m'} f_{c_\beta}$$

with $f_{c_\alpha}=a_{c_\alpha}$ if $\alpha<n$, $f_{c_\alpha}=a^*_{c_\alpha}$ otherwise, and similarly for f_{c_β}. From $\{a_\kappa,a^*_\lambda\}=-i\delta_{\kappa\lambda}$, $\{a_\kappa,a_\lambda\}=\{a^*_\kappa,a^*_\lambda\}=0$, and the correspondence between trees and polynomials we obtain the rule. ∎

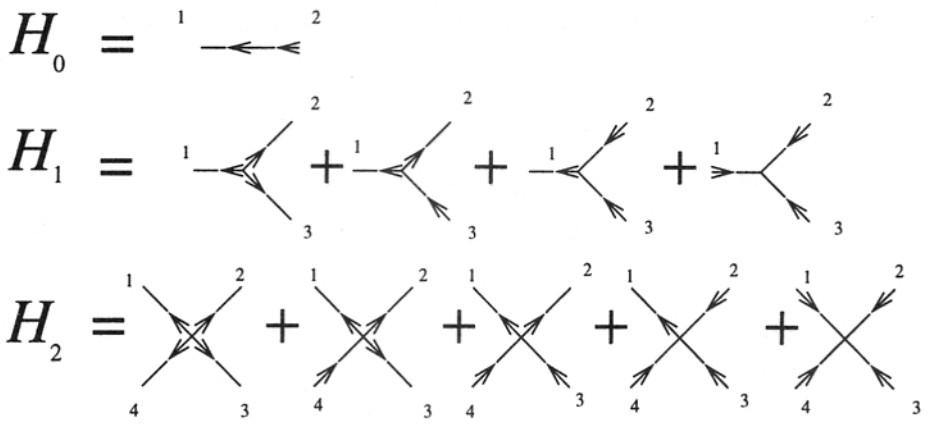

FIG. 1. The quartic water wave Hamiltonian.

The rules are essentially the same if we use the variables (q_γ, p_γ) or the well-known action-angle variables. Also, the diagrammatic notation can be compressed by considering diagrams without arrows or indices. One can calculate Poisson brackets with such trees and add arrows and indices afterwards.

III. AN APPLICATION TO FLUID MECHANICS

We indicate the use of diagrams with a normal form calculation for a Hamiltonian model of waves on the surface of a fluid layer surrounding a gravitating sphere. A detailed description of the model can be found in Ref. 10.

The canonical variables are the wave amplitude q and the surface hydrodynamic potential p, both functions on the two-sphere. The Hamiltonian is the total energy of the system. We denote the ith spherical harmonic coefficient of q,p by q_i, p_i, respectively. The index i runs over the pairs (l,m) with l a positive integer, $m=-l,-l+1,\ldots,l$. Using the frequencies of the linearized problem we also define the complex variables a_i and a_i^* as in (2.1). The Poisson bracket is (after a change of coordinates) as in (2.2). The Hamiltonian H can be written as $H=H_0+\epsilon H_1+\epsilon^2 H_2+\cdots$, with H_m homogeneous polynomials of degree $m+2$ in a_i, a_i^* and ϵ a small dimensionless parameter. Physically, ϵ is the ratio of the typical wave amplitude over the thickness of the fluid layer. The other dimensionless parameter of the problem, the ratio β of depth over radius, is set here to $O(1)$. Graphically H is as in Fig. 1.

The normal form calculation consists of eliminating the cubic and part of the quartic terms of H by canonical transformations. It is convenient to use the multi-index notation $z^k \bar{z}^{\bar{k}} a_1^{k_1}\cdots a_d^{k_d}\cdots (a_1^*)^{\bar{k}_1}\cdots (a_d^*)^{\bar{k}_d}\cdots$, with $|k|=k_1+k_2+\cdots$, $|\bar{k}|=\bar{k}_1+\bar{k}_2+\cdots$, and write $H_m=\Sigma_{|\kappa|+|\bar{\kappa}|=m+2} A^m_{|\kappa|,|\bar{\kappa}|} z^k \bar{z}^{\bar{k}}$. Following the Lie series method (in the version of Ref. 6), we seek a function S_1 for which $\exp \epsilon \mathrm{Ad}_{S_1} H$ has no cubic terms. We are led to the "homological equation" $\{S_1, H_0\}+H_1=0$, which is solved by

$$S_1=\sum_{\kappa+\bar{\kappa}=3} \frac{A^1_{\kappa,\bar{\kappa}}}{\Sigma_i \omega_i (k_i-\bar{k}_i)} \bar{z}^{\bar{k}} z^k,$$

i.e., the resonance condition is $\Sigma_i \omega_i (k_i-\bar{k}_i)=0$. In Ref. 10 we have shown that when the resonance condition is satisfied for some $k,\bar{k}$, the corresponding $A^1_{\kappa,\bar{\kappa}}$ must vanish, and thus ϵH_1 is formally eliminated. Next we eliminate the nonresonant terms of $\widetilde{H}_2$, the quartic terms of $\exp \epsilon \mathrm{Ad}_{S_1} H$. We have that $\widetilde{H}_2=H_2+\frac{1}{2}\{S_1, H_1\}$. Writing S_1 as in Fig. 2, we obtain $\widetilde{H}_2$ graphically. We have shown that the resonant part of $\widetilde{H}_2$ (denoted by $\bar{H}_2$) can only consist of terms corresponding to diagrams with two out-going and two in-going legs. $\bar{H}_2$ is represented in Fig. 3.

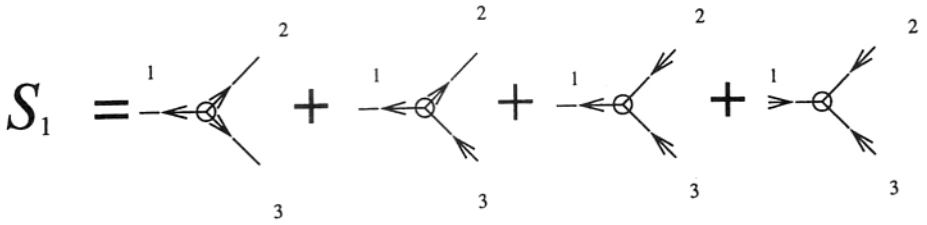

FIG. 2. The function S_1.

The normal form Hamiltonian $H_0+\bar{H}_2$ has several interesting properties. We can easily identify families of periodic and quasiperiodic orbits (the former representing traveling and standing waves) and finite-dimensional invariant manifolds. Also finite-dimensional truncations of $H_0+\bar{H}_2$, restricted to axisymmetric solutions, are completely integrable.

IV. SEMI-CLASSICAL DIAGRAMS

The rules for classical graphs have an interesting quantization that we now describe. As with the classical graphs, the natural application of the quantum diagrams is in semiclassical normal forms algorithm, for which we refer to Ref. 3.

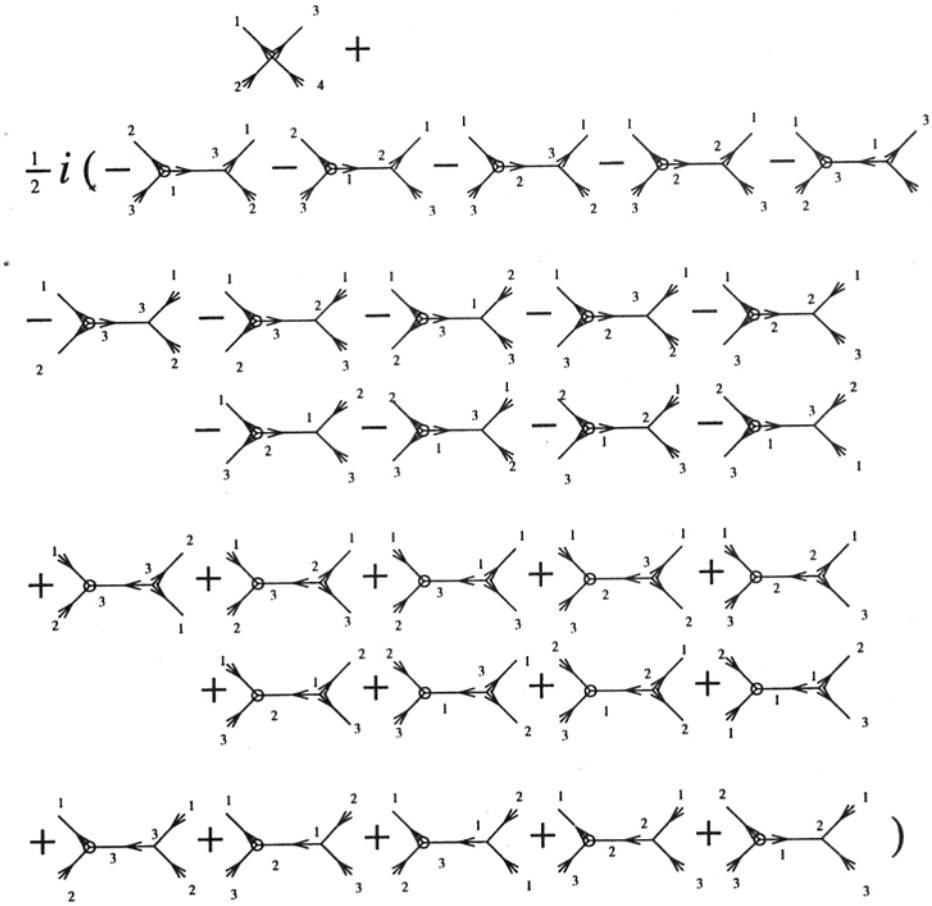

FIG. 3. The quartic part of the normal form Hamiltonian.

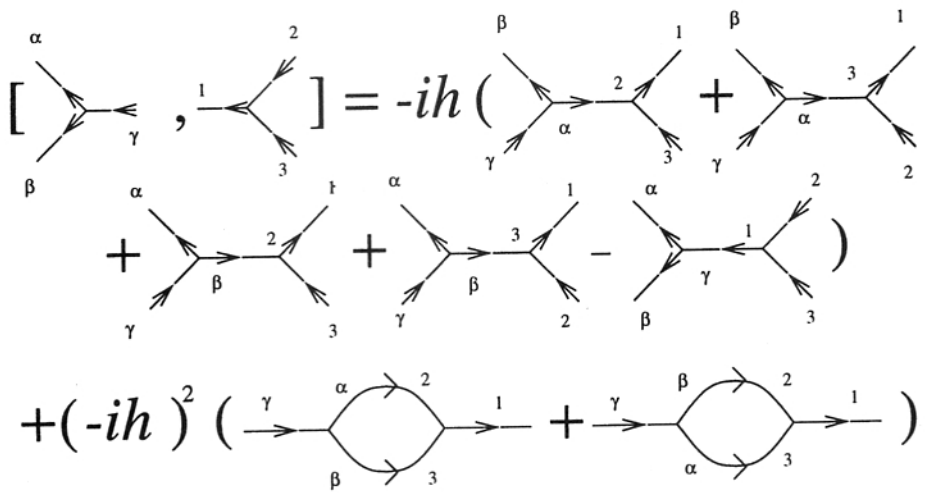

FIG. 4. Commutator of two quantum diagrams.

To describe the quantum diagrams, it is sufficient to consider the associative algebra W generated by the vectors $(a_j^*)\hat{},\hat{a}_i$, $i,j=1,2,...,d$, that also satisfy the commutation relations

$$[\hat{a}_i,\ (a_j^*)\hat{}]=-i\hbar\delta_{ij},\quad [\hat{a}_i,\ \hat{a}_j]=[(a_i^*)\hat{},\ (a_j^*)\hat{}]=0,\quad \forall i,j=1,2...,d, \tag{4.1}$$

with $[f,g]=fg-gf$, $f,g\in W$. Informally, the $(a_j^*)\hat{},\hat{a}_i$ are the ''creation–annihilation'' operators.

The graphical rules assign graphs to elements (polynomials) of W and also to the commutator of two graphs. Without loss of generality, we will assign graphs only to elements $\hat{w}$ of W that are Wick-ordered, i.e., with the $(a_j^*)\hat{}$ preceding the $\hat{a}_i$ in each monomial of $\hat{w}$. The rules are as follows:

(1) The set of graphs we consider will now be denoted by D_q. An element of D_q will be a directed tree with indices, constructed recursively in the following way: we take κ one-vertex elements t_i of D (as in Sec. II) and start by joining s_1 out-going (in-going) legs of t_1 to s in-going(out-going) legs of t_2. Denote this by $t_1\cup t_2$. At the ith step we join s_i out-going (in-going) legs of the $t_1\cup\cdots\cup t_i$ to s_i in-going(out-going) legs of t_{i+1}, until $i=\kappa-1$. The s_i are arbitrary. The external legs will carry one index, while internal legs will carry two indices, one for each vertex being joined. Note that $D\subset D_q$.

(2) We first discuss one-vertex trees. To a Wick-ordered homogeneous polynomial

$$\sum_{\kappa_1,\ldots,\kappa_n,\lambda_1,\ldots,\lambda_m} I_{\kappa_1\ldots\kappa_n,\lambda_1\ldots\lambda_m}(a_{\lambda_1}^*)\hat{}\cdots(a_{\lambda_m}^*)\hat{}\,\hat{a}_{\kappa_1}\cdots\hat{a}_{\kappa_n}$$

we assign a vertex with $n+m$ indexed legs with arrows, one out-going (in-going) leg for each $a_{k_i}(a_{k_j}^*)$. [This rule follows the classical one verbatim, with the $\hat{a}_i,(a_j^*)\hat{}$ playing the role of the a_i,a_j^*, respectively.]

The rule for assigning polynomials to multi-vertex graphs is similar to the one for the classical graphs. A multi-vertex tree represents a homogeneous polynomial in the variables indexed by the external legs of the tree. The out-going and in-going arrows represent the a_{κ_i} and $a_{\lambda_j}^*$, respectively. The coefficient of this polynomial will be the product of the coefficients of all the one-vertex subtrees of the multi-vertex tree, summed over all the indices appearing in external legs and contracted over the pairs of indices representing legs that connect vertices. Note that now multi-vertex graphs can be multiply connected. An example is in Fig. 4.

Proposition 4.1: The commutator $[F,G]$ of two graphs F,G is the sum of all graphs obtained by joining n in-going arrows of F to n out-going arrows of G and n out-going arrows of F to n in-going arrows of G, where $n=1,2,3,...$. The graphs will be multiplied by signs and powers of $\hbar$:

$(-i\hbar)^n$ for graphs obtained by joining n out-going legs from F to n in-going of G, and $-(-i\hbar)^n$ for graphs obtained by joining n in-going legs from F to n out-going from G.

Proof: We consider the commutator of two operators

$$\hat{F}=\sum A_{\bar{\kappa}_1,\ldots,\bar{\kappa}_{\bar{\mu}},\kappa_1,\ldots,\kappa_\mu}(a^*_{\bar{\kappa}_1})\hat{}\cdots(a^*_{\bar{\kappa}_{\bar{\mu}}})\hat{}\,\hat{a}_{\kappa_1}\cdots\hat{a}_{\kappa_\mu}$$

and

$$\hat{G}=\sum B_{\bar{\lambda}_1,\ldots,\bar{\lambda}_{\bar{\nu}},\lambda_1,\ldots,\lambda_\nu}(a^*_{\bar{\lambda}_1})\hat{}\cdots(a^*_{\bar{\lambda}_{\bar{\nu}}})\hat{}\,\hat{a}_{\lambda_1}\cdots\hat{a}_{\lambda_\nu}.$$

We first Wick-order $\hat{F}\hat{G}$ by passing the $\hat{a}_{\kappa_i}$ to the right of the $(a^*_{\bar{\lambda}_j})$ in a systematic way. We order the pairs of the subindices (i,j) of the $\hat{a}_{\kappa_i},(a^*_{\bar{\lambda}_j})\hat{}$ lexicographically, i.e., $(1,1)<(1,2)<\cdots<(\mu,\bar{\nu})$. Also we use the multi-index $\gamma=(i,j)$ and for $\gamma=(a,b)$ let $I(\gamma)=a$, $J(\gamma)=b$. Also $\Gamma_0=\{(i,j)|i=1,\ldots,\mu,j=1,\ldots,\bar{\nu}\}$. Define $L_{ij}\hat{F}\hat{G}$ to be $\hat{F}\hat{G}$ with $\hat{a}_{\kappa_i}$ and $(a^*_{\bar{\lambda}_j})\hat{}$ interchanged, and $R_{ij}\hat{F}\hat{G}$ to be $\hat{F}\hat{G}$ with $\hat{a}_{\kappa_i}$ and $(a^*_{\bar{\lambda}_j})\hat{}$ replaced by $[\hat{a}_{\kappa_i},(a_{\lambda_j})\hat{}]$. We write

$$\hat{F}\hat{G}=L_{1,1}\hat{F}\hat{G}+R_{1,1}\hat{F}\hat{G}=L_{1,2}L_{1,1}\hat{F}\hat{G}+R_{1,2}L_{1,1}\hat{F}\hat{G}+R_{1,1}\hat{F}=\cdots,$$

i.e., apply $L_{i,j}$ repeatedly, in the order induced by the (i,j), each time producing a commutator, and so that at most one commutator appears in each term. The procedure terminates after μ steps and we have $\hat{F}\hat{G}=S_1\hat{F}\hat{G}$ with

$$S_1\hat{F}\hat{G}=\sum_{\gamma_1\in\Gamma_1}\tilde{R}_{\gamma_1}\prod_{\tau_1\in T_1}L_\tau\hat{F}\hat{G},$$

where $\Gamma_1=\Gamma_0$ and $\tilde{R}_{\gamma_1}=L_{\gamma_1}$ if $\gamma_1=\max\{\gamma\in\Gamma_1\}$, R_{γ_1} otherwise, and $T_1\equiv T(\gamma_1)=\{\tau\in\Gamma_1|\tau<\gamma_1\}$. We repeat the procedure to terms of $S_1\hat{F}\hat{G}$ that are not Wick-ordered, so as to have at most two commutators. We get $S_2\hat{F}\hat{G}$, and similarly $\hat{F}\hat{G}=S_1\hat{F}\hat{G}=\cdots=S_n\hat{F}\hat{G}=\cdots$ with

$$S_n\hat{F}\hat{G}=\sum_{\gamma_1\in\Gamma_1}\left(\cdots\left(\sum_{\gamma_{n-1}\in\Gamma_{n-1}}\left(\sum_{\gamma_n\in\Gamma_n}\tilde{R}_{\gamma_n}\prod_{\tau_n\in T_n}L_{\tau_n}\right)\tilde{R}_{\gamma_{n-1}}\prod_{\tau_{n-1}\in T_{n-1}}L_{\tau_{n-1}}\right)\cdots\cdots\right)$$

$$\times\tilde{R}_{\gamma_1}\prod_{\tau_1\in T_1}L_{\tau_1}\hat{F}\hat{G},$$

where $\Gamma_p=\{\gamma\in\Gamma_0|I(\gamma)>I(\gamma_{p-1}),J(\gamma)\neq J(\gamma_{p-1}),\ldots,J(\gamma_1)\}$, $T_p\equiv T(\gamma_p)=\{\tau\in\Gamma_p|\tau<\gamma_p\}$ and $\tilde{R}_{\gamma_p}=L_{\gamma_p}$ if $\gamma_p=\max\{\gamma\in\Gamma_p\}$, R_{γ_p} otherwise.

Then note that, first in $S_n\hat{F}\hat{G}$ we encounter all the possible products of commutators $[\hat{a}_{\kappa_{\sigma_1}},(a^*_{\bar{\lambda}_{\rho_1}})\hat{}]\cdots[\hat{a}_{\kappa_{\sigma_n}},(a^*_{\bar{\lambda}_{\rho_n}})\hat{}]$ with $\sigma_1<\sigma_2<\cdots<\sigma_n$ and $\rho_j\neq\{\rho_1,\ldots,\rho_{j-1}\}$, $j=1,\ldots,n$, each such product appearing once as a summand of $S_n\hat{F}\hat{G}$. Moreover, in $S_{n+1}\hat{F}\hat{G}$ all these terms are Wick-ordered and therefore, from the diagrammatic interpretation at $S_{n+1}\hat{F}\hat{G}$, we have all the diagrams with m out-going legs of $\hat{F}$ joined to m in-going legs of $\hat{G}$, with $m=1,2,\ldots,n$, plus $\hat{F}\hat{G}$ Wick-ordered.

Applying the algorithm to $\hat{G}\hat{F}$ we similarly obtain the diagrams with m in-going legs of $\hat{F}$ joined to m out-going legs of $\hat{G}$, with $m=1,2,\ldots,n$, plus $\hat{F}\hat{G}$ Wick-ordered. Considering $\hat{F}\hat{G}-\hat{G}\hat{F}$, we have the proposition. ■

Remark 3.1: Comparing the last rule with its classical analog we have, graphically, the classical limit (see, e.g., Ref. 11)

$$\lim_{\hbar\to 0}\frac{i}{\hbar}[\hat{f},\hat{g}]=\{f,g\}.$$

In discussing the quantum graphs, quantization, i.e., the map from functions on the phase space to operators in a Hilbert space (see Ref. 11), enters only indirectly, through the commutation relations. In applying the graphs to the semi-classical normal form algorithm of Ref. 2, it is assumed that the quantization step is already taken and that the Hamiltonian operator has been Wick-ordered. Thus we only deal with Wick-ordered operators.

In conclusion, we have presented simple diagrammatic rules for classical and semi-classical normal forms. The rules highlight the combinatorial nature of the computations and can also be implemented in the computer.

ACKNOWLEDGMENTS

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