A DIAGRAMMATIC INTERPRETATION OF CLASSICAL AND SEMICLASSICAL PERTURBATION THEORY

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Abstract. We present a diagrammatic interpretation of the Lie-series classical perturbation theory and indicate the use of diagrams in a normal form calculation from fluid mechanics. We also extend the diagrammatic interpretation to the Rayleigh-Schrödinger perturbation theory of quantum mechanics. An advantage of the unified approach is that we have systematic expansions in $\hbar$, so that in the $\hbar \to 0$ limit we easily recover the classical diagrams.

1. Introduction

In this paper we present a diagrammatic method for computations in the perturbation theory of hamiltonian systems. The method can be thought of as a diagrammatic interpretation of the Lie-series perturbation theory of classical mechanics and is based on the properties of Poisson brackets. As will become clear our diagrammatic interpretation is elementary. Moreover, we have found it rather efficient in some lengthy computations, especially in infinite dimensional hamiltonian systems, and that was our original motivation for presenting it. We shall indicate the use of diagrams with an example drawn from a hamiltonian model of surface gravity waves (water waves).

Also we will present a quantized version of the diagrams using the analogy between the Rayleigh-Schrödinger perturbation theory of quantum mechanics and classical Lie-series. The analogy goes back to the origin of quantum mechanics but is also of recent interest especially from the point of view of relating small $\hbar$ asymptotics of the perturbed eigenvalues to features of the classical phase space of a near-integrable system (see for instance [EGH], [Ba]). ¿From our definition of the quantum graphical rules, it will be clear that in the limit $\hbar \to 0$ we recover classical ones.

A typical problem in canonical perturbation theory is the behaviour of a hamiltonian dynamical system near an elliptic fixed point. The problem arises, for instance, in the study of systems of weakly coupled harmonic oscillators and in non-linear wave equations. One of the tools used in the local study of such systems is the Poincare-Birkhoff method of successive elimination of the lowest order non-linear terms by changes of coordinates. In general there will be non-linear terms that can not be eliminated, the resonant terms. The reduced systems containing only resonant terms are said to be in normal form. Systems in normal form are frequently more tractable, and generally speaking the method is very useful for asymptotic calculations, for example approximating periodic and quasi-periodic orbits. In cases where the dynamical system under consideration satisfy extra conditions, normal form arguments can be strengthened to proofs of existence of periodic and quasiperiodic orbits.

For hamiltonian vector fields, since all the information is contained in the hamiltonian, the goal of Poincare-Birkhoff method is to simplify the hamiltonian by canonical transformations. Canonical transformations can be constructed by the the so-called Lie-series. In particular, letting M be the phase space, $\{,\}$ the Poisson bracket and χ and

f functions on M we define the map Ad_χ by $Ad_\chi f = \{\chi, f\}$ and its formal exponential $(\exp \epsilon Ad_\chi)$ by

$$(1.1) \qquad (\exp \epsilon Ad_\chi) f = f + \sum_{k=1}^{\infty} \frac{\epsilon^k}{k!} (Ad_\chi)^k f = f + \epsilon\{\chi, f\} + \frac{\epsilon^2}{2}\{\chi, \{\chi, f\}\} + \dots \quad .$$

The map $\exp \epsilon Ad_\chi$ is the formal time-ϵ map of the vector field with hamiltonian χ, acting on the functions on M. The convergence of the series for $\exp \epsilon Ad_\chi$ requires χ and f to be real analytic and χ or ϵ sufficiently small.

Let us outline the Poincare-Birkhoff procedure using Lie-series (referred to as Lie-series perturbation theory), following the version of Dragt-Finn (see [DF]). Initially we are given a hamiltonian $g = g_0 + \epsilon g_1$ with g_0 the hamiltonian of the linearised motion and ϵg_1 the non-linear perturbation (ϵ is small). The first step is to try to find a function χ_1 such that $(\exp \epsilon Ad_{\chi_1}) g$ has no terms of order ϵ. Using the series of (1.1) this means that we should have

$$(1.2) \qquad \{\chi_1, g_0\} + g_1 = 0$$

or $Ad_{g_0} \chi_1 = g_1$. After χ_1 is found the new hamiltonian is $(\exp \epsilon Ad_{\chi_1}) g = g_0 + \epsilon^2 \tilde{g}_2$ with $\tilde{g}_2$ calculated using (1.1). The procedure can be iterated: to find a function χ_2 so that $(\exp \epsilon^2 Ad_{\chi_2})(\exp \epsilon Ad_{\chi_1}) g$ has no terms of order ϵ^2 we must solve $Ad_{g_0} \chi_2 = \tilde{g}_2$ and so forth for higher orders. However in general the kernel of Ad_{g_0} will be non-empty, and to solve (1.2) we replace g_1 by its part belonging to the image of Ad_{g_0} (the non-resonant part), and χ_1 is chosen accordingly . The resonant terms of g_1 i.e those in the kernel of Ad_{g_0} can not be eliminated. (Note that some of the resonant terms are integrable.) Similar statements apply as we iterate to eliminate higher order terms. After iterating the procedure r times the transformed hamiltonian will contain only the resonant terms (to order ϵ^r). If we want to calculate the normal form Hamiltonian up to some order we have to evaluate repeated Poisson brackets between the functions χ_i and lowest order terms of the Hamiltonian. We have found that the manipulations are more efficient using the graphical method described below.

Note that there is another variant of the Lie-series method (see [D] or [C]) in which one looks for a function $\chi = \epsilon \chi_1 + \epsilon^2 \chi_2 + \cdots + \epsilon^r \chi_r$ so that $(\exp Ad_\chi) g$ will bring g to normal form up to order r. The χ_i are determined recursively, while the resonant terms are the same. The two formalisms are equivalent from the point of view of asymptotic expansions, but have different convergence and numerical stability properties (see Appendix C of [LMM]).

Also we would like to note that recently there has been been a lot of activity in diagrammatic methods in classical perturbation theories (see for instance [G]). These methods are quite different from the ones presented here as they concern convergent series expansions of parameterizations of invariant tori of fixed frequencies in near-integrable systems. Our Poincare-Birkhoff approach concerns a whole neighborhood of the origin and is asymptotic.

2. Diagrammatic interpretation

The diagrammatic interpretation 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 will define the complex variables a_i, a_i^* by

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

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

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

Hamilton's equations in the complex variables can be written as $\dot{a}_\gamma = -i\frac{\partial H}{\partial a_\gamma^*}$.

We may also consider infinite dimensional analogues of the above phase space. For instance the index i could be running over $\mathbf{Z}^n$ or $\mathbf{R}^n$ with sums replaced by integrals. We emphasize that what follows applies also to the infinite case, where the harmonic oscillator modes correspond to the sinusoidal plane waves of linear wave equation.

A real analytic observable (e.g. hamiltonian) H such that $H(0) = 0$ and $\nabla H(0) = 0$ can be written as

$$H = \sum_{\kappa_1,\kappa_2} \omega_{\kappa_1\kappa_2} a_{\kappa_1} a_{\kappa_2}^* + \sum_{\kappa_1,\kappa_2,\kappa_3} (A_{\kappa_1\kappa_2\kappa_3} a_{\kappa_1} a_{\kappa_2} a_{\kappa_3} + B_{\kappa_1\kappa_2\kappa_3} a_{\kappa_1} a_{\kappa_2} a_{\kappa_3}^* + \tag{2.3}$$

$$C_{\kappa_1\kappa_2\kappa_3}a_{\kappa_1}a^*_{\kappa_2}a^*_{\kappa_3} + D_{\kappa_1\kappa_2\kappa_3}a^*_{\kappa_1}a^*_{\kappa_2}a^*_{\kappa_3}) + \cdots$$

i.e. quartic and higher. (The coefficients $\omega_{\kappa\lambda}$, $A_{\kappa\lambda\mu}$ etc. are determined by the problem and typically H is real). We now describe the diagrammatic rules.

1) The set of graphs we consider 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

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

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.

For example, the hamiltonian of (2.3) will be, up to quartic terms, as in Figure 1

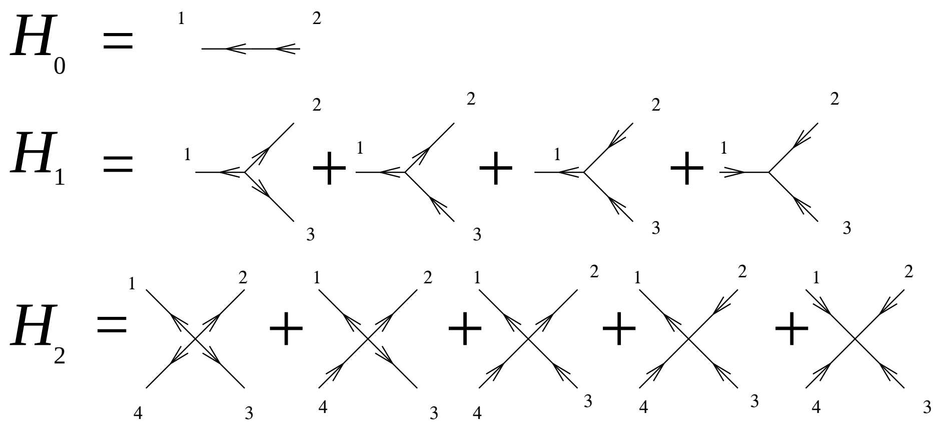

Figure 1

(here the legs are labeled by the sub-index i of the κ_i).

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 in general be represented by different symbols, for instance boxes, triangles etc. so that we can distinguish between graphs with the same number of in-going and out-going legs but different coefficients. In actual computations we need very few such symbols.

We now describe multi-vertex trees. A multi-vertex tree represents a homogeneous polynomial in the variables indexed by the external legs of the tree. The outgoing and ingoing 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. An example of a multi-vertex tree and its one-vertex sub-trees is shown in Figure 2.

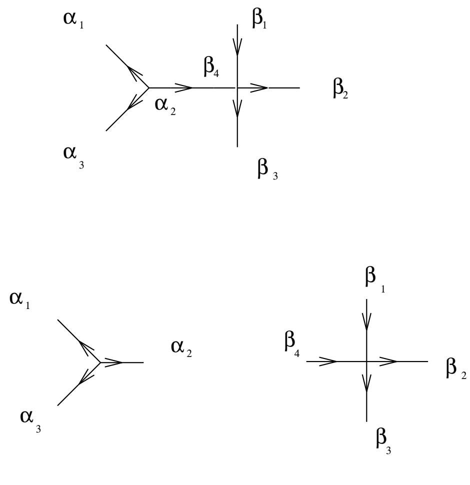

Figure 2

The one-vertex subtrees in Figure 2 represent the homogeneous polynomials

$$\sum_{\alpha_1,\alpha_2,\alpha_3} A_{\alpha_1\alpha_2\alpha_3} a_{\alpha_1} a_{\alpha_2} a_{\alpha_3} \quad \text{and} \quad \sum_{\beta_1,\beta_2,\beta_3,\beta_4} B_{\beta_1\beta_2\beta_3\beta_4} a^*_{\beta_1} a_{\beta_2} a_{\beta_3} a^*_{\beta_4}$$

respectively. The polynomial for the multi-index tree of Figure 2 is

$$\sum_{\alpha_1,\alpha_3,\beta_1,\beta_2,\beta_3,\lambda} A_{\alpha_1\lambda\alpha_3} B_{\beta_1\beta_2\beta_3\lambda} a_{\alpha_1} a_{\alpha_2} a^*_{\beta_1} a_{\beta_2} a_{\beta_3} \quad .$$

Note that the polynomial represented by multi-vertex tree may be alternatively viewed as 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 outgoing arrow of f to an in-going arrow of g and the trees obtained by joining an in-going arrow of f to an outgoing arrow of g. The trees obtained this way will also have signs: $(-i)$ for trees obtained by joining an outgoing 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 outgoing arrow of g. An example is in Figure 3.

Proof Recall that

(i) $\{a_\kappa, a^*_\lambda\} = -i\delta_{\kappa\lambda}, \quad \{a_\kappa, a_\lambda\} = \{a^*_\kappa, a^*_\lambda\} = 0$ for all indices κ, λ , and that

(ii) $\{\sum_i a_i f_i, \sum_j b_j g_j\} = \sum_{i,j} a_i b_j \{f_i, g_j\}, \quad \forall a_i, b_j \in \mathbf{C},\ f_i, g_j \in C^\infty(M)$,

(iii) $\{\prod_{i=1}^n f_i, \prod_{j=1}^m g_j\} = \sum_{i,j}^{n,m} \{f_i, g_j\} \prod_{r=1, r\neq i}^n f_r \prod_{s=1, s\neq j}^m g_s, \quad \forall f_i, g_j \in C^\infty(M)$,
from the linearity of the bracket and the product rule respectively. Applying (ii) and (iii) to

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

and F' same as F with the I, n and m primed we have

$$\{F, F'\} = \sum_{i,j} \sum_{\substack{c_1,\cdots,c_n,c_{n+1},\cdots,c_{n+m} \\ c_1,\cdots,c_{n'},c_{n'+1},\cdots,c_{n'+m'}}} I_{c_1\cdots c_n c_{n+1}\cdots c_{n+m}} I'_{c_1\cdots c'_n c_{n'+1}\cdots c_{n'+m'}} \{f_{c_i}, f_{c_j}\}$$

$$\prod_{\alpha=1,\alpha\neq i}^{n+m} f_{c_\alpha} \prod_{\beta=1,\beta\neq j}^{n'+m'} f_{c_\beta}$$

with $f_{c_\alpha} = a_{c_\alpha}$ if $\alpha < n$, $f_{c_\alpha} = a^*_{c_\alpha}$ otherwise, and similarly for f_{c_β} and from (i) and the correspondence between trees and polynomials we obtain the rule.

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An example is in Figure 3 below.

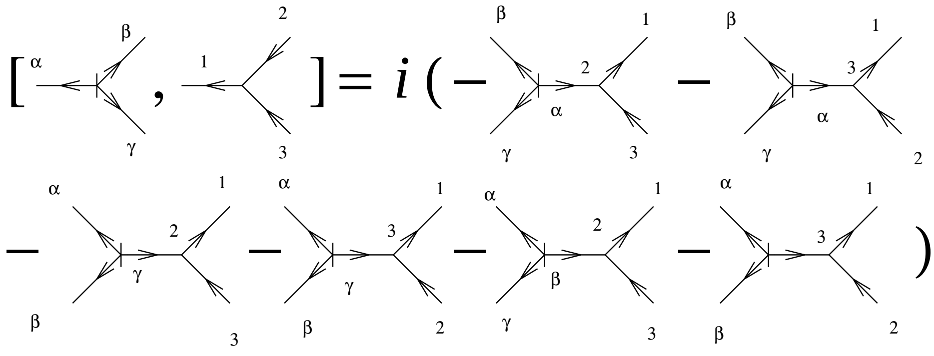

Figure 3

Remark 2.1 The rules are essentially the same if we use the variables (q_γ, p_γ) or the well known action-angle variables. Assigning inward arrows to the q_γ and outward arrows to the p_γ , the rules are the same, except that there are no i' s when we take the bracket of two graphs.

The diagrammatic notation can be compressed by considering diagrams without arrows or indices. We shall refer to these as bare trees and denote the set of bare trees by Δ. Each bare tree $\tau \in \Delta$ will represent a sum of graphs obtained by putting different combinations of arrows and indices to τ.

1) We describe the correspondence between bare trees and sums of trees by first discussing one-vertex bare trees. Letting μ, ν be the respective number of outgoing and in-going legs of a tree, we use a one-vertex bare tree with n legs to represent the sum of all one-vertex trees with different pairs μ, ν such that $\mu + \nu = n$. For example, the first terms of the hamiltonian of (2.3) is in Figure 4.

To a multi-vertex bare tree with n external legs and k one-vertex bare subtrees τ_i, $i = 1, \ldots, k$ we first assign the sum of un-indexed trees (directed trees) corresponding to the different allowed pairs $(\mu_1, \nu_1), (\mu_2, \nu_2), \ldots, (\mu_k, \nu_k)$ with μ_j, ν_j the respective number of outgoing and in-going legs of τ_j. Note that due to the presence of the internal legs not all pairs (μ_j, ν_j) are allowed. Then, to each of the un-indexed graphs we assign the sum of all the graphs corresponding to the different combinations of indices we can put on the legs. Specifically, given a one-vertex un-indexed subgraph τ with μ outgoing and ν in-going legs, of which there are $\tilde{\mu}$ outgoing and $\tilde{\nu}$ in-going legs that are internal, these are the combinations of putting $\tilde{\mu}$ numbered hats over the numbers $1, 2, \ldots, \mu$ and

$\tilde{\nu}$ numbered hats over $\mu+1, \mu+2, \ldots, \mu+\nu$, the hats representing the internal outgoing and in-going legs.

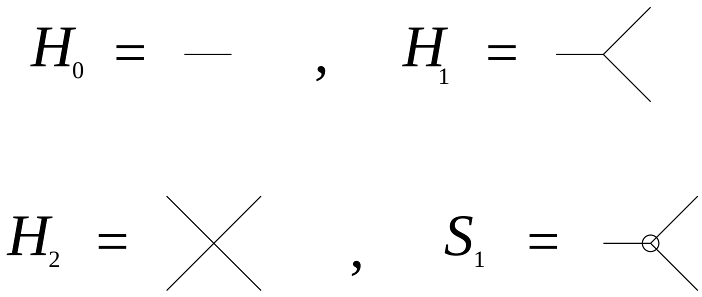

Figure 4

Proposition 2.1 The Poisson bracket between two bare trees θ, ϕ is the sum of the topologically distinct trees formed by joining an external leg of θ with an external leg of ϕ. The internal legs must be drawn so that the arrows we put on them will point either to the right or the left. Then we can give a $(-i)$ sign to arrows pointing to the right, $(+i)$ for arrows to the left. The sign of the whole multi-vertex graph will be the product of the signs of the internal (directed) legs.

Proof The rules for the Poisson bracket between bare trees are an implication of the rules for the Poisson bracket between trees. We need to check that by adding arrows and indices to bare trees θ, ϕ and taking the Poisson bracket of the resulting sums of trees we obtain the same trees as when using the rule for the bracket of θ and ϕ and then adding arrows and indices to obtain the trees. This is done by simply noticing each tree obtained in one way can be obtained in the other way as well.

■

For the r-th step of the normal form calculation we need to know $\tilde{H}_r$, the order r part of $(\exp \epsilon^{r-1} Ad_{S_{r-1}}) \ldots (\exp \epsilon Ad_{S_1}) H$. With $\tilde{H}_r$ we can determine the function S_r that eliminates the non-resonant part of $\tilde{H}_r$ and $\overline{H}_r$, the resonant part of $\tilde{H}_r$ and go to the next step. It is easy to express $\tilde{H}_r$ in terms of $H_1, \ldots, H_r$, $\overline{H}_1, \ldots, \overline{H}_{r-1}$ and $S_1, \ldots, S_{r-1}$. If we use one-vertex trees with $n+2$ legs and with the vertex circled and boxed to represent S_n and $\overline{H}_n$ respectively, then $\tilde{H}_2$, $\tilde{H}_3$ and $\tilde{H}_4$ are as in Figures 5a and 5b.

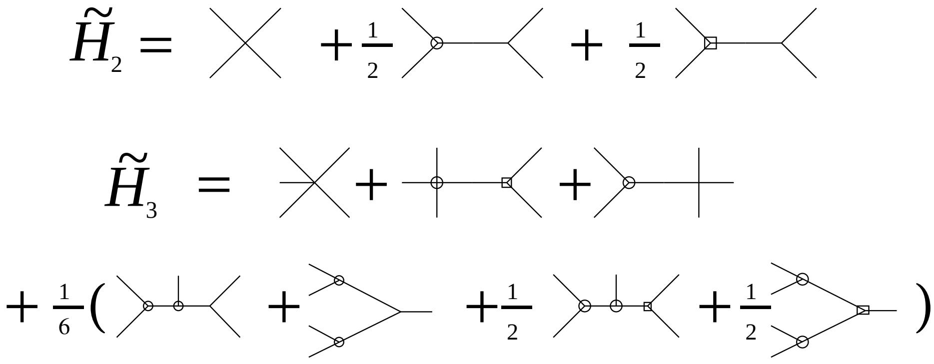

Figure 5a

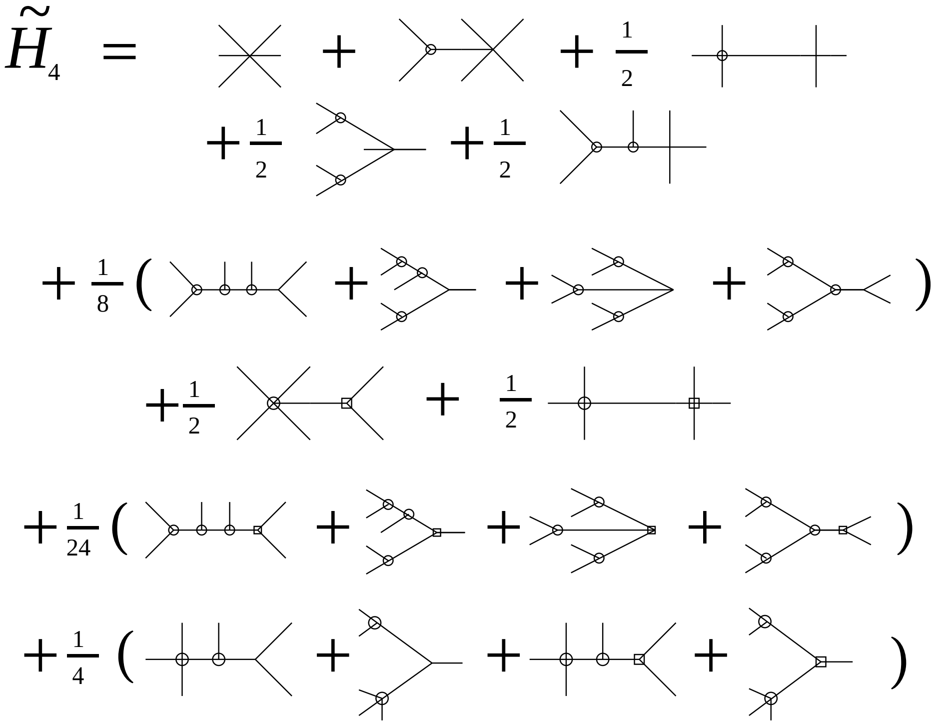

Figure 5b

3. An application to fluid mechanics

We shall indicate the use of diagrams with a normal form calculation for an infinite dimensional hamiltonian system. In particular, we will consider a hamiltonian model of waves on the surface of a fluid layer surrounding a gravitating sphere (water waves). A detailed description of the model and the computations can be found in [LP].

The evolution equation for this system can be written as an infinite analogue of Hamilton's equation. The canonical variables are the wave amplitude q and the surface hydrodynamic potential p, both functions on the 2-sphere, while the hamiltonian (functional) is the total energy of the system. We expand q and p in spherical harmonics Y_i and denote the coefficient of the i-th harmonic (or i-th mode) by q_i, p_i. (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 linearised 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 $H = H_0 + \epsilon H_1 + \epsilon^2 H_2 + \ldots$, with H_m homogeneous polynomials of degree $m+2$ in a_i, a_i^* and ϵ a small dimensionless parameter. Physically, 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 Figure 1.

Our calculation consists of eliminating the terms of order ϵ and some of the terms of order ϵ^2. It is convenient to use the multi-index notation

$$z^k \overline{z}^{\overline{k}} = a_1^{k_1} \ldots a_d^{k_d} \ldots (a_1^*)^{\overline{k}_1} \ldots (a_d^*)^{\overline{k}_d} \ldots \quad ,$$

with $|k| = k_1 + k_2 + \ldots$ $|\overline{k}| = \overline{k}_1 + \overline{k}_2 + \ldots$, and write $H_m = \sum_{|\kappa|+|\overline{\kappa}|=m+2} A^m_{|\kappa|,|\overline{\kappa}|} z^k \overline{z}^{\overline{k}}$. To find S_1 for which $\exp \epsilon Ad_{S_1} H$ has no terms of order ϵ we are led to $\{S_1, H_0\} + H_1 = 0$. Noting that

$$\{\overline{z}^{\overline{k}} z^k, H_0\} = -i(\sum_i \omega_i (k_i - \overline{k}_i)) \overline{z}^{\overline{k}} \hat{z}^k,$$

the solution is

$$\chi_1 = \sum_{\kappa+\overline{\kappa}=3} \frac{A^1_{\kappa,\overline{\kappa}}}{\sum_i \omega_i (k_i - \overline{k}_i)} \overline{z}^{\overline{k}} z^k,$$

i.e. the resonant terms are those satisfying $\sum_i \omega_i (k_i - \overline{k}_i) = 0$. Moreover, the hamiltonian is spherically symmetric and as a consequence every cubic monomial coupling three modes, say $a_{i_1}, a_{i_2}, a_{i_3}$ in H_1 is proportional to the integral of the product of the corresponding harmonics $Y_{i_1}, Y_{i_2}, Y_{i_3}$. Thus the resonant triples of modes must also satisfy the condition that these integrals do not vanish. In [LP] we have shown that H_1 contains no resonant terms and thus can be eliminated completely. Next, we eliminate the non-resonant terms of $\tilde{H}_2$, the order ϵ^2 terms of $\exp \epsilon Ad_{S_1} H$. ¿From (1.1) we have that $\tilde{H}_2 = H_2 + \frac{1}{2}\{S_1, H_1\}$. Writing S_1 as in Figure 6, we obtain $\tilde{H}_2$ graphically. Proceeding as before we find analogous resonance conditions (again involving conditions on integrals of spherical harmonics) for four modes and we have shown that the resonant terms of $\tilde{H}_2$ (denoted by $\overline{H}_2$) can only be of the type corresponding to diagrams with two outgoing and two in-going legs. $\overline{H}_2$ is represented in Figure 7.

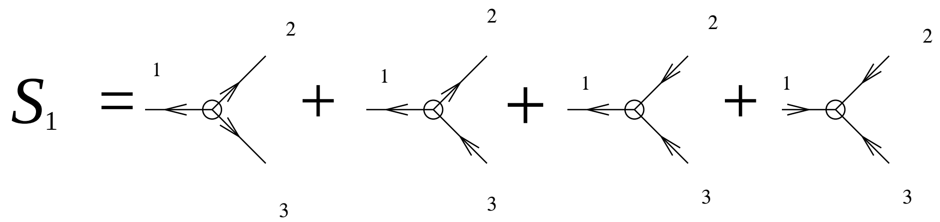

Figure 6

The result of this calculation is that we can now easily identify families of periodic solutions of the normal form system with hamiltonian $H_0 + \overline{H}_2$. These approximate solutions of the full system correspond to traveling and standing waves involving one or two modes. $\overline{H}_2$ calculated graphically gives us the relation between the amplitude and speed of these waves. Also, again using $\overline{H}_2$, we can identify invariant manifolds of solutions involving a finite number of modes. These manifolds are in fact invariant to higher order and on them we can find new families of periodic solutions of the water wave system.

Note that the resonance conditions can be read from the diagrams. For instance, the resonant terms of a diagram with m outgoing and n outgoing legs will be those satisfying $\omega_{\kappa_1} + \ldots + \omega_{\kappa_m} - \omega_{\lambda_1} - \ldots - \omega_{\lambda_n} = 0$. A similar statement can be made about the angular addition rules.

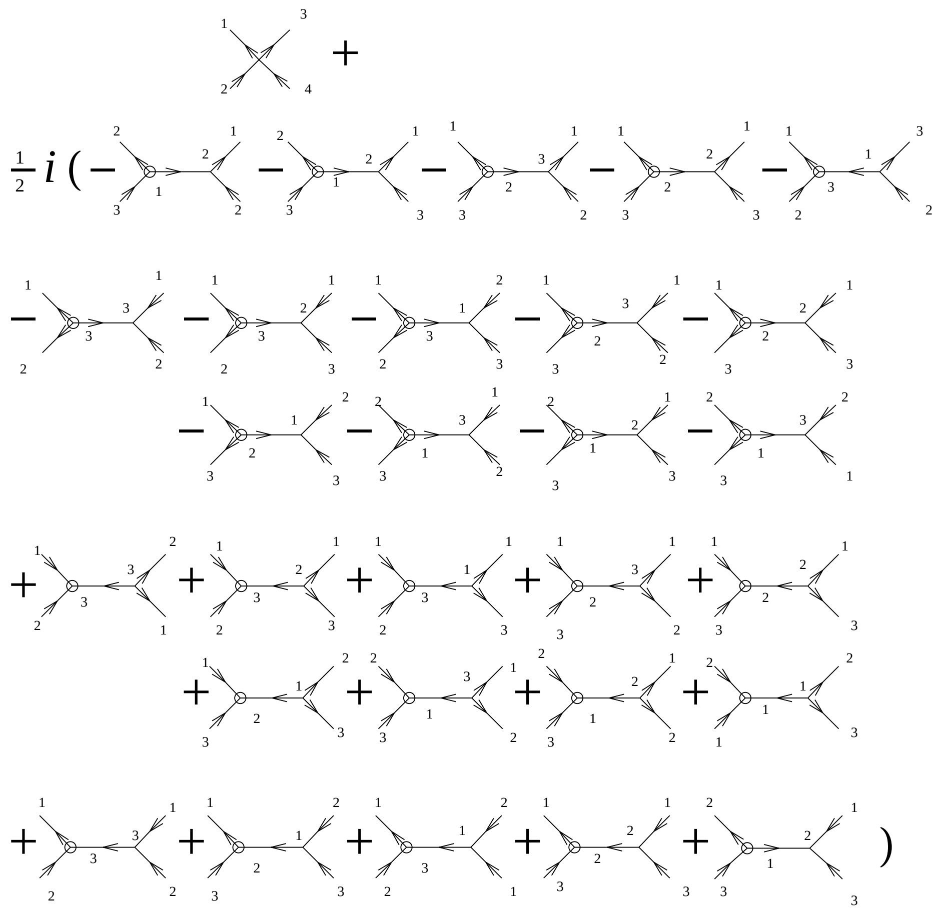

Figure 7

4. Semiclassical diagrams

As several authors have noted classical perturbation theories in the form of Lie-series or the Hamilton-Jacobi theory can be "quantized" to yield the Rayleigh-Schrödinger perturbation theory for the spectrum of the hamiltonian operator in quantum mechanics (see [GP1], [EGH], [BV]). Here we would like to show that the graphical interpretation can be extended to the quantized version of the Lie-series.

To describe the quantized Lie-series and the diagrammatic interpretation it is sufficient to consider the algebra W generated by polynomials in the $\hat{a}_i$ and $(a_j^*)\hat{}$, where $i, j = 1, 2 \ldots, d$. The $\hat{a}_i$ and $(a_j^*)\hat{}$ are required to satisfy the the commutation relations

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

where $[\hat{f}, \hat{g}] = \hat{f}\hat{g} - \hat{g}\hat{f}$. Also we will consider a quadratic polynomial $\hat{h}_0$ given by

$$\hat{h}_0 = \frac{1}{2}\sum_{i=1}^{d} \omega_i((a_i^*)\hat{}\hat{a}_i + \hat{a}_i(a_i^*)\hat{})$$

with $\omega_i \in \mathbf{R}$ and the polynomial $\hat{h} = \hat{h}_0 + \epsilon\hat{h}_1 + \epsilon^2\hat{h}_2 + \ldots$, with the $\hat{h}_\mu$ of order $\mu + 2$ in a_i and a_i^*. We will assume, without loss of generality that the products appearing in the $\hat{h}_\mu$ are in "Wick-ordered" form, that is, with the $(a_j^*)\hat{}$ preceding the $\hat{a}_i$.

In quantum mechanics the $\hat{a}_i$ and $(a_j^*)\hat{}$ are represented as operators in a Hilbert space, while $\hat{h}_0$ and $\hat{h}$ are the harmonic oscillator with frequencies $\omega = [\omega_1, \ldots, \omega_d]$ and perturbed harmonic oscillator hamiltonian operators respectively. In particular, we can take the Hilbert space of quantum states to be (the Bargmann space) $F_d(\mathbf{C}^d)$ of holomorphic functions $\psi : \mathbf{C}^d \to \mathbf{C}$ for which $\int_{R^{2d}} |\psi|^2 e^{-|z|^2/\hbar} dq dp$ is finite and represent $\hat{a}_i$ and $(a_j^*)\hat{}$ by

$$\hat{a}_i\psi = z_i\psi \quad , \quad (a_j^*)\hat{}\psi = \hbar\partial_{z_j}\psi \quad . \tag{4.2}$$

Note however that in the description of the perturbation theory and the diagrams that follows we only need the algebra W, the commutation relations (4.1) and $\hat{h}_0$ and $\hat{h}$.

The problem of quantum perturbation theory is the determination of the spectrum of $\hat{h}$. The spectral decomposition of $\hat{h}_0$ is known. ¿From the algebraic point of view we want to simplify $\hat{h}$ using transformations that preserve the commutators structure. In analogy with classical mechanics we define the map $\widehat{Ad}_{\hat{g}}$ by $\widehat{Ad}_{\hat{g}}\hat{f} = [\hat{g}, \hat{f}]$ and its formal exponential

$$(\exp \epsilon\widehat{Ad}_{\hat{g}})\hat{f} = \hat{f} + \epsilon[\hat{g}, \hat{f}] + \frac{1}{2}\epsilon^2[\hat{g}, [\hat{g}, \hat{f}]] + \ldots \tag{4.3}$$

As in the classical case we try to eliminate the $O(\epsilon)$ terms of $\hat{h}$, order by order, by a successive application of the map $\exp \epsilon\widehat{Ad}_{\hat{g}}$. We start by trying to find $\hat{\chi}_1$ so that $\exp \epsilon\widehat{Ad}_{\hat{\chi}_1}\hat{h}$ has no terms of order ϵ and we are led to

$$[\hat{\chi}_1, \hat{h}_0] + \hat{h}_1 = 0 \tag{4.4}$$

To solve (4.4), observe that for $\hat{h}_0$ quadratic we have that

$$[(\hat{\overline{z}})^{\overline{k}}\hat{z}^k, \hat{h}_0] = -i(\sum_{i=1}^{d} \omega_i(k_i - \overline{k}_i))(\hat{\overline{z}})^{\overline{k}}\hat{z}^k, \tag{4.5}$$

and recall that (using the multi-index notation)

$$\hat{h}_1 = \sum_{n=1}^{3} \sum_{\kappa+\overline{\kappa}=n} A^n_{\kappa,\overline{\kappa}} (\hat{\overline{z}})^{\overline{k}} (\hat{z})^k$$

and therefore

$$\hat{\chi}_1 = \sum_{n=1}^{3} \sum_{\kappa+\overline{\kappa}=n} \frac{A^n_{\kappa,\overline{\kappa}}}{\sum_i \omega_i (k_i - \overline{k}_i)} (\hat{\overline{z}})^{\overline{k}} (\hat{z})^k$$

The resonance condition is similar to the classical one, and χ_1 is chosen accordingly to eliminate the non-resonant terms of $\epsilon \hat{h}_1$. We repeat the procedure to remove the non-resonant terms ϵ^2 terms of $\exp \epsilon \widehat{Ad}_{\hat{\chi}_1} \hat{h}$ and similarly for higher orders in ϵ. The algorithm is clearly analogous to the classical Lie-series. After r steps the operator will be in "normal form". The relevance of the procedure is that if the frequencies are non-resonant to order r , i.e. if $< \omega, \nu > \neq 0$ for $\nu \in \mathbf{Z}^d$, $|\nu| < r+2$, the transformed operator will be diagonal to $o(\epsilon^r)$ in the basis of the eigenfunctions of $\hat{h}_0$. Thus the quantized Lie-series algorithm is in effect the (non-degenerate) Rayleigh-Schrödinger perturbation theory. In the case of resonance, some off-diagonal terms will remain. These are the classical resonant terms plus corrections of $O(\hbar)$. A semiclassical version of degenerate Rayleigh-Schrödinger series, corresponding to the Poincare "secular" perturbation theory of classical mechanics is also possible along similar lines (see [Ba], also [GP2]).

The graphical interpretation consists of a rule for assigning graphs to polynomial operators and a rule for assigning a graph to the commutators of two graphs. Graphs will be assigned to Wick-ordered operators only. ¿From the above, after Wick-ordering a quantized observable $\hat{h}$, and provided that we can Wick-order the commutator of two Wick-ordered terms, we only have to deal with Wick-ordered polynomials only.

The rules are as follows:

1) The set of graphs under consideration 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 chapter 2) and start by joining s_1 outgoing (ingoing)legs of t_1 to s ingoing(outgoing) legs of t_2. Denote this by $t_1 \cup t_2$. At the i-th step we join s_i outgoing (ingoing) legs of the $t_1 \cup \ldots t_i$ to s_i ingoing(outgoing) 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, one for each vertex being joined. Note that $D \subset D_q$.

Examples are in Figure 8 below.

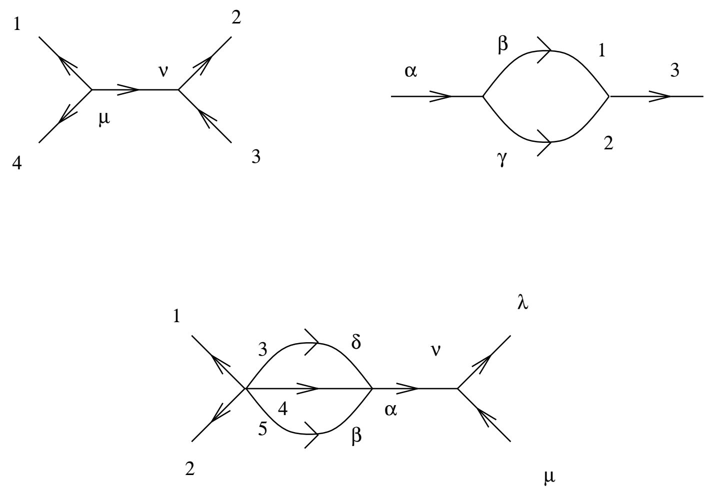

Figure 8

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

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

we assign a vertex with $n+m$ indexed legs with arrows, one outgoing (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 outgoing and ingoing 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 Figure 9.

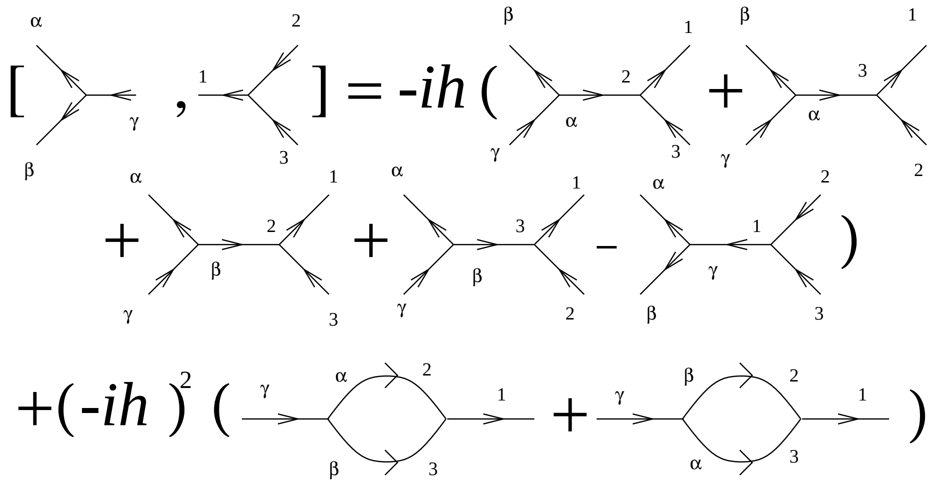

Figure 9

Proposition 4.1 We form the commutator $[F, G]$ of two graphs F, G by adding all the graphs obtained by joining n in-going arrows of F to n outgoing arrows of G and n outgoing arrows of F to n in-going arrows of G, where $n = 1, 2, 3, \ldots$. The graphs will be multiplied by signs and powers of $\hbar$: $(-i\hbar)^n$ for graphs obtained by joining n outgoing 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 outgoing from G.

Proof We consider the commutator of two operators

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

and

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

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

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

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

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

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 $T_1 \equiv T(\gamma_1) = \{\tau \in \Gamma_1 | \tau \prec \gamma_1\}$. 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

$$\hat{F}\hat{G} = S_1\hat{F}\hat{G} = \ldots = S_n\hat{F}\hat{G} = \ldots$$

with

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

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

with $\Gamma_p \equiv \Gamma_p(\gamma_{p-1}, \ldots, \gamma_1) = \{\gamma \in \Gamma_0 | I(\gamma) > I(\gamma_{p-1}), J(\gamma) \neq J(\gamma_{p-1}), \ldots, J(\gamma_1)\}$, $T_p \equiv T(\gamma_p) = \{\tau \in \Gamma_p | \tau \prec \gamma_p\}$ 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 $[\hat{a}_{\kappa_{\sigma_1}}, (a^*_{\lambda_{\rho_1}})\hat{\ }] \ldots [\hat{a}_{\kappa_{\sigma_n}}, (a^*_{\lambda_{\rho_n}})\hat{\ }]$ with $\sigma_1 < \sigma_2 < \ldots < \sigma_n$ 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 outgoing 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 ingoing legs of $\hat{F}$ joined to m outgoing 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

$\blacksquare$

Remark 3.1 Note that comparing the last rule with its classical analogue we have the classical limit that, graphically

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

Note that the quantum "normal form" hamiltonian obtained after r steps of the algorithm will contain polynomials that are multiplied by powers of $\hbar$. This is clear, for instance from the rule for the commutator of two graphs. Therefore the dependence of the perturbed eigenvalues on $\hbar$ will be explicit. In the case of non-resonance the eigenvalues obtained from the quantum Lie-series will be those given by the semiclassical EBK values (see [EGH]) plus $O(\hbar)$ corrections.

We would like to point out that the analogy between the classical and quantum Lie-series above can be discussed more fully within the framework of pseudodifferential operators, where we can consider explicit ways to map classical observables (f) to linear operators ($\hat{f}$), i.e. quantizations (for a heuristic introduction see [BS], ch. 5). In particular, under certain assumptions on the classical hamiltonian $h_0 + \epsilon g$, the frequencies of h_0 (and using the Weyl quantization) we can make error estimates for the eigenvalues obtained using the above semiclassical expansions, and show that the error is small uniformly in $\hbar$. (this follows from [Ba] with some modifications, see also [BV] for a different approach). In our presentation we assume that the quantization step is already taken, and that the operators have been Wick-ordered. It is in fact possible to discuss diagrams for polynomials that are not Wick-ordered, by introducing a convention that takes into account the order of the $\hat{a}_i$ and $(a_j^*)\hat{}$, e.g. numbering the external legs. The advantage of using Wick-ordered polynomials is that the ordering of the $\hat{a}_i$ and $(a_j^*)\hat{}$ is taken into account and the correspondence between graphs and polynomials is similar to the one for the classical case.

In summary, we have presented a simple graphical interpretation of the classical Lie-series algorithm and its quantized version, which takes the form of the Rayleigh-Schrödinger perturbation theory. Also we gave an application to an asymptotic calculations in a problem of classical fields (hydrodynamics).

5. Acknowledgments

I would like to thank Professor de la Llave for encouraging me to write this note and for several suggestions. I would also like to acknowledge partial support from NSF and TARP grants.

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