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A.S.Nikolaev¹

ON THE DIAGONALIZATION OF THE QUANTUM
BIRKHOFF-GUSTAVSON NORMAL FORM²

SW 9607

¹nikolaev@mx.ihep.su

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Abstract

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An application to quantum mechanics of one of classical perturbation theory methods – the Birkhoff-Gustavson normal form (BGNF) is described. In the quantum case it results in the Van Vleck perturbation theory performed upon Wick normal ordered operators. Algebraic aspects of this procedure and formal construction of invariants (integrals of motion) for a perturbed system are considered. It turned out that a larger set of such operators existed in the quantum mechanics, rather than in the classical one. Demonstrated that, according to general results of the quantum mechanical perturbation theory, the quantum BGNF may always be diagonalized, and two formal processes for such diagonalization are constructed. On the opposite case, the classical BGNF is, in general, non-diagonalizable. This reflects the fact that the classical perturbation theory can't handle a system with two or more resonances. Possible reasons for such different behavior of two very close, in spirit, perturbation procedures are discussed. Results of the described procedure, entirely performed upon the Wick normal ordered operators, are equivalent to those of Rayleigh-Schrödinger perturbation expansion.

Аннотация

Николаев А.С. О диагонализации квантовой нормальной формы Бирхгофа-Густавсона: Препринт ИФВЭ 94-143. – Протвино, 1994. – 21 с., библиогр.: 26.

Обсуждается приложение к квантовой механике одного из методов классической теории возмущений – нормальной формы Бирхгофа-Густавсона (BGNF). В квантовом случае он сводится к теории возмущений Ван Флека, производимой над нормально упорядоченными операторами. Обсуждаются алгебраические аспекты этой процедуры и формальное построение интегралов движения возмущенной системы. Оказывается, в квантовой механике существует больший набор таких операторов, чем в классическом случае. Затем демонстрируется, что согласно общим результатам квантово-механической теории возмущений квантовая BGNF всегда может быть диагонализирована, и обсуждаются два формальных процесса такой диагонализации. В противоположность этому классическая BGNF, вообще говоря, недиагонализуема. Это отражает тот факт, что классическая теория возмущений не позволяет аналитически рассмотреть систему с двумя и более резонансами. Обсуждаются возможные причины такого различного поведения двух очень близких по духу процедур теории возмущений. Результаты описанной теоретико-возмущенческой процедуры, полностью производимой над нормально упорядоченными по Вику операторами, эквивалентны теории возмущений Рэлея-Шрёдингера.

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Introduction

Birkhoff method [1] in classical mechanics provides a procedure to transform the original nonseparable $\mathbf{d}$ -dimensional oscillator Hamiltonian canonically into the normal form consisting of a power series in one-dimensional uncoupled harmonic oscillator Hamiltonians

$$H(p_1, q_1, \dots, p_d, q_d) \rightarrow \mathcal{H}(\zeta_1^2 + \eta_1^2, \dots, \zeta_d^2 + \eta_d^2),$$

where ζ_k and η_k are canonical coordinates and momenta, and $\mathcal{H}$ is a formal power series in $\zeta_k^2 + \eta_k^2$. If the series $\mathcal{H}$ were to converge, the new equation could be easily integrated, $\mathbf{d}$ independent isolating invariants would exist, and the motion would be multiple periodic. Unfortunately it was shown that the Birkhoff normal form diverged in general because of small divisors in the coefficients.

The Birkhoff method was applied by Gustavson [2] in order to obtain power series expressions for invariants and analytically predict the Poincare surfaces of section for the Henon–Heiles system. Doing that Gustavson had to modify the original Birkhoff method in order to include resonances. Such calculations showed that, despite the known divergence of the power series representing the normal form, a truncated series could give accurate approximations to regular trajectories [7].

The Birkhoff-Gustavson normal form was successfully applied to the semiclassical Einstein-Brillouin-Kemmer quantization of various systems, such as the Henon-Heiles system [8,9] and the hydrogen atom (Stark and Stark-Zeeman effects [10]) up to very high order of coupling constant.

Ali [11] and then Eckhard [12] showed that formalism of the so-called Lie-algebraic perturbation theory in classical mechanics [3,4] might be applied to Birkhoff-Gustavson normalization and extended to quantum mechanical systems, resulting in the expansion which, in the classical limit, is reduced to the Birkhoff-Gustavson normal form. They mention that the results of this procedure coincide with those obtained by Rayleigh-Schrödinger perturbation expansion. However their discussion was mainly limited to the systems with nondegenerate energy levels.

An opposite trend of investigations originates from the canonical Van Vleck perturbation theory [14,25]. This procedure is a quantum mechanical analogue of the classical Lie-algebraic perturbation method. Surprisingly it dates back about 40 years before the corresponding procedures in classical mechanics [5,6] become available. Now the Van Vleck perturbation theory is widely used in quantum chemistry both for the analytical and numerical treatment of electronic degrees of freedom and analyses of molecular vibrations (see [23,24] and referencies therein). Several equivalent forms of such perturbation expansions were reviewed in [26]. We choose here the most conceptually simple iterative order by order reduction of the Hamiltonian.

In this paper we will review algebraic aspects of the Birkhoff-Gustavson normalization for polynomially perturbed quantum mechanical harmonic oscillator. We describe it as a procedure to construct unitary transformation of an initial Hamiltonian into an operator belonging to the algebra of invariants for an unperturbed problem. Both the transformation and the transformed Hamiltonian are obtained as a (formal) power series in the perturbation constant. Doing this, we discuss Gustavson invariants, their validity in the quantum case and a set of new, specific to quantum mechanics, invariants. Then, we demonstrate that, unlike the classical case, we can construct a formal process of diagonalization of the quantum mechanical Birkhoff-Gustavson normal form. In fact this process is a standard block diagonalization used in the Rayleigh-Schrödinger perturbation theory, recasted in the form of Wick normal ordered operators. We also describe another diagonalization process, which is a generalization of Bogolyubov transformations used for the diagonalization of finite dimensional bilinear operator forms [17]. After this we discuss possible origins of the different behavior of classical and quantum mechanical perturbation procedures. Thus the Birkhoff-Gustavson normalization procedure for perturbed quantum mechanical harmonic oscillator is extended to a full equivalent of the Rayleigh-Schrödinger perturbation expansion applied for such system³. All steps of the described procedure are entirely made with the Wick normal ordered operators.

Note that all calculations here are only formal, in a sense that neither discussion of power series convergence nor conditions for the existence of constructed operators are present.

Let us consider a d dimensional system with a Hamiltonian

$$\hat{H}(\hat{p}, \hat{q}) = \sum_{k=0}^d \left(\hat{p}_k^2 + \omega_k^2 \hat{q}_k^2 \right) + \alpha \hat{H}_i(\hat{p}, \hat{q}), \quad (1)$$

where $\hat{H}_i(\hat{p}, \hat{q})$ is some polynomial in $\hat{p}_i, \hat{q}_i$. These operators of momentum and coordinate have the canonical commutation relations

$$[\hat{p}_i, \hat{q}_j] = -i\delta_{ij}.$$

We will simplify the Hamiltonian performing subsequent unitary transformations according to Van Vleck [14] method.

³Under the Rayleigh-Schrödinger perturbation expansion we assume the standard quantum mechanical perturbation treatment, including the expansion of operator resolvent and the subsequent diagonalization of energy shift operator by degenerate blocks [13,16].

A first step in the reduction of our Hamiltonian to the Birkhoff-Gustavson normal form will be the diagonalization of the unperturbed harmonic oscillator Hamiltonian. To do this, we had to perform the canonical transformation to the representation of ladder operators

$$\begin{cases} \hat{a}_k &= \frac{1}{\sqrt{2\omega_k}}(\hat{p}_k - i\omega_k \hat{q}_k), \\ \hat{a}_k^+ &= \frac{1}{\sqrt{2\omega_k}}(\hat{p}_k + i\omega_k \hat{q}_k), \end{cases} \quad k = 1, \dots, d \quad (2)$$

with commutation relations

$$[\hat{a}_k, \hat{a}_l^+] = \delta_{kl},$$

and all other commutators identical to zero.

In terms of the "number" operators $\hat{N}_k = \hat{a}_k^+ \hat{a}_k$, the initial Hamiltonian will take the form

$$\hat{H} = \sum_{k=0}^n \omega_k (\hat{N}_k + \frac{1}{2}) + \alpha \hat{H}_i(\hat{a}_k^+, \hat{a}_k) = \hat{H}_0 + \alpha \hat{H}_i,$$

where $\hat{H}_i(\hat{a}_k^+, \hat{a}_k)$ is a polynomial in $\hat{a}_k^+, \hat{a}_k$.

Before describing the Birkhoff-Gustavson perturbative treatment of the above system, let us remind some facts about its zero order approximation.

I. Unperturbed System – Multidimensional Harmonic Oscillator

In what follows it will be very convenient for us to use a compact "vector" notation for multiindices. We will write: $\bar{n}$ as an abbreviation for a set of d integer indices $(n_1, \dots, n_d)$. We will use other related notations:

- "scalar" product

$$(\bar{\omega} \bar{n}) \stackrel{\text{def}}{=} \sum_{i=1}^d \omega_i n_i,$$

- multiindex factorials and binomial coefficients

$$\begin{aligned} \bar{n}! &\stackrel{\text{def}}{=} n_1! \dots n_d!, \\ C_{\bar{n}}^{\bar{m}} &\stackrel{\text{def}}{=} \prod_{k=1}^d C_{n_k}^{m_k}. \end{aligned}$$

- product of operators

$$\hat{a}^{\bar{m}} \stackrel{\text{def}}{=} \hat{a}_1^{m_1} \dots \hat{a}_d^{m_d},$$

- and as a compact form for the system of inequalities we will write

$$\bar{n} \leq \bar{m} \stackrel{\text{def}}{=} \begin{cases} n_1 \leq m_1 \\ \dots \\ n_d \leq m_d \end{cases}.$$

Before performing any actions on operators polynomial in $\hat{a}_k^+$, $\hat{a}_k$, we must, at first, reduce these operators to some standard ordering in constituent ladder operators. We will use the Wick normal ordering prescription, in which any raising operator must be moved, using commutation relations, to the left and any lowering operator remains on the right. The Wick normal ordered form of the operator $\hat{A}$ will look like

$$\hat{A} = \sum A_{\vec{m}, \vec{n}}^{(W)} \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} \frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}}. \quad (3)$$

Note that we explicitly write out here normalizing denominators. This will be convenient for us when discussing the Rayleigh-Schrödinger transformations. Besides, several identities in this section will take the remarkably symmetrical form with such normalization.

The reduction to the Wick normal ordering may be extremely efficiently realized with the computer algebra system, since one may take full advantage of the following identity

$$\hat{a}^{\vec{n}} \hat{a}^{+\vec{m}} = \sum_{\substack{\vec{k} \leq \vec{n} \\ \vec{k} \leq \vec{m}}} \vec{k}! C_{\vec{m}}^{\vec{k}} C_{\vec{n}}^{\vec{k}} \hat{a}^{+\vec{m}-\vec{k}} \hat{a}^{\vec{n}-\vec{k}}. \quad (4)$$

This identity is a direct consequence of the Wick theorem on the product of two normal ordered operators. The theorem states that the Wick normal form of this product is equal to the sum of normal operator products with *all possible couplings* between operators. For any k couplings between multipliers, one has $C_n^k C_m^k$ different choices of two sets consisting of k indices of $\hat{a}$ and $\hat{a}^+$ in multipliers and $k!$ different couplings between these sets. The generalization to many dimensional cases using the "vector" notation is straightforward.

Explicitly writing out a normalizing denominators, we will use this reordering identity in the form

$$\frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}} \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} = \sum_{\substack{\vec{k} \leq \vec{n} \\ \vec{k} \leq \vec{m}}} \sqrt{C_{\vec{m}}^{\vec{k}} C_{\vec{n}}^{\vec{k}}} \frac{\hat{a}^{+\vec{m}-\vec{k}}}{\sqrt{(\vec{m}-\vec{k})!}} \frac{\hat{a}^{\vec{n}-\vec{k}}}{\sqrt{(\vec{n}-\vec{k})!}}. \quad (5)$$

Now let us more closely consider the structure of the harmonic oscillator Hilbert space (Fock space) and operators on it[15]. This space has a ground state $|\vec{0}\rangle$ and a complete orthonormal basis set created by powers of the raising operator

$$|\vec{m}\rangle = \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} |\vec{0}\rangle.$$

This basis naturally induces the corresponding basis for operators. Indeed, any operator on Fock space may be decomposed as

$$\hat{A} = \sum_{\vec{m}, \vec{n}} A_{\vec{m}, \vec{n}}^{(M)} |\vec{m}\rangle \langle \vec{n}| = \sum_{\vec{m}, \vec{n}} A_{\vec{m}, \vec{n}}^{(M)} \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} \hat{P}_0 \frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}}, \quad (6)$$

where $\hat{P}_0 = |\vec{0}\rangle \langle \vec{0}|$ is a projector on the ground state. This decomposition is the "matrix" form of the operator $\hat{A}$.

For any Wick normal ordered operator one may obtain its matrix form inserting an identity expansion

$$\begin{aligned}\hat{A} &= \sum_{\vec{m}, \vec{n}} A_{\vec{m}, \vec{n}}^{(W)} \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} \frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}} = \sum_{\vec{m}, \vec{n}} A_{\vec{m}, \vec{n}}^{(W)} \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} \left\{ \sum_{\vec{k}} |\vec{k}\rangle \langle \vec{k}| \right\} \frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}} = \\ &= \sum_{\vec{m}, \vec{n}, \vec{k}} A_{\vec{m}, \vec{n}}^{(W)} \frac{\hat{a}^{+\vec{m}+\vec{k}}}{\sqrt{\vec{m}! \vec{k}!}} \hat{P}_0 \frac{\hat{a}^{\vec{n}+\vec{k}}}{\sqrt{\vec{n}! \vec{k}!}}.\end{aligned}$$

Changing summation indices, we conclude matrix elements of the operator $\hat{A}$ to be

$$A_{\vec{m}, \vec{n}}^{(M)} = \sum_{\substack{\vec{k} \leq \vec{n} \\ \vec{k} \leq \vec{m}}} \sqrt{C_{\vec{m}}^{\vec{k}} C_{\vec{n}}^{\vec{k}}} A_{\vec{m}-\vec{k}, \vec{n}-\vec{k}}^{(W)}. \quad (7)$$

One may obtain the inverse transformation from the matrix to the Wick normal ordered form of an operator using the following formula for the normal ordered form of the ground state projector [15]

$$\hat{P}_0 =: \exp(-\hat{a}^+ a) := \sum_{\vec{n}} (-1)^{\sum_i n_i} \frac{\hat{a}^{+\vec{n}} \hat{a}^{\vec{n}}}{\vec{n}!}. \quad (8)$$

It is easy to check that the only nonzero matrix element of the above operator will be between a ground state wavefunctions. The substitution of this ground state projector into the definition of matrix form (6) results in the following connection between coefficients of normal and matrix forms of the operator

$$A_{\vec{m}, \vec{n}}^{(W)} = \sum_{\substack{\vec{k} \leq \vec{m} \\ \vec{k} \leq \vec{n}}} (-1)^{\sum_{i=1}^d k_i} \sqrt{C_{\vec{m}}^{\vec{k}} C_{\vec{n}}^{\vec{k}}} A_{\vec{m}-\vec{k}, \vec{n}-\vec{k}}^{(M)}. \quad (9)$$

Note the similarity of coefficients in (5), (7) and (9).

Now we proceed to the discussion of dynamical features of the harmonic oscillator. It is amazing that all in the rest of this section is a consequence of the following two commutators

$$\begin{cases} [N_k, \hat{a}_k^m] &= -m \hat{a}_k^m, \\ [N_k, \hat{a}_k^{+m}] &= m \hat{a}_k^{+m}. \end{cases} \quad (10)$$

Commutation properties and unitary transformations of operators may be treated in a convenient way with the help of the superoperator formalism [25]. Here we will only outline some basics of it. For any operator $\hat{H}$ one may introduce the quantum Liouville superoperator⁴ which acts on the operator space

$$\hat{L}_{\hat{H}} = [\hat{H}, \cdot], \quad \hat{L}_{\hat{H}} \hat{A} = [\hat{H}, \hat{A}].$$

⁴Corresponding Liouville operator in the classical mechanics acts upon any function on the phase space resulting in the Poisson bracket with H : $L_H^c A = \{H, A\} = \sum_k \left(\frac{\partial H}{\partial p_k} \frac{\partial A}{\partial q_k} - \frac{\partial A}{\partial p_k} \frac{\partial H}{\partial q_k} \right)$.

An interest to the study $\hat{L}_{\hat{H}}$ originates from the well-known fact that the exponent of this superoperator is a unitary map in the operator space

$$\tilde{A} = e^{i\alpha\hat{L}_{\hat{H}}} \hat{A} = e^{i\alpha\hat{H}} \hat{A} e^{-i\alpha\hat{H}}.$$

Some properties of the general Liouville superoperator are summarized in Appendix 1.

Here, in the harmonic oscillator context, we are particularly interested in $\hat{L}_{\hat{H}_0} = [\sum_0^n \omega_k \hat{N}_k, \cdot]$. Using the commutation properties (10) one can verify that any Wick normal ordered monomial is an eigenoperator of $\hat{L}_{\hat{H}_0}$

$$\hat{L}_{\hat{H}_0} \hat{a}^{+\bar{\mathbf{m}}} \hat{a}^{\bar{\mathbf{n}}} = (\bar{\omega}, \bar{\mathbf{m}} - \bar{\mathbf{n}}) \hat{a}^{+\bar{\mathbf{m}}} \hat{a}^{\bar{\mathbf{n}}}. \quad (11)$$

Since it is linear, the superoperator $\hat{L}_{\hat{H}_0}$ admits the decomposition of its domain $\mathcal{D}$ into the direct sum $\mathcal{D} = \mathcal{N} \oplus \mathcal{R}$, where $\mathcal{N}$ or $\mathcal{R}$ are the kernel and the range space, respectively. The decomposition of the domain $\mathcal{D}$ into the desired form means that any element of it can be written uniquely as the sum of an element in the kernel space and an element in the range space. Now it may be easily seen that the linear superoperator $\hat{L}_{\hat{H}_0}$ has the above decomposition, since each term in $\mathcal{D}$ is a linear combination of monomial terms, and since each monomial belongs to the kernel (range) space of $\hat{L}_{\hat{H}_0}$ if and only if $(\bar{\omega}, \bar{\mathbf{m}} - \bar{\mathbf{n}})$ equals (does not equal) zero.

In other words, every polynomial operator $\hat{P}$ on the harmonic oscillator Hilbert space may be uniquely decomposed into parts commutative and noncommutative with $\hat{H}_0$

$$\begin{cases} \hat{P} = \langle \hat{P} \rangle + \{ \hat{P} \}, \\ \hat{L}_{\hat{H}_0} \langle \hat{P} \rangle = 0, & \langle \hat{P} \rangle \in \mathcal{N}, \\ \hat{L}_{\hat{H}_0} \{ \hat{P} \} \neq 0, & \{ \hat{P} \} \in \mathcal{R}. \end{cases} \quad (12)$$

In the classical mechanics the above appears as the decomposition of function on the phase space into the *secular* and the *periodical* parts.

For the perturbation theory which we will discuss further, it is crucial that on the range space of $\hat{L}_{\hat{H}_0}$ this superoperator may be inverted. This means that for any polynomial operator $\hat{P}$ there exists another polynomial operator $\hat{G} \in \mathcal{R}$, such that

$$\hat{L}_{\hat{H}_0} \hat{G} = -\hat{L}_{\hat{G}} \hat{H}_0 = \{ \hat{P} \}.$$

We will denote this operator as $\hat{G} = \hat{L}_{\hat{H}_0}^{-1} \hat{P}$. If we demand that $\hat{L}_{\hat{H}_0}^{-1} \langle \hat{P} \rangle = 0$, then the explicit construction of $\hat{G}$ for $\hat{P}$ will be

$$\hat{L}_{\hat{H}_0}^{-1} \hat{P} = \sum' \frac{1}{(\bar{\omega}, \bar{\mathbf{m}} - \bar{\mathbf{n}})} P_{\bar{\mathbf{m}}, \bar{\mathbf{n}}}^{(W)} \hat{a}^{+\bar{\mathbf{m}}} \hat{a}^{\bar{\mathbf{n}}}, \quad (13)$$

where the prime indicates that all the terms with the vanishing denominators must be omitted from the sum.

One may easily check that for any Hermitian polynomial operator $\hat{P}$, operators $\hat{L}_{\hat{H}_0} \hat{P}$ and $\hat{L}_{\hat{H}_0}^{-1} \hat{P}$ are anti-Hermitian. We also mention here the superoperators $\hat{\mathcal{P}}_{\mathcal{R}} = \hat{L}_{\hat{H}_0}^{-1} \hat{L}_{\hat{H}_0}$

and $\hat{\mathcal{P}}_{\mathcal{N}} = 1 - \hat{\mathcal{P}}_{\mathcal{R}}$, projectors on $\mathcal{R}$ and $\mathcal{N}$ spaces, respectively. Primas [25] established formal expressions for these superoperators without any explicit reference to the matrix or the Wick normal ordered forms

$$\begin{aligned}\hat{\mathcal{P}}_{\mathcal{N}} &= \lim_{\alpha \rightarrow 0} \alpha \int_0^\infty dt e^{-\alpha t} e^{-it\hat{L}_{\hat{H}_0}}, \\ \hat{L}_{\hat{H}_0}^{-1} &= i \lim_{\alpha \rightarrow 0} \int_0^\infty dt e^{-\alpha t} e^{-it\hat{L}_{\hat{H}_0}} (1 - \hat{\mathcal{P}}_{\mathcal{N}}).\end{aligned}\tag{14}$$

Let us describe now a null subspace $\mathcal{N}$. This is the space of operators commutative with $\hat{H}_0$ – a space of invariants of the harmonic oscillator. Due to the linearity of $\hat{L}_{\hat{H}_0}$ and the Liebniz property

$$\hat{L}_{\hat{H}}(\hat{A}\hat{B}) = \hat{A}(\hat{L}_{\hat{H}}\hat{B}) + (\hat{L}_{\hat{H}}\hat{A})\hat{B},$$

this space receives an algebraic structure. In fact $\mathcal{N}$ is the representation of the algebra of invariants for the harmonic oscillator, and we are going to describe now its basis.

First of all, there are $\mathbf{d}$ commutative with each other invariants which corresponded to the individual dimensions

$$\begin{aligned}\hat{N}_i &= \hat{a}_i^\dagger \hat{a}_i, \quad i, j = 1, \dots, \mathbf{d}, \\ [\hat{N}_i, \hat{N}_j] &= 0.\end{aligned}\tag{15}$$

The oscillator hamiltonian $\hat{H}_0$ is the function of these invariants. In the classical mechanics the corresponding invariants are called *actions*.

At this point we will distinguish between degenerate (resonance in classical mechanics) and non-degenerate case. One has $\mathbf{r}^{th}$ -fold degeneracy whenever the ω_i , $i = 1, \dots, \mathbf{d}$, are connected by $\mathbf{r}$ (and only $\mathbf{r}$) linearly independent relations of commensurability

$$\sum_{i=1}^{\mathbf{d}} D_{ki} \omega_i = 0, \quad k = 1, \dots, \mathbf{r},\tag{16}$$

where all D_{ki} are integers. We will use this in more convenient vector form

$$(\omega, \vec{D}_k) = 0,\tag{17}$$

where $\vec{D}_k$ is the set of $\mathbf{r}$ independent vectors with integer coefficients. If ω_i are rationally independent, the problem is nondegenerate (nonresonance).

As is known from the classical mechanics, otherwise ergodic on the surface of constant actions (N_i), the phase space trajectory of the classical oscillator with commensurability relations between frequencies will be bounded to the lower dimensional tori. In the coordinate space of 2-dimensional oscillator, for example, this leads to the famous Lissajous figures. The quantum mechanical oscillator with commensurable frequencies will have the degenerate energy levels.

In the nondegenerate case operators $\hat{N}_i$ form a full system of $\mathbf{d}$ invariants for anisotropic harmonic oscillator with incommensurable frequencies. But in the degenerate case the harmonic oscillator has some hidden symmetry, which reveals itself in the existence of $2\mathbf{r}$ additional noncommutative nonhermitian invariants $\hat{K}_i$ and $\hat{K}_i^+$

$$\hat{K}_i = \prod_{k=1}^{\mathbf{d}} \hat{b}_k^{[D_{ik}]} (\text{sign } D_{ik}), \quad \hat{b}_k(l) = \begin{cases} \hat{a}_k^+ & l = +1, \\ \hat{a}_k & l = -1, \end{cases} \quad i = 1, \dots, \mathbf{r}. \quad (18)$$

In general not all of these invariants ($\hat{N}$'s, $\hat{K}$'s and $\hat{K}^+$'s) are independent. We will neither construct here a maximal set of independent hermitian invariants, nor explicitly establish their algebraic properties. We only note that in the classical mechanics the corresponding polynomials form a Lie algebra, but the quantum mechanical case is more complicated, and non-linear extensions or quantum deformations of this Lie algebra arise [21].

Instead we will focus our attention on the set of operators that form the center of the above algebra – the set of invariants commutative with all other invariants of the harmonic oscillator. As was explicitly shown in [22] any operator commutative with all written above invariants ($\hat{N}$'s, $\hat{K}$'s and $\hat{K}^+$'s) for the $\mathbf{d}$ dimensional harmonic oscillator with $\mathbf{r}$ commensurability relations between frequencies is a function of $\mathbf{d}$ independent operators. These operators are divided into two distinct subgroups

- $\mathbf{d} - \mathbf{r}$ operators of form:

$$\hat{\mathcal{G}}_i = \sum_{j=1}^{\mathbf{d}} \alpha_{ij} \hat{N}_j, \quad i = 1, \dots, \mathbf{d} - \mathbf{r}. \quad (19)$$

Here $\vec{\alpha}_i$ is any set of $\mathbf{d} - \mathbf{r}$ independent vectors orthogonal to all $\mathbf{r}$ commensurability vectors $\vec{D}_k$

$$\sum_{j=1}^{\mathbf{d}} \alpha_{ij} D_{kj} = 0, \quad \begin{matrix} i = 1, \dots, \mathbf{d} - \mathbf{r}, \\ k = 1, \dots, \mathbf{r}. \end{matrix}$$

A classical version of these invariants appeared in [2] as "integrals of motions for normal form". Since $(\vec{\omega}, \vec{D}_k) = 0$, it is clear that the oscillator hamiltonian $\hat{H}_0$ is a linear function of these invariants $\hat{\mathcal{G}}_i$. Sometimes such operators are named the "first order Casimirs".

- New complementary $\mathbf{r}$ periodic invariants ("generalized parities" [22]), without the classical counterpart, of the form

$$\hat{\mathcal{V}}_i = \exp(2\pi i \sum_{j=0}^{\mathbf{d}} \beta_{ij} \hat{N}_j), \quad i = 1, \dots, \mathbf{r}. \quad (20)$$

Here $\vec{\beta}_i$ is a set of $\mathbf{d}$ vectors dual to $\vec{D}_k$. Such β_{ij} satisfy the system

$$\sum_j \beta_{ij} D_{kj} = \delta_{ik}, \quad i = 1, \dots, \mathbf{r}.$$

The existence of these invariants for the quantum mechanical oscillator is a direct consequence of the general commutation relation $\hat{F}(\hat{N})\hat{a}^{+m}\hat{a}^n = \hat{a}^{+m}\hat{a}^n\hat{F}(\hat{N}+m-n)$ which may be proven for any operator function $\hat{F}$ if one compares matrix elements in both sides of the identity.

As we will see further, these invariants ($\hat{\mathcal{G}}_j$ and $\hat{\mathcal{V}}_j$) will survive under the general perturbation of the harmonic oscillator. Unlike them, the invariants $\hat{N}_k$ and $\hat{K}_i$ will be destroyed under the perturbation. This means that there is no analytical extension of these invariants to the perturbed case.

Now, having described the unperturbed system we will return to the perturbed one.

II. The Birkhoff-Gustavson Normalization

In this section we will briefly describe the formal reduction of the general Hamiltonian

$$\hat{H} = \sum_{i=0}^{\infty} \alpha^i \hat{H}_i, \quad (21)$$

into a simpler form by unitary transformations with generators chosen from the range of $\hat{L}_{\hat{H}_0}$. As we will see further, the word "simpler" means that the transformed Hamiltonian will have the diagonal or the block-diagonal matrix form. Since we deal now with the Wick normal ordered operators, we will use the following definition by Gustavson [2] for the Hamiltonian in the Birkhoff-Gustavson normal form (BGNF):

The Hamiltonian $\hat{H} = \sum_{i=0}^{\infty} \alpha^i \hat{H}_i$ is in BGNF up to the order α^n if all terms in it of the order α^i , $i < n$ belong to the kernel subspace of $\hat{L}_{\hat{H}_0}$.

In other words part of our Hamiltonian transformed into the BGNF will be commutative with the unperturbed Hamiltonian, and thus belongs to the algebra of invariants for the unperturbed problem. Note that by assumption our Hamiltonian is normalized (is in BGNF) at least up to the first order ($\hat{H}_0 \in \ker \hat{L}_{\hat{H}_0}$).

This definition of the normalized Hamiltonian was used by Gustavson in the case of the classical mechanics to describe the formal process of the reduction of the classical Hamiltonian to a simpler (integrable) form. The original version of normalization process used the formalism of *generating functions*, which in quantum mechanics leads to additional complications due to the noncommutability of operators. An example of a similar approach may be found in [20]. Fortunately, the original Gustavson algorithm was modified [12] using formalism of *generators* of symplectic transformations [3], which has the direct quantum mechanical counterpart. Let us now describe it.

Assume that quantum mechanical Hamiltonian of type (21) is in BGNF up to the order n . Our aim is to find such unitary transformation, after applying of which, the original Hamiltonian will be normalized up to the order $n+1$

$$\hat{\mathcal{H}} = e^{i\alpha^n \hat{G}_n} \hat{H} e^{-i\alpha^n \hat{G}_n} = e^{i\alpha^n \hat{L}_{\hat{G}_n}} \left(\sum_{m=0}^{\infty} \alpha^m \hat{H}_m \right) =$$

$$\begin{aligned}
&= \sum_{m=0}^{\infty} \alpha^m \left(\sum_{k=0}^{[m/n]} \frac{1}{k!} \hat{L}_{i\hat{G}_n}^k \hat{H}_{m-nk} \right) = \\
&= \hat{H}_0 + \alpha \hat{H}_1 + \dots + \alpha^{n-1} \hat{H}_{n-1} + \alpha^n (\hat{H}_n + \hat{L}_{i\hat{G}_n} \hat{H}_0) + O(\alpha^{n+1}) \\
&= (\text{already normalized terms}) + \alpha^n (\hat{H}_n - i \hat{L}_{\hat{H}_0} \hat{G}_n) + O(\alpha^{n+1}),
\end{aligned}$$

here $[m/n]$ denote an integer part of this quotient.

As was demonstrated in the previous section, we may always find the hermitian operator $\hat{G}_n = -i \hat{L}_{\hat{H}_0}^{-1} \{\hat{H}_n\}$ from $\mathcal{R}$ such that

$$\hat{L}_{\hat{H}_0} \hat{G}_n = -i \{\hat{H}_n\}.$$

After the unitary transformation with generator $\hat{G}_n$ our Hamiltonian becomes normalized up to the order $n+1$ too

$$\widehat{\mathcal{H}} = \hat{H}_0 + \alpha \langle \hat{H}_1 \rangle + \dots + \alpha^{n-1} \langle \hat{H}_{n-1} \rangle + \alpha^n \langle \hat{H}_n \rangle + O(\alpha^{n+1}).$$

It is clear from the above that repeating the procedure for $n+1$, etc., we obtain a formal process of normalization of the original Hamiltonian to subsequently higher orders.

In summary, we describe the construction for initial Hamiltonian (21) and any number n of such unitary transformation

$$e^{i\alpha \widehat{\Gamma}^{(n)}(\alpha)} = e^{i\alpha^n \hat{G}_n} \dots e^{i\alpha^2 \hat{G}_2} e^{i\alpha \hat{G}_1}, \quad (22)$$

that our Hamiltonian will be in the Birkhoff-Gustavson normal form up to the order $n+1$. Now we will demonstrate an application of the above defined procedure to two general classes of quantum mechanical systems.

II.A. Nondegenerate Systems

In the case when no commensurability relations (16) exist, the unperturbed system has commutative symmetry algebra, and the kernel subspace of $\hat{L}_{\hat{H}_0}$ consists only of polynomials of $\hat{N}_k$. In this case the Hamiltonian reduced to Birkhoff-Gustavson normal form became diagonal in representation of $\hat{N}_k$ operators.

A normalized part of nondegenerate Hamiltonian will be a function of $\mathbf{d}$ hermitian operators $\hat{N}_k$, each being commutative with all others (and the normalized part of Hamiltonian). These $\mathbf{d}$ operators form a Complete Set of Commutative Operators for such system. The explicit form of these operators in the initial representation is

$$\widehat{\mathcal{N}}_k = e^{-i\alpha \widehat{\Gamma}^{(n)}(\alpha)} \hat{N}_k = e^{-i\alpha \hat{G}_1} \dots e^{-i\alpha^n \hat{G}_n} \hat{N}_k e^{i\alpha^n \hat{G}_n} \dots e^{i\alpha \hat{G}_1}, \quad (23)$$

and may be easily calculated as a power series expansions up to the desired order in α .

Approximations of perturbed eigenvalues and eigenfunctions up to $o(\alpha^n)$ are classified by the complete set of $\mathbf{d}$ quantum numbers n_k and are given by:

$$\begin{aligned}
E_{\tilde{\mathbf{n}}} &= \mathcal{H}(n_1, \dots, n_{\mathbf{d}}), \\
|\tilde{\mathbf{n}}\rangle &= e^{-i\alpha \widehat{\Gamma}^{(n)}(\alpha)} |\mathbf{n}\rangle.
\end{aligned} \quad (24)$$

Due to the uniqueness of asymptotic power series in α , the results of the above procedure coincide with the Rayleigh-Schrödinger perturbation expansion for eigenvalues and eigenfunctions of the perturbed quantum mechanical system.

Note that, if we restore powers of $\hbar$ in the above formulas, operators $\widehat{\mathcal{N}}_k$ will naturally realize the program of the Einstein-Brillouin-Kemmer quantization for all orders of α in the quasi-classical approximation [20]. This fact leads also to the success of the so-called quasi-classical quantization of the Birkhoff normal form [8].

Example 1. One-dimensional anharmonic oscillator.

The system described by Hamiltonian

$$\hat{H} = \hat{p}^2 + \hat{q}^2 + \alpha \hat{q}^4.$$

After normalization of Hamiltonian up to α^6

$$\begin{aligned} \hat{\mathcal{H}} = & 2(\hat{N} + \frac{1}{2}) + \\ & + \alpha \left(\frac{3}{8} + \frac{3}{2}(\hat{N} + \frac{1}{2})^2 \right) - \\ & - \alpha^2 \left(\frac{67}{32}(\hat{N} + \frac{1}{2}) + \frac{17}{8}(\hat{N} + \frac{1}{2})^3 \right) + \\ & + \alpha^3 \left(\frac{1539}{1024} + \frac{1707}{128}(\hat{N} + \frac{1}{2})^2 + \frac{375}{64}(\hat{N} + \frac{1}{2})^4 \right) - \\ & - \alpha^4 \left(\frac{305141}{8192}(\hat{N} + \frac{1}{2}) + \frac{89165}{1024}(\hat{N} + \frac{1}{2})^3 + \frac{10689}{512}(\hat{N} + \frac{1}{2})^5 \right) + \\ & + \alpha^5 \left(\frac{1456569}{32768} + \frac{9317949}{16384}(\hat{N} + \frac{1}{2})^2 + \frac{587265}{1024}(\hat{N} + \frac{1}{2})^4 + \frac{87549}{1024}(\hat{N} + \frac{1}{2})^6 \right) \\ & + \dots \end{aligned}$$

Here we see the first terms of the Rayleigh-Schrödinger perturbation expansion for the anharmonic oscillator. The growth of numerical coefficients in higher order terms reflects an asymptotic behavior of perturbative approximations. Using (25) we obtain perturbed eigenfunctions (not presented here).

The discussion of perturbation expansion for the quartic anharmonic oscillator and the reasons why coefficients in eigenvalues series are polynomials with the definite parity of $(\hat{N} + \frac{1}{2})$ alone, may be found in [18].

II.B. Systems with Degenerate Energy Levels

Now we will consider a case of non-zero number of commensurability vectors (16). The unperturbed quantum mechanical system in such a case will have degenerate energy levels, and, as we have previously discussed, additional noncommutative invariants. Now the kernel subspace of $\hat{L}_{\hat{H}_0}$ consists of not only polynomials of $\hat{N}_k$, but also include all the Wick normal ordered monomials for which $(\omega, \bar{\mathbf{m}} - \bar{\mathbf{n}}) = 0$. The corresponding classical system referred to as resonance.

Here and in what follows we will suppose that Hamiltonian is in BGNF up to sufficiently high order in α , and will usually omit unnormalized part of it, dealing only with the normalized one.

It is clear from the previous section that the normalized Hamiltonian may be written in the form of power series in invariants of the unperturbed system. Due to noncommutativity of these invariants, some ordering for any term in this series must be imposed. Since not all of the above invariants are independent, this power series may be even non-unique. Series of such type appear as the "standard form" of the classical BGNF in [19] (in fact no connection was established in this paper between such series and the invariants of the unperturbed system).

Because $\mathbf{d}$ invariants $\hat{\mathcal{G}}$ and $\hat{\mathcal{V}}$ are commutative with all other invariants of the unperturbed problem, these operators will be commutative with the normalized Hamiltonian as well. This means that for the degenerate system we again have $\mathbf{d}$ commutative with each other and the Hamiltonian operators⁵. But now the reduced Hamiltonian $\hat{\mathcal{H}}$ is *not* a function of $\hat{\mathcal{G}}$ and $\hat{\mathcal{V}}$ operators only, and these $\mathbf{d}$ commutative operators *do not* form the Complete Set of Commutative Operators for degenerate system.

Note, that any degenerate eigensubspace of the oscillator Hamiltonian is the degenerate eigensubspace for each of the $\mathbf{d}$ invariant operators $\hat{\mathcal{G}}$ and $\hat{\mathcal{V}}$ as well. This follows from the fact that quantum numbers $\vec{N}$ for two eigenvectors of $\hat{H}_0$ with the same eigenvalue may differ only in integer coefficient combination of $\vec{D}_i$. As a result eigenvalues of $\mathbf{d}$ operators $\hat{\mathcal{G}}$ and $\hat{\mathcal{V}}$ will *not* classify degenerate eigenstates of the perturbed system. This is not surprising, since the splitting of $\hat{H}$ eigenvalues depends on the *perturbation* $\hat{H}_i$, and can't be described by operators originating from the center of the algebra of invariants for the *unperturbed* system. One may obtain these perturbative invariants in the initial representation similar to those in (23).

Example 2. The Henon-Heiles system.

The Henon-Heiles two-dimensional system was originally used by Gustavson [2] as the first example of BGNF. This system is described by (1:1) resonance Hamiltonian:

$$\hat{H} = \frac{1}{2}(\hat{p}_1^2 + \hat{q}_1^2 + \hat{p}_2^2 + \hat{q}_2^2) + \alpha(\hat{q}_2^3 - \frac{1}{3}\hat{q}_1^2\hat{q}_2).$$

After normalization of Hamiltonian up to α^4

$$\begin{aligned} \hat{\mathcal{H}} = & (1 - \frac{1}{9}\alpha^2 - \frac{11}{108}\alpha^4) + (1 - \frac{2}{3}\alpha^2 - \frac{61}{54}\alpha^4) (\hat{a}_1^+\hat{a}_1 + \hat{a}_2^+\hat{a}_2) - \\ & - \frac{\alpha^2}{12}(5 + \frac{47}{4}\alpha^2) (\hat{a}_1^{+2}\hat{a}_1^2 + \hat{a}_2^{+2}\hat{a}_2^2) - \frac{7\alpha^2}{12}(1 - \frac{1}{4}\alpha^2) (\hat{a}_1^{+2}\hat{a}_2^2 + \hat{a}_2^{+2}\hat{a}_1^2) + \\ & + \frac{\alpha^2}{3}(1 - \frac{27}{4}\alpha^2) \hat{a}_1^+\hat{a}_2^+\hat{a}_1\hat{a}_2 + \\ & + \alpha^4(+\frac{101}{432}\hat{a}_1^{+3}\hat{a}_1^3 - \frac{161}{144}\hat{a}_1^{+3}\hat{a}_1\hat{a}_2^2 - \frac{65}{16}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_1^2\hat{a}_2 + \frac{175}{144}\hat{a}_1^{+2}\hat{a}_2^+\hat{a}_2^3 - \\ & - \frac{235}{432}\hat{a}_2^{+3}\hat{a}_2^3 - \frac{161}{144}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1^3 + \frac{47}{16}\hat{a}_1^+\hat{a}_2^{+2}\hat{a}_1\hat{a}_2^2 + \frac{175}{144}\hat{a}_2^{+3}\hat{a}_1^2\hat{a}_2) + \dots \end{aligned} \quad (25)$$

The above discussion systematizes the structure of the normalized Hamiltonian, but unfortunately was not answered the question about eigenvalues and eigenfunctions of the

⁵Only $\mathbf{d} - \mathbf{r}$ Gustavson invariants exist for the corresponding classical system.

perturbed system. The definite solution of this may be obtained following the guidelines of the Rayleigh-Schrödinger perturbation theory for degenerate systems.

As we have already noticed, in the degenerate case the Hamiltonian reduced to the BGNF is, in general, not diagonal in the $\hat{N}_k$ representation. But, since the normalized part of the Hamiltonian $\hat{\mathcal{H}}$ is *commutative* with the unperturbed Hamiltonian $\hat{H}_0$, matrix of $\hat{\mathcal{H}}$ must be *block-diagonal* in this representation, with blocks corresponding to degenerate eigenstates of $\hat{H}_0$. This apparently becomes evident if one converts $\hat{\mathcal{H}}$ into the matrix form. Doing this, it is easy to recognize that the condition $(\bar{\omega}, \bar{\mathbf{n}}) = (\bar{\omega}, \bar{\mathbf{m}})$ means that all non-zero matrix elements of $\hat{\mathcal{H}}$ must connect only states corresponding to the same energy of the unperturbed system.

At this point one usually performs the standard procedure for the Rayleigh-Schrödinger perturbation theory:

With account for the matrix form of $\hat{\mathcal{H}}$ being block-diagonal, one needs solve secular equations for these blocks and perform an unitary diagonalizing transformation inside each block independently, obtaining eigenvalues and eigenvectors for the perturbed system.

This procedure supposes the conversion of $\hat{\mathcal{H}}$ into the matrix form. But it is interesting that we can perform essentially the same diagonalization in the Wick normal form of operators as well. This leads to an unusual class of unitary transformations, not infinitesimal in nature, which we will also refer to as the Rayleigh-Schrödinger transformations.

III. Rayleigh-Schrödinger transformations

We will utilize now the obvious fact that the kernel subspace of $\hat{L}_{\hat{H}_0}$ is stable against unitary transformations from it. For any monomial, belonging to the kernel subspace $\mathcal{N}$ of $\hat{L}_{\hat{H}_0}$ (or, equivalently, the algebra of invariants for the harmonic oscillator), we introduce the characteristic functional Λ

$$\Lambda(\hat{a}^{+\bar{\mathbf{n}}} \hat{a}^{\bar{\mathbf{m}}}) = (\bar{\omega}, \bar{\mathbf{m}}) = (\bar{\omega}, \bar{\mathbf{n}}). \quad (26)$$

This characteristic functional will take values of energy levels of the unperturbed system. The value of this characteristic functional for a polynomial operator will be the minimum of Λ values for individual monomials in that operator.

Now we can group the terms of the reduced Hamiltonian by Λ values

$$\hat{\mathcal{H}} = \sum_{\Lambda} \sum_{\substack{(\bar{\omega}, \bar{\mathbf{n}}) = \Lambda \\ (\bar{\omega}, \bar{\mathbf{m}}) = \Lambda}} H_{\bar{\mathbf{m}}, \bar{\mathbf{n}}}^{(W)} \frac{\hat{a}^{+\bar{\mathbf{m}}} \hat{a}^{\bar{\mathbf{n}}}}{\sqrt{\bar{\mathbf{m}}!} \sqrt{\bar{\mathbf{n}}!}}. \quad (27)$$

We note here that the expansion of any operator belonging to $\mathcal{N}$ into the power series in $\hat{a}^+$ and $\hat{a}$ leads to the expansion in monomials with increasing values of characteristic functional Λ .

Whereas all presented in this section is quite clear from the matrix form point of view, it is not the case with the Wick normal ordered form of operators. Appendix 2 will shed

some light on the underlying mathematics for products of Wick normal ordered operators belonging to $\mathcal{N}$.

We demonstrate that

- The value of characteristic functional Λ for the product of two operators is greater or equal to that of multipliers

$$\Lambda(\hat{A}\hat{B}) \geq \max(\Lambda(\hat{A}), \Lambda(\hat{B})).$$

- Terms having the minimal allowed value of $\Lambda = \Lambda_0$ in product of two homogenous operators: $\hat{A}, \hat{B} \in \mathcal{N}$, $\Lambda(\hat{A}) = \Lambda(\hat{B}) = \Lambda_0$, will obey the matrix multiplication law

$$\sum_{\mathbf{k} \in \mathcal{I}} A_{\mathbf{k} \mathcal{I}} \frac{\hat{a}^{+\mathbf{k}}}{\sqrt{\mathbf{k}!}} \frac{\hat{a}^{\mathcal{I}}}{\sqrt{\mathcal{I}!}} \sum_{\mathbf{m} \mathbf{n}} B_{\mathbf{m} \mathbf{n}} \frac{\hat{a}^{+\mathbf{m}}}{\sqrt{\mathbf{m}!}} \frac{\hat{a}^{\mathbf{n}}}{\sqrt{\mathbf{n}!}} = \sum_{\mathbf{k} \mathbf{n}} \left(\sum_{\mathbf{m}} A_{\mathbf{k} \mathbf{m}} B_{\mathbf{m} \mathbf{n}} \right) \frac{\hat{a}^{+\mathbf{k}}}{\sqrt{\mathbf{k}!}} \frac{\hat{a}^{\mathbf{n}}}{\sqrt{\mathbf{n}!}} + (\dots).$$

We proceed now to the explicit construction of the diagonalizing transformation. Let us consider, for any possible value of $\Lambda = \Lambda_0$, a subspace of our Hilbert space spanned by eigenvectors of $\hat{H}_0$ with an eigenvalue equal to Λ_0 . The orthogonal projector on this finite-dimensional subspace is

$$\hat{P} = \sum_{\substack{\mathbf{n} \\ (\omega, \mathbf{n}) = \Lambda}} |\mathbf{n}\rangle \langle \mathbf{n}|.$$

Using (9) we convert this projector into the Wick normal ordered form

$$\hat{P} = \sum_{\Lambda \geq \Lambda_0} \sum_{\substack{\mathbf{n} \\ (\omega, \mathbf{n}) = \Lambda}} \left\{ \sum_{\substack{\mathbf{k} \leq \mathbf{n} \\ (\omega, \mathbf{k}) = \Lambda - \Lambda_0}} (-1)^{\sum_i k_i} C_{\mathbf{n}}^{\mathbf{k}} \right\} \frac{\hat{a}^{+\mathbf{n}} \hat{a}^{\mathbf{n}}}{\mathbf{n}!}. \quad (28)$$

For any unitary matrix $u_{\mathbf{m} \mathbf{n}}$ with dimensions equal to those of this Λ_0 subspace we construct an operator $\hat{u} = \sum u_{\mathbf{m} \mathbf{n}} |\mathbf{m}\rangle \langle \mathbf{n}|$ with the properties

$$\begin{cases} \hat{u}^+ \hat{u} = \hat{P}, \\ \hat{u} \hat{P} = \hat{P} \hat{u} = \hat{u}, \\ [\hat{H}_0, \hat{u}] = 0. \end{cases}$$

Again we convert this "unitary inside block" operator into the Wick normal ordered form as

$$\hat{u} = \sum_{\Lambda \geq \Lambda_0} \left\{ \sum_{\substack{\mathbf{m}, \mathbf{n}, \mathbf{k} \\ (\omega, \mathbf{n}) = \Lambda_0 \\ (\omega, \mathbf{m}) = \Lambda_0 \\ (\omega, \mathbf{k}) = \Lambda - \Lambda_0}} (-1)^{\sum_i k_i} u_{\mathbf{m}, \mathbf{n}} \sqrt{C_{\mathbf{m} + \mathbf{k}}^{\mathbf{k}} C_{\mathbf{n} + \mathbf{k}}^{\mathbf{k}}} \frac{\hat{a}^{+\mathbf{m} + \mathbf{k}}}{\sqrt{(\mathbf{m} + \mathbf{k})!}} \frac{\hat{a}^{\mathbf{n} + \mathbf{k}}}{\sqrt{(\mathbf{n} + \mathbf{k})!}} \right\}. \quad (29)$$

To finish the construction of commutative with $\hat{H}_0$ unitary operator we must extend $\hat{u}$ to our full Hilbert space as

$$\hat{U} = 1 - \hat{P} + \hat{u}. \quad (30)$$

This operator is the normal form of the unitary transformation performed in Λ_0 block of the matrix form independently. The transformation of this type is used in the Rayleigh-Schrödinger perturbation theory for the final diagonalization of degenerate block in the Hamiltonian. We explicitly present here expressions (28 – 30) to outline the cumbersome structure of $\hat{U}$ in the Wick normal ordered form. The construction of the above operator makes it clear, that performing the subsequent unitary transformations of type (30) we will diagonalize the Hamiltonian reduced to BGNF by blocks with increasing values of characteristic functional Λ .

Indeed, suppose that all terms in our Hamiltonian with the value of characteristic functional $\Lambda < \Lambda_0$ are already diagonalized

$$\widehat{\mathcal{H}} = \sum_{(\omega, \vec{k}) < \Lambda_0} \mathcal{H}_{\vec{k}\vec{k}}^{(\Lambda)} \frac{\hat{a}^{\dagger \vec{k}} \hat{a}^{\vec{k}}}{\vec{k}!} + \sum_{\substack{(\omega, \vec{n}) = \Lambda_0 \\ (\omega, \vec{m}) = \Lambda_0}} \mathcal{H}_{\vec{m}\vec{n}}^{(\Lambda_0)} \frac{\hat{a}^{\dagger \vec{m}}}{\sqrt{\vec{m}!}} \frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}} + (\dots). \quad (31)$$

In order to construct the diagonalizing transformation $\hat{U}$ we must solve the following secular equation

$$\det \left(\mathcal{H}_{\vec{m}\vec{n}}^{(\Lambda_0)} + \sum_{(\omega, \vec{k}) < \Lambda_0} \mathcal{H}_{\vec{k}\vec{k}}^{(\Lambda)} C_{\vec{n}}^{\vec{k}} \delta_{\vec{m}\vec{n}} - E_{\vec{n}\vec{n}} \delta_{\vec{m}\vec{n}} \right) = 0. \quad (32)$$

Suppose that we can obtain its solution at least as a power series in some rational power of α (Puizeaux series). After this we will have the diagonalizing unitary finite-dimensional matrix $u_{\vec{m}\vec{n}}$ and construct its normal form (30). In the transformed operator

$$\tilde{\mathcal{H}} = \hat{U} \widehat{\mathcal{H}} \hat{U}^+,$$

all terms with the characteristic value $\Lambda = \Lambda_0$ will be also diagonal.

This process results in the expansion of the Hamiltonian in diagonal operators with increasing characteristic values of Λ , or equivalently, the increasing powers of raising and lowering operators. If we cut this expansion on some value of $\Lambda = \Lambda_0$, then analytical expressions for all excited states originating from states of the unperturbed Hamiltonian with the energy $E \leq \Lambda_0$ will be obtained up to the desired order of perturbation parameter α .

After such transformation the diagonalized part of $\tilde{\mathcal{H}}$ will be an (operator) function of d commutative operators $\tilde{N}_i$. Eigenvalues of these operators will classify eigenvalues of the perturbed system with the complete set of d quantum numbers.

Example 2 (cont.). Complete diagonalization of the Henon-Heiles system. As one may see from the previous example, for the reduced to the BGNF Henon-Heiles Hamiltonian (25), the first excited state, corresponding to $\Lambda = 1$, is doubly degenerate. But the reduced Hamiltonian is already diagonal on the subspace spanned by kets $\hat{a}_1^\dagger |\vec{0}\rangle$ and $\hat{a}_2^\dagger |\vec{0}\rangle$.

On subspaces of the next excited states, corresponding to $\Lambda = 2$ and 3 this Hamiltonian will be diagonalized by the unitary transformation $\tilde{\mathcal{H}} = U \widehat{\mathcal{H}} U^+$, where

$$\hat{U} = 1 + \frac{\sqrt{2}}{4} \hat{a}_1^{\dagger 2} \hat{a}_1^2 - \frac{1}{2} (1 - \frac{\sqrt{2}}{2}) \hat{a}_2^{\dagger 2} \hat{a}_2^2 - \frac{\sqrt{2}}{4} \hat{a}_1^{\dagger 2} \hat{a}_2^2 - \frac{1}{2} (1 - \frac{\sqrt{2}}{2}) \hat{a}_1^{\dagger 2} \hat{a}_1^2 +$$

$$\begin{aligned}
& + \left(\frac{1}{3} - \frac{\sqrt{2}}{4}\right) \hat{a}_1^{+3} \hat{a}_1^3 + \frac{1}{4} \hat{a}_1^{+3} \hat{a}_1^2 \hat{a}_2^1 + \frac{\sqrt{2}}{4} \hat{a}_1^{+3} \hat{a}_1^1 \hat{a}_2^2 - \frac{1}{12} \hat{a}_1^{+3} \hat{a}_2^3 + \\
& + \frac{1}{4} \hat{a}_1^{+2} \hat{a}_2^{+1} \hat{a}_1^3 - \frac{\sqrt{2}}{4} \hat{a}_1^{+2} \hat{a}_2^{+1} \hat{a}_1^2 \hat{a}_2^1 + \frac{1}{4} \hat{a}_1^{+2} \hat{a}_2^{+1} \hat{a}_1^1 \hat{a}_2^2 + \frac{\sqrt{2}}{4} \hat{a}_1^{+2} \hat{a}_2^{+1} \hat{a}_2^3 - \\
& - \frac{\sqrt{2}}{4} \hat{a}_1^{+1} \hat{a}_2^{+2} \hat{a}_1^3 + \frac{1}{4} \hat{a}_1^{+1} \hat{a}_2^{+2} \hat{a}_1^2 \hat{a}_2^1 - \frac{\sqrt{2}}{4} \hat{a}_1^{+1} \hat{a}_2^{+2} \hat{a}_1^1 \hat{a}_2^2 + \frac{1}{4} \hat{a}_1^{+1} \hat{a}_2^{+2} \hat{a}_2^3 + \\
& + \frac{1}{12} \hat{a}_2^{+3} \hat{a}_1^3 - \frac{\sqrt{2}}{4} \hat{a}_2^{+3} \hat{a}_1^2 \hat{a}_2^1 - \frac{1}{4} \hat{a}_2^{+3} \hat{a}_1^1 \hat{a}_2^2 + \left(\frac{1}{3} - \frac{\sqrt{2}}{4}\right) \hat{a}_2^{+3} \hat{a}_2^3 + (\dots).
\end{aligned} \tag{33}$$

Here the first row diagonalizes $\Lambda = 2$ part of $\hat{\mathcal{H}}$. It is easy to check the unitarity (up to $\Lambda = 3$) of the above transformation. The transformed Hamiltonian will now take the following diagonal form

$$\begin{aligned}
\tilde{\mathcal{H}} = & \left(1 - \frac{1}{9}\alpha^2 - \frac{11}{108}\alpha^4\right) + \left(1 - \frac{2}{3}\alpha^2 - \frac{61}{54}\alpha^4\right) \hat{N}_1 + \left(1 - \frac{2}{3}\alpha^2 - \frac{61}{54}\alpha^4\right) \alpha^4 \hat{N}_2 + \\
& + \alpha^2 \left(\frac{1}{3} - \frac{9}{4}\alpha^2\right) \hat{N}_1 \hat{N}_2 + \\
& + \frac{\alpha^2}{2} \left(\frac{1}{3} - \frac{9}{4}\alpha^2\right) \left(\hat{N}_1 - 1\right)_2 - \alpha^2 \left(1 + \frac{5}{6}\alpha^2\right) \left(\hat{N}_2 - 1\right)_2 + \\
& + \alpha^2 \left(\frac{7}{6} + \frac{229}{216}\alpha^2\right) \left(\hat{N}_2 - 2\right)_3 - \frac{95}{54}\alpha^4 \left(\hat{N}_1 - 2\right)_3 - \\
& - \alpha^2 \left(\frac{7}{6} + \frac{\alpha^2}{8}\right) \hat{N}_1 \left(\hat{N}_2 - 1\right)_2 - \alpha^2 \left(\frac{7}{3} - \frac{\alpha^2}{6}\right) \hat{N}_2 \left(\hat{N}_1 - 1\right)_2 + \dots
\end{aligned} \tag{34}$$

Notation $(x)_n$ is used here for the Pochhammer polynomial

$$(x)_n = x(x+1) \dots (x+n-1).$$

Note that (34) holds only for the values of quantum numbers n_1 and n_2 such that $n_1 + n_2 \leq 3$. This formula provides us with analytical expressions up to $o(\alpha^4)$ for 10 lowest eigenvalues of the Henon-Heiles system.

An alternative to the above diagonalization process may be established. Since we deal with the Wick normal ordered operators, it is even more natural to diagonalize $\Lambda = \Lambda_0$ terms in (31) using the explicitly unitary operator

$$\hat{\mathcal{H}} = e^{i\hat{L}_\psi} \hat{\mathcal{H}} = \hat{U} \hat{\mathcal{H}} \hat{U}^\dagger,$$

where

$$\hat{U} = e^{i\hat{w}} = \exp \left(i \sum_{\substack{(\omega, \bar{\mathbf{n}}) = \Lambda_0 \\ (\omega, \bar{\mathbf{m}}) = \Lambda_0}} w_{\bar{\mathbf{m}}\bar{\mathbf{n}}} \frac{\hat{a}^{+\bar{\mathbf{m}}}}{\sqrt{\bar{\mathbf{m}}!}} \frac{\hat{a}^{\bar{\mathbf{n}}}}{\sqrt{\bar{\mathbf{n}}!}} \right) \tag{35}$$

and $w_{\bar{\mathbf{m}}\bar{\mathbf{n}}}$ is a finite dimensional hermitian matrix such that the exponent of it coincides with the used above finite dimensional diagonalizing unitary matrix $u_{\bar{\mathbf{m}}\bar{\mathbf{n}}}$

$$u_{\bar{\mathbf{m}}\bar{\mathbf{n}}} = \left(e^{i\omega} \right)_{\bar{\mathbf{m}}\bar{\mathbf{n}}}. \tag{36}$$

It immediately follows from the results of Appendix 2 that $\Lambda = \Lambda_0$ terms in operator (35) coincide with those of the Rayleigh-Schrödinger transformation (28 – 30), and therefore the transformed Hamiltonian will also become diagonal in Λ_0 terms. To continue the diagonalization process, we need to calculate terms with characteristic value $\Lambda > \Lambda_0$ in operator exponent (35). We can perform this exponentiation using the block-diagonality of the operator

$$\hat{w} = \sum_{\substack{(\omega, \vec{n}) = \Lambda_0 \\ (\omega, \vec{m}) = \Lambda_0}} w_{\vec{m}\vec{n}} \frac{\hat{a}^{+\vec{m}}}{\sqrt{\vec{m}!}} \frac{\hat{a}^{\vec{n}}}{\sqrt{\vec{n}!}}.$$

At first we convert the operator $\hat{w}$ into the matrix form. Since it is block-diagonal, the exponent of $\hat{w}$ is reduced to exponentiation of independent finite-dimensional blocks, and may be performed by algebraic methods. The last step will be to convert the resulting operator again into the Wick normal ordered form. Unfortunately secular equations appeared during the application of this process are, in general, more complicated.

Example 3. Exponent of block diagonal operator.

Diagonalization of $\Lambda = 2$ terms in the Hamiltonian of Henon-Heiles system (25) was done in Example 2 by the first row of (33). Alternatively we will use the operator:

$$\hat{U} = e^{\frac{\pi}{4}(\hat{a}_2^{+2}\hat{a}_1^2 - \hat{a}_1^{+2}\hat{a}_2^2)}.$$

For the illustration purposes we calculate the Wick normal ordered form of this operator up to $\Lambda = 3$ terms using the above procedure

$$\begin{aligned} \hat{U} = & 1 + \frac{\sqrt{2}}{4}\hat{a}_2^{+2}\hat{a}_1^2 - \frac{1}{2}\left(1 - \frac{\sqrt{2}}{2}\right)\hat{a}_2^{+2}\hat{a}_2^2 - \frac{\sqrt{2}}{4}\hat{a}_1^{+2}\hat{a}_2^2 - \frac{1}{2}\left(1 - \frac{\sqrt{2}}{2}\right)\hat{a}_1^{+2}\hat{a}_1^2 + \\ & + \left(\frac{1}{3} - \frac{\sqrt{2}}{4} + \frac{1}{6}\cos\left(\frac{\sqrt{3}}{4}\pi\right)\right)(\hat{a}_2^{+3}\hat{a}_2^3 + \hat{a}_1^{+3}\hat{a}_1^3) + \\ & + \left(\frac{\sqrt{2}}{4} - \frac{\sqrt{3}}{6}\sin\left(\frac{\sqrt{3}}{4}\pi\right)\right)(\hat{a}_1^{+3}\hat{a}_1^1\hat{a}_2^2 + \hat{a}_1^{+2}\hat{a}_2^{+1}\hat{a}_2^3 - \hat{a}_1^{+1}\hat{a}_2^{+2}\hat{a}_1^3 - \hat{a}_2^{+3}\hat{a}_1^2\hat{a}_2^1) + \\ & + \left(\frac{1}{2}\cos\left(\frac{\sqrt{3}}{4}\pi\right) - \frac{\sqrt{2}}{4}\right)(\hat{a}_1^{+1}\hat{a}_2^{+2}\hat{a}_1^1\hat{a}_2^2 + \hat{a}_1^{+2}\hat{a}_2^{+1}\hat{a}_1^2\hat{a}_2^1) + (\dots). \end{aligned}$$

We note that (35) is a straightforward generalization of the transformation used by Bogolyubov and Bogolyubov [17] for the diagonalization of $\Lambda = 1$ bilinear operator forms.

IV. Summary and discussion

In this paper we have described the Birkhoff-Gustavson normalization as a procedure to transform the Hamiltonian of d -dimensional harmonic oscillator with polynomial perturbation into the operator belonging to the algebra of invariants for the unperturbed problem. The transformed Hamiltonian was obtained (at least formally) as an expansion in powers of perturbation constant and generators of this algebra.

It is known [4] that in the classical perturbation theory the d dimensional system with the r resonance conditions between frequencies may be (formally) reduced to the

a dimensional system. This reduction is made using $\mathbf{d} - \mathbf{r}$ Gustavson invariants, since each of them may be analytically continued to the invariant of perturbed system. But the classical Hamiltonian with more than one degree of freedom is, in general, nonintegrable. This means that, in general, the classical perturbation theory failed to give analytical predictions for the system with two or more resonance conditions. The perturbative description of such systems is possible only for very special classes of resonance conditions and/or perturbations.

Unlike this, the quantum mechanical perturbation theory has not this conceptual difficulty and always results in definite (formal) approximations to eigenvalues and eigenvectors of the perturbed system. As has been shown in the previous section, this leads to the fact, that we can always construct the process of diagonalization of the quantum mechanical Birkhoff-Gustavson normal form. Possibly, this rather different behavior of two very close in spirit procedures may be attributed to the existence of $\mathbf{r}$ additional quantum mechanical invariants.

From the other point of view, we note that the described diagonalization of the quantum mechanical BGNF is achieved using two different power series expansions. One of them was made in powers of the perturbation constant α , and the other in powers of ladder operators $\hat{a}$ and $\hat{a}^+$. Classical mechanics is more restrictive. Since all classical variables are commutative, the BGNF expansion in powers of α coincides with the expansion in powers of a and a^+ . Moreover, the original definitions by Birkhoff [1] and Gustavson [2] of normalization procedure were made in terms of power series in variables, rather than the perturbation constant. Due to this, one can't, in general, diagonalize the reduced to BGNF classical Hamiltonian.

It is worth to mention that the described diagonalization process, when applied to the Wick normal ordered operators, include the construction of very interesting, not infinitesimally close to unity, unitary transformations. These transformations may be treated as non-linear generalizations of the finite-dimensional Bogolyubov transformations.

In summary, we demonstrate that the Birkhoff-Gustavson normalization procedure for the perturbed multi-dimensional harmonic oscillator may be extended, in the quantum mechanics, to full equivalent of the Rayleigh-Schrödinger perturbation expansion for such system. All steps of this procedure are performed upon Wick normal ordered operators.

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Appendix 1

The Liouville superoperator

We summarize here some of the properties of general Liouville superoperator $\hat{L}_{\hat{H}}$ (α , β and ϵ constants):

1. $\hat{L}_{\hat{H}}$ is linear: $\hat{L}_{\hat{H}}(\alpha\hat{A} + \beta\hat{B}) = \alpha\hat{L}_{\hat{H}}\hat{A} + \beta\hat{L}_{\hat{H}}\hat{B}$,
2. and antisymmetric: $\hat{L}_{\hat{A}}\hat{B} = -\hat{L}_{\hat{B}}\hat{A}$,
3. it obeys the Liebniz rule: $\hat{L}_{\hat{H}}(\hat{A}\hat{B}) = \hat{A}(\hat{L}_{\hat{H}}\hat{B}) + (\hat{L}_{\hat{H}}\hat{A})\hat{B}$,
4. and the Jakoby identities: $\hat{L}_{\hat{H}}([\hat{A}, \hat{B}]) = [\hat{A}, \hat{L}_{\hat{H}}\hat{B}] + [\hat{L}_{\hat{H}}\hat{A}, \hat{B}]$,
5. $\hat{L}_{[\hat{A}, \hat{B}]} = [\hat{L}_{\hat{A}}, \hat{L}_{\hat{B}}]$,
6. $\hat{L}_{\hat{H}}^n[\hat{A}, \hat{B}] = \sum_{m=0}^n C_n^m [\hat{L}_{\hat{H}}^m \hat{A}, \hat{L}_{\hat{H}}^{n-m} \hat{B}]$,
an exponent of it is the linear map and preserves algebraic properties of operators:
7. $e^{\epsilon\hat{L}_{\hat{H}}}(\alpha\hat{A} + \beta\hat{B}) = \alpha e^{\epsilon\hat{L}_{\hat{H}}}\hat{A} + \beta e^{\epsilon\hat{L}_{\hat{H}}}\hat{B}$,
8. $e^{\epsilon\hat{L}_{\hat{H}}}(\hat{A}\hat{B}) = (e^{\epsilon\hat{L}_{\hat{H}}}\hat{A})(e^{\epsilon\hat{L}_{\hat{H}}}\hat{B})$,
9. $e^{\epsilon\hat{L}_{\hat{H}}}[\hat{A}, \hat{B}] = [e^{\epsilon\hat{L}_{\hat{H}}}\hat{A}, e^{\epsilon\hat{L}_{\hat{H}}}\hat{B}]$,
10. and may be decomposed as: $e^{\epsilon\hat{L}_{\hat{H}}}\hat{A} = e^{\epsilon\hat{H}}\hat{A}e^{-\epsilon\hat{H}}$.

Properties 1-9 take place both in quantum and classical case with the corresponding change, whenever needed, of the commutator to the Poisson bracket $([\cdot, \cdot] \rightarrow \{\cdot, \cdot\})$.

Appendix 2

Products of invariant polynomials

Consider the product of two operators $\hat{A}$ and $\hat{B}$ belonging to the kernel subspace of $\hat{L}_{\hat{H}_0}$. We assume that minimal values of the characteristic functional $\Lambda(\hat{a}^{+\bar{\mathbf{m}}}\hat{a}^{\bar{\mathbf{n}}}) = (\bar{\omega}, \bar{\mathbf{m}}) = (\bar{\omega}, \bar{\mathbf{n}})$ for monomials in each of the above operators are Λ_A and Λ_B , respectively. We are interested in terms with the minimal value of Λ in this product. Using (4) we may write down these terms as

$$\begin{aligned}
 & \sum_{\bar{\mathbf{k}} \bar{\mathbf{l}}} \frac{A_{\bar{\mathbf{k}} \bar{\mathbf{l}}}}{\sqrt{\bar{\mathbf{k}}! \bar{\mathbf{l}}!}} \hat{a}^{+\bar{\mathbf{k}}} \hat{a}^{\bar{\mathbf{l}}} \sum_{\bar{\mathbf{m}} \bar{\mathbf{n}}} \frac{B_{\bar{\mathbf{m}} \bar{\mathbf{n}}}}{\sqrt{\bar{\mathbf{m}}! \bar{\mathbf{n}}!}} \hat{a}^{+\bar{\mathbf{m}}} \hat{a}^{\bar{\mathbf{n}}} = \\
 & = \sum_{\bar{\mathbf{k}} \bar{\mathbf{l}} \bar{\mathbf{m}} \bar{\mathbf{n}}} D_{\bar{\mathbf{k}} \bar{\mathbf{l}} \bar{\mathbf{m}} \bar{\mathbf{n}}} \hat{a}^{+\bar{\mathbf{k}}+\bar{\mathbf{m}}-\min(\bar{\mathbf{l}}, \bar{\mathbf{m}})} \hat{a}^{\bar{\mathbf{n}}+\bar{\mathbf{l}}-\min(\bar{\mathbf{l}}, \bar{\mathbf{m}})} + (\dots) = \\
 & = \sum_{\bar{\mathbf{k}} \bar{\mathbf{l}} \bar{\mathbf{m}} \bar{\mathbf{n}}} D_{\bar{\mathbf{k}} \bar{\mathbf{l}} \bar{\mathbf{m}} \bar{\mathbf{n}}} \hat{a}^{+\bar{\mathbf{k}}-\bar{\mathbf{l}}+\max(\bar{\mathbf{l}}, \bar{\mathbf{m}})} \hat{a}^{\bar{\mathbf{n}}-\bar{\mathbf{m}}+\max(\bar{\mathbf{l}}, \bar{\mathbf{m}})} + (\dots), \tag{37}
 \end{aligned}$$

where terms with the greater value of characteristic functional Λ are denoted by $(\dots)$. The notation " $\max(\bar{\mathbf{l}}, \bar{\mathbf{m}})$ " is used for the vector, each component of which is the maximum of the correspondent component of $\bar{\mathbf{l}}$ and $\bar{\mathbf{m}}$. Coefficients D are

$$D_{\bar{\mathbf{k}} \bar{\mathbf{l}} \bar{\mathbf{m}} \bar{\mathbf{n}}} = \frac{A_{\bar{\mathbf{k}} \bar{\mathbf{l}}}}{\sqrt{\bar{\mathbf{k}}! \bar{\mathbf{l}}!}} \frac{B_{\bar{\mathbf{m}} \bar{\mathbf{n}}}}{\sqrt{\bar{\mathbf{m}}! \bar{\mathbf{n}}!}} (\min(\bar{\mathbf{l}}, \bar{\mathbf{m}}))! C_{\bar{\mathbf{m}}}^{\bar{\mathbf{m}}-\min(\bar{\mathbf{l}}, \bar{\mathbf{m}})} C_{\bar{\mathbf{l}}}^{\bar{\mathbf{l}}-\min(\bar{\mathbf{l}}, \bar{\mathbf{m}})}.$$

Let us calculate characteristic values Λ for explicitly written terms in (37)

$$\Lambda = (\bar{\omega}, \bar{n} - \bar{m} + \max(\bar{l}, \bar{m})) = (\bar{\omega}, \max(\bar{l}, \bar{m})) \geq \begin{cases} (\omega, \bar{l}) = \Lambda_A, \\ (\omega, \bar{m}) = \Lambda_B, \end{cases}$$

since all $\omega_i > 0$.

Consider now the homogenous case, whenever each monomial in both operators has equal characteristic value Λ_0 . The minimal allowed value of Λ in product $\hat{A}\hat{B}$ will have terms with $\Lambda = \Lambda_0$, or

$$\begin{cases} (\bar{\omega}, \max(\bar{l}, \bar{m})) = (\bar{\omega}, \bar{l}), \\ (\bar{\omega}, \max(\bar{l}, \bar{m})) = (\bar{\omega}, \bar{m}). \end{cases}$$

The above equalities may take place only for $\bar{l} = \bar{m}$. So, the product of homogenous in Λ polynomials will take the form

$$\sum_{\bar{k}\bar{l}} A_{\bar{k}\bar{l}} \frac{\hat{a}^{+\bar{k}}}{\sqrt{\bar{k}!}} \frac{\hat{a}^{\bar{l}}}{\sqrt{\bar{l}!}} \sum_{\bar{m}\bar{n}} B_{\bar{m}\bar{n}} \frac{\hat{a}^{+\bar{m}}}{\sqrt{\bar{m}!}} \frac{\hat{a}^{\bar{n}}}{\sqrt{\bar{n}!}} = \sum_{\bar{k}\bar{n}} \left(\sum_{\bar{m}} A_{\bar{k}\bar{m}} B_{\bar{m}\bar{n}} \right) \frac{\hat{a}^{+\bar{k}}}{\sqrt{\bar{k}!}} \frac{\hat{a}^{\bar{n}}}{\sqrt{\bar{n}!}} + (\dots). \quad (38)$$

This is the standard matrix multiplication law.

А.С.Николаев.

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