# Small denominators, frequency operators, and Lie transforms for nearly integrable quantum spin systems

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Based on the previously proposed notions of action operators and of quantum integrability, *frequency operators* are introduced in a fully quantum-mechanical setting. They are conceptually useful because another formulation can be given to unitary perturbation theory. When worked out for quantum spin systems, this variant is found to be formally equivalent to canonical perturbation theory applied to nearly integrable systems consisting of classical spins. In particular, it becomes possible to locate the quantum-mechanical operator-valued equivalent of the *frequency denominators* that may cause divergence of the classical perturbation series. The results that are established here link the concept of quantum-mechanical integrability to a technical question, namely, the behavior of specific perturbation series.

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## I. INTRODUCTION

In classical mechanics, the distinction between integrable and nonintegrable Hamiltonian systems is clear cut. On the one hand, for a system to be integrable, the existence of $N$ smooth, involutive, and functionally independent constants of the motion is required. Then, its $2N$-dimensional phase space is guaranteed to be foliated into $N$-dimensional tori, and the resulting almost periodic motion of the system is very simple. On the other hand, a nonintegrable system may explore a $(2N-1)$-dimensional region of phase space in the course of time if (except for the energy) there are no invariants that restrict the motion to lower-dimensional manifolds. Accordingly, the time evolution of a nonintegrable system is extremely complicated [1].

Much is known about the properties of quantum systems obtained by quantizing classically integrable and nonintegrable systems, respectively [2]. Nevertheless, no rigorously established and generally accepted features have emerged that would allow one to unambiguously distinguish integrable and nonintegrable quantum systems in analogy to classical mechanics. While the concept of integrability is important in classical mechanics (for example, the KAM theorem deals with the influence of a perturbation on *integrable* systems), it appears, for the time being, to be much less fertile in quantum mechanics.

A new concept of *quantum integrability* has been proposed in [3] that is based on quantum-mechanical *action operators* without any reference to classical mechanics. Incorporating criticism of earlier concepts of quantum integrability [4], this notion relies only on the *algebraic* structure of a quantum system provided by the commutation relations of the basic operators. It is the objective of the present paper to explore the features of nearly quantum integrable systems: a perturbation is added to a system that qualifies as quantum integrable in the above sense, and a method is given to successively remove the disturbance. By using the quantum actions in a framework of Lie transforms it becomes possible to lay open strong formal analogies to the corresponding classical perturbational approach. In particular, with *frequency operators* being defined for integrable quantum systems, it will become obvious that quantum-mechanical ''counterparts'' of the classical *frequency denominators* show up in this perturbational treatment. The results of the present work are *formal*, i.e., questions of convergence have not yet been dealt with. Fortunately, the structural similarity of the results to classical mechanics allows one to already imagine possible scenarios.

Two general remarks are in order before turning to the detailed presentation. The investigations are carried out for *spin* systems but the generalization of the results to particle systems is not expected to provide substantial difficulties. Then, it should be pointed out that no part of this work relies on semiclassical approximations.

In brief, the paper is organized as follows. In Sec. II, the notion of quantum integrability used here is recapitulated. Frequency operators are introduced in Sec. III, and they are recognized to naturally generalize the classical frequencies known from integrable systems. The main part of the paper, Sec. IV, consists of formulating the theory of Lie transforms for nearly quantum integrable systems. Applications to systems with one and two degrees of freedom follow in Sec. V. Finally, the results are summarized in Sec. VI, and connections to other work are discussed.

## II. ALGEBRAIC VIEW OF QUANTUM INTEGRABILITY

It will be useful to summarize the algebraic view of quantum integrability in order to motivate the investigations of the subsequent chapters. Only the essential points will be mentioned; details have been elaborated on in Ref. [3].

Let us outline the concept of integrability with a view on the algebraic structure of classical mechanics. For a system of $N$ degrees of freedom there are canonical variables $q=(q_1,\ldots,q_N)$ and $p=(p_1,\ldots,p_N)$. They provide a basis for the algebra of (smooth) phase-space functions $f(p,q)$ since each such function can be approximated arbitrarily well by summing products of $p_n,q_n$ with appropriate coefficients. They can be multiplied by real coefficients, and one can add them; any two phase-space functions define a third one via the Poisson bracket, turning the set of all phase-

 

space functions into a Lie algebra. This framework is the same for all classical mechanical systems. A particular physical system is described by selecting one specific phase-space function and by calling it the Hamiltonian. Its role is to generate the time evolution of the system by defining a flow in phase space. Integrability comes in as follows. Typically, the Hamiltonian function will depend on all components of momentum $p$ and coordinate $q$. However, it is possible to perform a canonical change of basis, $(p,q)\rightarrow(p',q')$, as a result of which the Hamiltonian will turn into a different function if expressed in terms of the primed variables. It may happen that such a change of basis leads to a particular form of the new Hamiltonian function, namely, that it depends on only half of the number of variables, $N$. One has found a particularly convenient basis of the algebra because it becomes obvious that the flow in phase space decomposes into $N$ decoupled flows. A system with such a *trivial* flow is called *integrable*. As is well known, this situation is very rare: typically, no decoupling basis exists, and the phase-space flow is extremely intricate.

It is straightforward to rephrase this line of thought for quantum-mechanical systems. Now the basis of the algebra of operators is given by $\hat{p}=(\hat{p}_1,\ldots,\hat{p}_N)$ and $\hat{q}=(\hat{q}_1,\ldots,\hat{q}_N)$, and each operator in the algebra can be represented by an appropriate sum of products of $\hat{p}_n,\hat{q}_n$. The commutator of two operators defines a third one, and Jacobi's identity holds in general: one is dealing with a Lie algebra of operators. If one particular operator of the algebra is chosen as Hamiltonian, a quantum system and its time evolution are determined. A generic Hamiltonian operator will depend on all components of $\hat{p}$ and $\hat{q}$. In special cases, however, a *unitary* transformation exists that allows one to express the Hamiltonian as a function of only half of the number of basic operators, $N$. By analogy, the system will then be called *quantum integrable*. Part of the purpose of the present work is to show that, in an appropriate sense, the corresponding quantum-mechanical flow is *trivial*, and that this situation is not generic.

It should be noted that in the context of quantum mechanics the term ''algebraic'' will be understood as ''independent of the representation.'' The idea is to only use relations that have a counterpart in the classical algebra. For example, within each finite-dimensional matrix representation of the spin algebra there exist relations between different powers of spin matrices that are specific to the representation at hand. Such relations do not exist in the classical algebra and, thus, they should not be used. An instructive discussion of the common algebraic structure underlying classical and quantum mechanics has been given by Falk [5].

For convenience, the definition of quantum integrability for spin systems proposed in [3] will be reproduced. The description of a quantum spin system with $N$ degrees of freedom is based on $N$ copies of the one-spin commutation relations,

$$[\hat{S}_{j\alpha},\hat{S}_{j'\beta}]=i\hbar\,\delta_{jj'}\sum_{\gamma=xyz}\varepsilon_{\alpha\beta\gamma}\hat{S}_{j\gamma},\quad j,j'=1,2,\ldots N. \tag{1}$$

Here is the criterion for integrability of quantum spin systems, denoted by *QJ*:

QJ: A given $N$-spin Hamiltonian $\hat{H}=H(\hat{\mathbf{S}}_1,\ldots,\hat{\mathbf{S}}_N)$ is *quantum integrable* if there exists a unitary transformation $\mathscr{U}(\hat{\mathbf{S}}_1,\ldots,\hat{\mathbf{S}}_N)$ that converts the spin operators $\hat{\mathbf{S}}_j$, $j=1,\ldots,N$, into new spin operators,

$$\hat{\mathscr{S}}_j=\hat{\mathscr{U}}\,\hat{\mathbf{S}}_j\,\hat{\mathscr{U}}^\dagger=\mathscr{S}_j(\hat{\mathbf{S}}_1,\ldots\hat{\mathbf{S}}_N),\quad j=1,\ldots,N, \tag{2}$$

such that the Hamiltonian turns into a function of $N$ quantum actions $\hat{J}_j=\hat{\mathscr{S}}_{jz}$:

$$H(\hat{\mathbf{S}}_1,\ldots,\hat{\mathbf{S}}_N)=\mathscr{H}(\hat{J}_1,\ldots,\hat{J}_N). \tag{3}$$

The spectra of the operators $\hat{J}_j,j=1,\ldots,N$, in each $(2s+1)$-dimensional representation $\Gamma_s$ consist of uniformly spaced levels:

$$\hat{J}_j^s=\sum_{m_j=-s}^{+s}|\ldots,m_j,\ldots;s\rangle m_j\hbar\langle\ldots,m_j,\ldots;s|,$$

$$j=1,\ldots,N. \tag{4}$$

If the transformation (3) has been achieved, the eigenvalues of the Hamiltonian can be read off immediately, and its eigenfunctions are known as well. In spite of the reference to the representation $\Gamma_s$, Eq. (4) is an algebraic statement since it is required to hold in *all* representations, $s=1/2,1,3/2,\ldots$ As will become clear in Sec. IV, condition (3) defines a program that can be carried out in strong analogy to classical mechanics.

## III. FREQUENCY OPERATORS

Frequency operators, to be defined for quantum integrable systems in a straightforward way, are introduced in this section. The main objective of Ref. [3] has been to provide numerical and analytical support for the existence of quantum-mechanical action operators, and to use them as building blocks for quantum-mechanical integrability. These arguments will not be repeated here; instead, an independent approach will be presented that illustrates the idea of action operators from a different perspective. To arrive at the definition of frequency operators will then be a small step.

As a starter, a classical spin system with one degree of freedom is considered. Its Hamiltonian is assumed to depend on a single spin component only, $S_z$, say:

$$H=H(S_z). \tag{5}$$

The complex quantities

$$S_\pm=S_x\pm iS_y \tag{6}$$

are classical counterparts of ladder operators for a quantum spin. In these variables the Poisson brackets for a single spin read

$$\{S_z,S_\pm\}=\pm iS_\pm,\quad \{S_+,S_-\}=2iS_z, \tag{7}$$

as obtained from the replacement $[\ ,\ ]\rightarrow-i\hbar\{\ ,\ \}$ in (1). The equations of motion are given by

$$\frac{d\mathbf{S}}{dt}=\{H,\mathbf{S}\}, \tag{8}$$

and for the Hamiltonian (5) they read explicitly

$$\frac{dS_z}{dt}=\{H,S_z\}=0, \tag{9}$$

$$\frac{dS_+}{dt}=\{H,S_+\}=iS_+\omega(S_z), \tag{10}$$

the equation of motion for $S_-$ being complex conjugate to that of $S_+$. When expressing the spin as $\mathbf{S}=(\sqrt{S^2-p_\varphi^2}\cos\varphi,\sqrt{S^2-p_\varphi^2}\sin\varphi,p_\varphi)$ in terms of canonical coordinates with $\{p_\varphi,\varphi\}=1$, it becomes obvious that the third component, $S_z$, plays the role of an action: it is both a canonical variable and a constant of the motion. The phase-space functions $S_\pm$ are proportional to the exponentiated angle variable. In view of later developments it is useful to stick with the periodic functions of time, $S_\pm(t)$, instead of using the canonical variable $\varphi$. The frequency

$$\omega(S_z)=\frac{dH(S_z)}{dS_z} \tag{11}$$

is completely determined by the Hamiltonian and thus depends on the action $S_z$ only. The time evolution of integer powers $k=2,3,\ldots$ of $S_+(t)$ is obtained from (10) as

$$\frac{dS_+^k}{dt}=\{H,S_+^k\}=iS_+^k\omega_k(S_z), \tag{12}$$

and similarly for $S_-$. The notation

$$\omega_k(S_z)\equiv k\omega(S_z), \tag{13}$$

used here will simplify comparison with quantum-mechanical expressions.

Consider now a quantum-mechanical spin system with one degree of freedom, i.e., one copy of the commutation relations (1) only occurs. The Hamiltonian of the system is assumed to depend on the third component of the spin operator $\hat{\mathbf{S}}$ only,

$$\hat{H}=H(\hat{S}_z). \tag{14}$$

Again, ladder operators are useful: $\hat{S}_\pm=\hat{S}_x\pm i\hat{S}_y$, leading to commutators similar to (7):

$$[\hat{S}_z,\hat{S}_\pm]=\pm\hbar\hat{S}_\pm,\quad [\hat{S}_+,\hat{S}_-]=2\hbar\hat{S}_z. \tag{15}$$

Heisenberg's equations of motion for the quantum spin are

$$\frac{d\hat{\mathbf{S}}}{dt}=\frac{i}{\hbar}[\hat{H},\hat{\mathbf{S}}], \tag{16}$$

and for the Hamiltonian (14) they read

$$\frac{d\hat{S}_z}{dt}=\frac{i}{\hbar}[\hat{H},\hat{S}_z]=0, \tag{17}$$

$$\frac{d\hat{S}_+}{dt}=\frac{i}{\hbar}[\hat{H},\hat{S}_+]=i\hat{S}_+\omega(\hat{S}_z), \tag{18}$$

and the equation for $\hat{S}_-=(\hat{S}_+)^\dagger$ is the adjoint of the last equation,

$$\frac{d\hat{S}_-}{dt}=\frac{i}{\hbar}[\hat{H},\hat{S}_-]=-i\omega(\hat{S}_z)\hat{S}_-. \tag{19}$$

The self-adjoint operator $\hat{\omega}\equiv\omega(\hat{S}_z)$ depends on the $z$ component of the spin operator $\hat{\mathbf{S}}$ only; explicitly, one has

$$\omega(\hat{S}_z)=\frac{1}{\hbar}(H(\hat{S}_z+\hbar)-H(\hat{S}_z)), \tag{20}$$

thus providing the definition of a quantum-mechanical *frequency operator*. Its form is suggested by requiring that the operator $\hat{S}_+$ stand on the left of everything else in Eq. (18). The derivation of (20) hinges on the fact that the Hamilton operator depends on the operator $\hat{S}_z$ only because in (16) one can then use the relation

$$\begin{aligned}[f(\hat{S}_z),\hat{S}_+^k]&=\hat{S}_+^k(f(\hat{S}_z+k\hbar)-f(\hat{S}_z))\\&=\hat{S}_+^k[\exp(k\hbar\partial_z)-1]f(\hat{S}_z),\end{aligned} \tag{21}$$

where $\partial_z$ denotes the (formal) derivative with respect to the operator $\hat{S}_z$. An algebraic proof of (21) is given in Appendix A for functions $f(x)$ that have a power-series expansion in $x$, and another one for arbitrary functions $f(x)$ that holds in each representation. A different but equivalent definition of the frequency operator can be given if one moves $\hat{S}_+$ to the right in Eq. (18). Either convention is unambiguous; in the following, the version occurring in (18) will be used.

Comparing the classical and the quantum-mechanical equations of motion, (10) and (18), it becomes plausible to call the operator $\hat{S}_z$ an *action operator*: it is both a constant of the motion and (the closest analog of) a canonical momentum in the spin algebra. It is reasonable to consider the Hamiltonian (14) as *quantum integrable* since it depends on nothing but an action operator. This also fits well with conceiving $\hat{\omega}$ given in (20) as a frequency operator because (20) is the discretized version of (11).

On this basis, the notion of quantum-mechanical integrability as defined in QJ makes sense: a system with Hamilton operator $\hat{\mathscr{H}}$ will be called quantum integrable if a unitary transformation $\hat{\mathscr{U}}$ can be found such that the Hamiltonian turns into a function of commuting $z$ components of the different spins only while the commutation relations (1) remain invariant. As a consequence, the equations of motion in the Heisenberg picture strongly resemble those of classically integrable systems. In addition, frequency operators are defined in analogy to the classical frequencies, both of which are determined completely by the Hamiltonian. It is not for the first time that operator-valued analogs of the classical frequencies do occur: as early as 1925, Dirac introduced a similar concept for particle systems [6].

It is important to look at the time evolution of powers of $\hat{S}_+$ (and $\hat{S}_-$). One finds

$$\frac{d\hat{S}_+^k}{dt}=\frac{i}{\hbar}[\hat{H},\hat{S}_+^k]=i\hat{S}_+^k\omega_k(\hat{S}_z), \tag{22}$$

where now

$$\omega_k(\hat{S}_z)=\frac{1}{\hbar}(H(\hat{S}_z+k\hbar)-H(\hat{S}_z)). \tag{23}$$

Since generally

$$\hat{\omega}_k \neq k\hat{\omega}, \tag{24}$$

a difference to the classical relation (13) arises that will have interesting consequences for the perturbative approach to be studied later on. When formally expanding both sides of (24) in powers of $\hbar$, however, the leading order reflects the classical relation.

The generalization to systems consisting of $N$ spins, $\hat{\mathbf{S}}_j, j=1,\ldots,N$, is straightforward. The components of each individual spin fulfill commutation relations (1), and operators associated with different spins $\hat{S}_{j\alpha},\hat{S}_{j'\beta}$ commute. The Hamiltonian now will depend on all spins, $\hat{H}=H(\hat{\mathbf{S}}_1,\ldots,\hat{\mathbf{S}}_N)$ and the equations of motion read

$$\frac{d\hat{S}_{j\alpha}}{dt}=\frac{i}{\hbar}[\hat{H},\hat{S}_{j\alpha}], \quad \alpha=x,y,z. \tag{25}$$

For a quantum integrable $N$-spin Hamiltonian there are $N$ frequency operators generalizing the expressions (20) and (23):

$$\omega_k^{(j)}(\hat{\mathbf{S}}_z)=\frac{1}{\hbar}(H(\hat{S}_{1z},\ldots,\hat{S}_{jz}+k\hbar,\ldots,\hat{S}_{Nz})-H(\hat{\mathbf{S}}_z)), \tag{26}$$

and the time evolution of the ladder operators is simply given by

$$\frac{d\hat{S}_{j+}^k}{dt}=\frac{i}{\hbar}[\hat{H},\hat{S}_{j+}^k]=i\hat{S}_{j+}^k\hat{\omega}_k^{(j)}, \quad k=1,2,\ldots, \tag{27}$$

and their adjoints.

## IV. PERTURBATION THEORY

Having established a concept of integrability for quantum systems, the program to be carried out is as follows. In classical mechanics, a small perturbation is added to an integrable system and it is investigated whether, by successive canonical transformations, the perturbation can be removed completely; this would render the system integrable. As is known from the KAM theorem, however, integrability is destroyed by a generic perturbation: any perturbation series is doomed to diverge in finite fractions of phase space. A quantum-mechanical implementation of this approach aims at transforming a perturbed quantum integrable system into an integrable one by applying a sequence of unitary transformations. Lie transforms are a convenient tool here since they are adapted to the algebraic structure of the theory. Moreover, they facilitate comparison with canonical perturbation theory, the relevant formulas of which are gathered in Appendix B.

A quantum system consisting of $N$ spins with constant length $\hat{S}_j^2$ is assumed to be described by a Hamiltonian operator of the form

$$\hat{H}_\varepsilon=H(\hat{\mathbf{S}},\varepsilon)=H_0(\hat{\mathbf{S}}_z)+\tilde{H}(\hat{\mathbf{S}},\varepsilon), \tag{28}$$

where $\hat{H}_0$ is a quantum integrable system, depending only on the $z$ components of the spins [if not indicated otherwise, $\hat{\mathbf{S}}$ denotes the collection $(\hat{\mathbf{S}}_1,\ldots,\hat{\mathbf{S}}_N)$ of operators].

The perturbation $\tilde{H}(\hat{\mathbf{S}},\varepsilon)$ may depend on all components of the $N$ spins and it contains a real expansion parameter $\varepsilon$ such that the perturbation vanishes for $\varepsilon=0$: $\tilde{H}(\hat{\mathbf{S}},0)=0$. Furthermore, it is assumed that the unperturbed Hamiltonian $\hat{H}_0$ is not degenerate. In the following, a possible dependence of operators on the invariants $\hat{S}_j^2$ will not be made explicit.

### A. Unitary transformations

To begin with, it is useful to study the effect of unitarily transforming the spin operators by an operator $\hat{U}_\varepsilon=U(\hat{\mathbf{S}},\varepsilon)$ with $U(\hat{\mathbf{S}},\varepsilon=0)=1$. New spin operators $\hat{\mathbf{S}}'$ (throughout this paper the prime does not denote a derivative) are introduced by

$$\hat{\mathbf{S}}'_\varepsilon=U_\varepsilon(\hat{\mathbf{S}})\ \hat{\mathbf{S}}\ U_\varepsilon^\dagger(\hat{\mathbf{S}}), \tag{29}$$

and the induced transformation of the Hamiltonian reads

$$H(\hat{\mathbf{S}},\varepsilon)=H'(\hat{\mathbf{S}}'_\varepsilon,\varepsilon), \tag{30}$$

that is, in terms of the primed operators, $\hat{\mathbf{S}}'_\varepsilon$, the Hamiltonian is given by a new function $H'$. By using the inverse of (29) in the form

$$\hat{\mathbf{S}}=U_\varepsilon^\dagger(\hat{\mathbf{S}})\ \hat{\mathbf{S}}'_\varepsilon\ U_\varepsilon(\hat{\mathbf{S}})=U_\varepsilon'^\dagger(\hat{\mathbf{S}}'_\varepsilon)\ \hat{\mathbf{S}}'_\varepsilon\ U'_\varepsilon(\hat{\mathbf{S}}'_\varepsilon), \tag{31}$$

relation (30) can be written as

$$U'^\dagger_\varepsilon(\hat{\mathbf{S}}'_\varepsilon)H(\hat{\mathbf{S}}'_\varepsilon,\varepsilon)U'_\varepsilon(\hat{\mathbf{S}}'_\varepsilon)=H'(\hat{\mathbf{S}}'_\varepsilon,\varepsilon). \tag{32}$$

This equation holds for any unitary transformation $\hat{U}_\varepsilon$. In view of the criterion for quantum integrability, QJ, the new Hamiltonian $\hat{\mathscr{H}}=\hat{H}'$ is required to depend on the $z$ components of the primed spin operators $\hat{\mathscr{S}}=\hat{\mathbf{S}}'$ only, so that (30) assumes the special form

$$H(\hat{\mathbf{S}},\varepsilon)=\mathscr{H}(\hat{\mathscr{S}}_z,\varepsilon). \tag{33}$$

Defining $\mathscr{U}_\varepsilon(\hat{\mathscr{S}})=U'_\varepsilon(\hat{\mathscr{S}})$, Eq. (32) turns into

$$\mathscr{U}_\varepsilon^\dagger(\hat{\mathscr{S}})\ H(\hat{\mathscr{S}},\varepsilon)\ \mathscr{U}_\varepsilon(\hat{\mathscr{S}})=\mathscr{H}(\hat{\mathscr{S}}_z,\varepsilon). \tag{34}$$

In order to distinguish quantities related to a general transformation as in (30) from those associated with (33), curly symbols such as $\hat{\mathscr{U}}$ and $\hat{\mathscr{H}}$ have been used. It will be convenient to rename the curly operators $\hat{\mathscr{S}}$ by $\hat{\mathbf{S}}$ in Eq. (34).

### B. Perturbation expansion

The construction of the unitary transformation $\hat{\mathscr{U}}_\varepsilon$ achieving (34) is at stake now. Under three assumptions it can be reduced formally to the successive solution of an infinite set of hierarchical equations determined by the unperturbed Hamiltonian $H_0(\hat{\mathbf{S}}_z)$ and the perturbation $\tilde{H}(\hat{\mathbf{S}},\varepsilon)$. First, it is

assumed that the perturbation in (28) can be expanded in a power series of the parameter $\varepsilon$:

$$\widetilde{H}(\hat{\mathbf{S}},\varepsilon)=\sum_{p=1}^{\infty}\varepsilon^{p}H_{p}(\hat{\mathbf{S}}). \tag{35}$$

When writing the operator $\hat{\mathscr{U}}_{\varepsilon}$ as a Lie transform,

$$\mathscr{U}(\hat{\mathbf{S}},\varepsilon)=\exp[-iu(\hat{\mathbf{S}},\varepsilon)/\hbar], \tag{36}$$

a similar expansion is required to exist for the Hermitian operator $\hat{u}_{\varepsilon}$:

$$u(\hat{\mathbf{S}},\varepsilon)=\sum_{p=1}^{\infty}\varepsilon^{p}u_{p}(\hat{\mathbf{S}}). \tag{37}$$

The operator $\hat{u}_{\varepsilon}$ is called the generator (or generating operator) of the unitary transformation $\hat{\mathscr{U}}_{\varepsilon}$. Finally, it must be possible to expand the new Hamiltonian operator, $\hat{\mathscr{H}}$, in powers of $\varepsilon$:

$$\mathscr{H}(\hat{S}_{z},\varepsilon)=\sum_{p=0}^{\infty}\varepsilon^{p}\mathscr{H}_{p}(\hat{S}_{z}). \tag{38}$$

Plugging these expansions into requirement (34) and collecting the terms multiplied by equal powers of the parameter $\varepsilon$, one obtains the following set of equations:

$$\begin{aligned}
&0=\hat{H}_{0}-\hat{\mathscr{H}}_{0},\quad \frac{i}{\hbar}[\hat{H}_{0},\hat{u}_{1}]=\hat{H}_{1}-\hat{\mathscr{H}}_{1},\\
&\frac{i}{\hbar}[\hat{H}_{0},\hat{u}_{2}]=\hat{H}_{2}-\frac{i}{2\hbar}[\hat{u}_{1},\hat{\mathscr{H}}_{1}+\hat{H}_{1}]-\hat{\mathscr{H}}_{2},\\
&\vdots\\
&\frac{i}{\hbar}[\hat{H}_{0},\hat{u}_{p}]\\
&\quad=R_{p}(\hat{u}_{1},\ldots,\hat{u}_{p-1},\hat{H}_{1},\ldots,\hat{H}_{p},\hat{\mathscr{H}}_{1},\ldots,\hat{\mathscr{H}}_{p-1})\\
&\qquad-\hat{\mathscr{H}}_{p},\\
&\vdots
\end{aligned} \tag{39}$$

For convenience, each equation has been solved for the commutators of the unperturbed Hamiltonian, $\hat{H}_{0}$, with the generator of the highest index, $\hat{u}_{p}$. Equations (39) constitute a nested hierarchy: at the $p$th level the quantities $\hat{\mathscr{H}}_{p}$ and $\hat{u}_{p}$ can be determined if all quantities with smaller indices have been found; the operator $\hat{R}_{p}$ contains only quantities know from the beginning or determined when solving the equations of the lower levels. Such a structure is typical for perturbation theory formulated in terms of Lie transforms. It is possible to discuss the method to solve the equations (39) in full generality [7–9]. For simplicity, the procedure is carried out here for a system with a single degree of freedom first; generalization to two (or more) spins is then straightforward.

### C. One degree of freedom

For a single-spin system with Hamiltonian

$$H(\hat{\mathbf{S}},\varepsilon)=H_{0}(\hat{S}_{z})+\widetilde{H}(\hat{\mathbf{S}},\varepsilon), \tag{40}$$

the unknowns $\hat{u}_{p}$ and $\hat{\mathscr{H}}_{p}$ are determined from the nested hierarchy (39) as follows.

Solving the first equation of the hierarchy is particularly simple because it states that the old and the new Hamiltonian, $\hat{H}_{0}$ and $\hat{\mathscr{H}}_{0}$, respectively, coincide. By assumption, $\hat{H}_{0}$ depends on the $z$ component of $\hat{\mathbf{S}}$ only, and, thus, $\hat{\mathscr{H}}_{0}$ has this property, too, while $\hat{\mathscr{S}}$ and $\hat{\mathbf{S}}$ are identical to order $\varepsilon^{0}$. This is consistent, as is easily seen from the limit of vanishing perturbation, $\varepsilon=0$.

The remaining equations are all of the same type:

$$\frac{i}{\hbar}[H_{0}(\hat{S}_{z}),u_{p}(\hat{S}_{\pm},\hat{S}_{z})]=R_{p}(\hat{S}_{\pm},\hat{S}_{z})-\mathscr{H}_{p}(\hat{S}_{z}). \tag{41}$$

The operator $\hat{R}_{p}$ can be written as a power series in the operators $\hat{S}_{\pm}$ [cf. Eq. (84) in Appendix C]:

$$R_{p}(\hat{S}_{\pm},\hat{S}_{z})=R_{p,0}(\hat{S}_{z})+\sum_{k=1}^{\infty}(\hat{S}_{+}^{k}R_{p,k}^{+}(\hat{S}_{z})+R_{p,k}^{-}(\hat{S}_{z})\hat{S}_{-}^{k}), \tag{42}$$

with uniquely defined operators $\hat{R}_{p,k}^{+}=(\hat{R}_{p,k}^{-})^{\dagger}$ and $\hat{R}_{p,0}$ that depend on $\hat{S}_{z}$ only.

However, expanding $u_{p}(\hat{S}_{\pm},\hat{S}_{z})$ as in (42),

$$u_{p}(\hat{S}_{\pm},\hat{S}_{z})=u_{p,0}(\hat{S}_{z})+\sum_{k=1}^{\infty}(\hat{S}_{+}^{k}u_{p,k}^{+}(\hat{S}_{z})+u_{p,k}^{-}(\hat{S}_{z})\hat{S}_{-}^{k}), \tag{43}$$

one obtains for the commutator in (41)

$$\frac{i}{\hbar}[\hat{H}_{0},\hat{u}_{p}]=\sum_{k=1}^{\infty}(\hat{S}_{+}^{k}\hat{u}_{p,k}^{+}i\hat{\omega}_{k}+(-i\hat{\omega}_{k})\hat{u}_{p,k}^{-}\hat{S}_{-}^{k}), \tag{44}$$

where Eq. (22) has been used. The order of the operators $\hat{u}_{p,k}^{\pm}$ and the frequency operator of the unperturbed system, $\hat{\omega}_{k}$, is immaterial since they depend on $\hat{S}_{z}$ only. Obviously, there is no term depending on $\hat{S}_{z}$ alone; hence, for (41) to hold one must have

$$\mathscr{H}_{p}(\hat{S}_{z})=R_{p,0}(\hat{S}_{z}). \tag{45}$$

Furthermore, the operators $\hat{u}_{p,k}^{\pm}$ follow from comparing (42) and (44):

$$u_{p}(\hat{S}_{\pm},\hat{S}_{z})=u_{p,0}(\hat{S}_{z})+\sum_{k=1}^{\infty}\left(\hat{S}_{+}^{k}\frac{\hat{R}_{p,k}^{+}}{i\hat{\omega}_{k}}+\frac{\hat{R}_{p,k}^{-}}{-i\hat{\omega}_{k}}\hat{S}_{-}^{k}\right), \tag{46}$$

where the inverse of the operator $\hat{\omega}_{k}$ is well-defined only if the operator $\hat{\omega}_{k}$ does not have a zero eigenvalue; this, however, is guaranteed by the assumption that the unperturbed Hamiltonian has no degenerate eigenvalues. Therefore, an operator $\hat{u}_{p}$ solving Eq. (41) has been found in terms of $\hat{R}_{p}$

and $\hat{\omega}_k$. Its ''diagonal'' part $u_{p,0}(\hat{S}_z)$ (corresponding to a phase shift when acting on eigenstates of $\hat{S}_z$) remains undetermined—for simplicity, it will be chosen equal to zero for all $p$. As a result, the possibility to solve the hierarchy of Eqs. (39) has been established. The similarity of Eq. (46) with the classical formula, Eq. (B5), is striking.

It is important to note that the expression (46) for the generator $\hat{u}_p$ exhibits factors inversely proportional to the frequency operators $\omega_k(\hat{S}_z)$, as is familiar from classical perturbation theory (cf. Appendix B). As can be read off from the structure of the hierarchy (39), the operators $\hat{R}_p$ are linear in $\hat{u}_{p-1}$: thus, they contain terms proportional to $1/\hat{\omega}_k^{p-1}$. Solving (46) for the generating operator of $p$th order, $\hat{u}_p$, one finds it to be proportional to the inverse of the $p$th power of frequency operators. The structurally similar classical expansion is bound to converge to a well-defined canonical transformation since all classical systems with one degree of freedom are integrable. By analogy, it is expected that the individual generating operators $\hat{u}_p$ will add up to a sensible expression for the unitary transformation $\hat{\mathscr{U}}_\varepsilon$. If classical systems with two degrees of freedom are studied, the impact of a perturbation is known to be disastrous in most cases.

### D. Two degrees of freedom

For a nearly integrable quantum system with two degrees of freedom

$$H(\hat{\mathbf{S}}_1,\hat{\mathbf{S}}_2,\varepsilon)=H_0(\hat{S}_{1z},\hat{S}_{2z})+\widetilde{H}(\hat{\mathbf{S}}_1,\hat{\mathbf{S}}_2,\varepsilon), \tag{47}$$

the transformed Hamiltonian operator should depend on two new spin components only, $\hat{\mathscr{S}}_{1z}$ and $\hat{\mathscr{S}}_{2z}$. As before, the lowest order of the hierarchy (39) is easily solved by defining $\hat{\mathscr{H}}_0$ to be identical with the unperturbed Hamiltonian, $\hat{H}_0$. For $p\geqslant 1$, the equations to be solved read:

$$\begin{aligned}&\frac{i}{\hbar}[H_0(\hat{S}_{1z},\hat{S}_{2z}),u_p(\hat{S}_{1\pm},\hat{S}_{2\pm},\hat{S}_{1z},\hat{S}_{2z})]\\&\quad=R_p(\hat{S}_{1\pm},\hat{S}_{2\pm},\hat{S}_{1z},\hat{S}_{2z})-\mathscr{H}_p(\hat{S}_{1z},\hat{S}_{2z}).\end{aligned} \tag{48}$$

Using expansions for the operators $\hat{R}_p$ and $\hat{u}_p$ (cf. Appendix C) in analogy to (42) and (43), respectively, one finds for the generator

$$\hat{u}_p(\hat{\mathbf{S}}_\pm,\hat{\mathbf{S}}_z)=\sum_{\substack{k,l=0\\(k,l)\neq(0,0)}}^{\infty}\left(\hat{S}_{1+}^k\hat{S}_{2+}^l\frac{R_{p,kl}^+(\hat{\mathbf{S}}_z)}{i(\omega_k^{(1)}(\hat{S}_{1z},\hat{S}_{2z}+l\hbar)+\omega_l^{(2)}(\hat{S}_{1z},\hat{S}_{2z}))}+\hat{S}_{1+}^k\frac{R_{p,kl}^\pm(\hat{\mathbf{S}}_z)}{i(\omega_k^{(1)}(\hat{\mathbf{S}}_z)-\omega_l^{(2)}(\hat{\mathbf{S}}_z))}\hat{S}_{2-}^l+\text{H.c.}\right). \tag{49}$$

Again, the generator $\hat{u}_p$ is determined up to an arbitrary function of $\hat{\mathbf{S}}_z$ only which is chosen equal to zero. When expressing the denominators in terms of the unperturbed Hamiltonian, it becomes obvious that both spins enter symmetrically in (49): the first one reads

$$\hat{\Delta}_{kl}^+=\frac{1}{\hbar}(H_0(\hat{S}_{1z}+k\hbar,\hat{S}_{2z}+l\hbar)-H_0(\hat{S}_{1z},\hat{S}_{2z})), \tag{50}$$

and the second one is equal to

$$\hat{\Delta}_{kl}^-=\frac{1}{\hbar}(H_0(\hat{S}_{1z}+k\hbar,\hat{S}_{2z})-H_0(\hat{S}_{1z},\hat{S}_{2z}+l\hbar)). \tag{51}$$

Equation (49) belongs to the main results of the present paper. For systems with two (or more) degrees of freedom the generators contain terms proportional to the inverse of *linear combinations* of frequency operators. The expansion (49) makes sense only if the denominators $\hat{\Delta}_{kl}^\pm$ do not have a zero eigenvalue, which will be assumed from now on. When dealing with the convergence of the perturbation series, it will be necessary to proceed in two steps: first, the existence of each generator $\hat{u}_p$ has to be shown, and subsequently it has to be checked that the sum of all $\hat{u}_p$ leads to a sensible result.

## V. EXAMPLES

The perturbation theory as developed in the preceding section is applied here to explicit examples. Systems with one and two degrees of freedom will be studied in order to obtain more detailed insight into the structure of the denominators.

### A. One degree of freedom

The Hamiltonian to be studied is defined as follows:

$$\begin{aligned}H(\hat{\mathbf{S}},\varepsilon)&=\alpha\hat{S}_z+\frac{1}{2}\beta\hat{S}_z^2+\frac{\varepsilon}{2}\hat{S}_x^2\\&=\alpha\hat{S}_z+\frac{1}{2}\beta\hat{S}_z^2+\frac{\varepsilon}{4}(\hat{\mathbf{S}}^2-\hat{S}_z^2)+\frac{\varepsilon}{8}(\hat{S}_+^2+\hat{S}_-^2),\end{aligned} \tag{52}$$

the nonzero constants $\alpha$ and $\beta$ being real numbers, and the quantum integrable part, $\hat{H}_0=\alpha\hat{S}_z+\beta\hat{S}_z^2/2$, is assumed to have no degenerate eigenvalue. The perturbation $\widetilde{H}(\hat{\mathbf{S}},\varepsilon)=\varepsilon\hat{S}_x^2/2$ is particularly simple because it consists of just one single term being proportional to $\varepsilon$.

It is straightforward to calculate the frequency operators according to (23):

$$\hat{\omega}_k = k(\alpha + \beta \hat{S}_z) + \tfrac{1}{2}\beta k^2 \hbar, \quad k = 1,2, \ldots . \tag{53}$$

The first term on the right-hand side defines a function $\omega_k$ of the operator $\hat{S}_z$ which coincides with the expression for the classical frequency: $\omega_k(S_z) = k\omega(S_z) = k(\alpha + \beta S_z)$. Due to the discretization of the derivative an additional term proportional to $\hbar$ shows up in (53).

According to (45) the new first-order Hamiltonian is equal to the diagonal part of the perturbation:

$$\mathscr{H}_1(\hat{S}_z) = \tfrac{1}{4}(\hat{\mathbf{S}}^2 - \hat{S}_z^2), \tag{54}$$

as can be read off from Eq. (52). When expanding the off-diagonal part of the perturbation the only nonvanishing coefficients are found to be

$$R_{1,2}^{\pm}(\hat{S}_z) = \tfrac{1}{8}, \tag{55}$$

leading to the following expression for the first-order generator:

$$\hat{u}_1 = \frac{1}{8}\left( \hat{S}_+^2 \frac{1}{i\hat{\omega}_2} + \frac{1}{-i\hat{\omega}_2} \hat{S}_-^2 \right), \tag{56}$$

with $\hat{\omega}_2$ from (53). Since the energy eigenvalues of the Hamiltonian $\hat{H}_0$ in (52) have been assumed not to be degenerate, the expectation value of the denominators in Eq. (56) will not have zero eigenvalues. Consequently, there is no principal obstacle which would destroy the convergence of the perturbation series for the unitary transformation $\hat{\mathscr{U}}$, similar to classical mechanics.

### B. Two degrees of freedom

Consider a two-spin Hamiltonian (47) with

$$H(\hat{\mathbf{S}}_1, \hat{\mathbf{S}}_2, \varepsilon) = f_1(\hat{S}_{1z}) + f_2(\hat{S}_{2z}) + \gamma \hat{S}_{1z}\hat{S}_{2z} + \tilde{H}(\hat{\mathbf{S}}_1, \hat{\mathbf{S}}_2, \varepsilon), \tag{57}$$

where

$$f_j(x) = \alpha_j x + \frac{1}{2}\beta_j x^2, \quad j = 1,2. \tag{58}$$

The quantum integrable Hamiltonian consisting of the first three terms on the right-hand side of Eq. (57) is quadratic in the $z$ components of the spin. With a view to the structure of the denominators present in the generating operator—which are completely determined by the frequencies of the unperturbed system as seen from Eq. (49)—the form of the perturbation $\tilde{H}(\hat{\mathbf{S}}_1, \hat{\mathbf{S}}_2, \varepsilon)$ must not be specified in detail. On evaluating (26) one finds

$$\hat{\omega}_k^{(1)} = k(\alpha_1 + \beta_1 \hat{S}_{1z} + \gamma \hat{S}_{2z}) + \tfrac{1}{2}\beta_1 k^2 \hbar, \tag{59}$$

and $\hat{\omega}_k^{(2)}$ follows from exchanging the indices $(1 \leftrightarrow 2)$. The first term is closely related to the classical frequency,

$$\begin{aligned} \omega_k^{(1)}(S_{1z}, S_{2z}) &= k\omega^{(1)}(S_{1z}, S_{2z}) \\ &= k \frac{\partial H_0(S_{1z}, S_{2z})}{\partial S_{1z}} \\ &= k(\alpha_1 + \beta_1 S_{1z} + \gamma S_{2z}), \end{aligned} \tag{60}$$

and analogously for $\omega_k^{(2)}(S_{1z}, S_{2z})$. In formula (49), the expansion of the generator $\hat{u}_p$ has been given in general terms. Focus now on the second term of its right-hand side containing the difference of the frequency operators in the denominator. Its matrix elements in the product basis $|m_1, m_2\rangle$, consisting of eigenstates of the operators $\hat{S}_{jz}$, are given by

$$\begin{aligned} &\langle m_1, m_2 | \hat{S}_{1+}^k \frac{\hat{R}_{p,kl}^+}{\hat{\Delta}_{kl}^-} \hat{S}_{2-}^l | m_1', m_2' \rangle \\ &= \langle m_1', m_2 | \frac{\hat{R}_{p,kl}^+}{\hat{\Delta}_{kl}^-} | m_1', m_2 \rangle \, \delta_{m_1 m_1' + k} \delta_{m_2 m_2' - l}, \end{aligned} \tag{61}$$

where, as before, $\hat{\Delta}_{kl}^- = \hat{\omega}_k^{(1)} - \hat{\omega}_l^{(2)}$, which in the present case reads explicitly

$$\begin{aligned} \hat{\Delta}_{kl}^- = &[k(\alpha_1 + \beta_1 \hat{S}_{1z} + \gamma \hat{S}_{2z}) - l(\alpha_2 + \beta_2 \hat{S}_{2z} + \gamma \hat{S}_{1z})] \\ &+ \frac{\hbar}{2}(\beta_1 k^2 - \beta_2 l^2). \end{aligned} \tag{62}$$

Since both operators, $\hat{R}_{p,kl}^+$ and $\hat{\Delta}_{kl}^-$, depend on the $z$ components only, the expectation value of their ratio, $\langle \hat{R}/\hat{\Delta} \rangle$, is equal to the ratio of their expectation value, $\langle \hat{R} \rangle / \langle \hat{\Delta} \rangle$. Consequently, the convergence of the power series defining the first-order generator for the system (57), will be controlled by matrix elements of operators such as $\hat{\Delta}_{kl}^-$ in Eq. (62). They are made up of two contributions with different origins. The operator in square brackets is recognized as the difference of the frequency operators that one would obtain if in the classical formula (60) one were to replace the variables $S_{jz}$ by their operator equivalents, $\hat{S}_{jz}$. The possibility to approximate arbitrarily well the ratio of the frequencies $\omega^{(2)}/\omega^{(1)}$ for a given torus (i.e., fixed values of $S_{1z}$ and $S_{2z}$) by $k/l$ leads to the problem of small denominators in classical mechanics (cf. [10]).

Then, the difference $\hat{\Delta}_{kl}^-$ contains a term proportional to Planck's constant: the occurrence of a term *linear* in $\hbar$ follows from studying a Hamiltonian $\hat{H}$ being quadratic in the $z$ components of the spins. Polynomials of degree $r$ for the Hamiltonian lead to terms of at most $\hbar^{r-1}$, etc. The presence of such terms has been noted already by Robnik [11] in a similar treatment of particle systems. He suggested that these additional terms will have the effect to move the system away from the classical resonance, however small the value of $\hbar$. But looking at the *exact* expression (62) for a fixed value of Planck's constant, $\hbar = 1$, say, one can also conceive it as a new type of resonance condition that is no longer *linear* in the indices $k$ and $l$: a quantum-mechanical *nonlinear* resonance condition arises that has to be studied in its own right for all possible representations.

The relevant matrix elements of the operator $\hat{\Delta}_{kl}^-$ [cf. (61)] read explicitly

$$\langle m_1-k,m_2'-l|\hat{\Delta}_{kl}^{-}|m_1-k,m_2'-l\rangle = k(\alpha_1+\beta_1\hbar m_1+\gamma\hbar m_2')-l(\alpha_2+\beta_2\hbar m_2'+\gamma\hbar m_1) - \frac{\hbar}{2}(\beta_1 k^2-\beta_2 l^2), \tag{63}$$

[note the sign change of the last term relative to (62)]. In each individual representation, there is an important difference compared to classical mechanics. The range of the numbers $k$ and $l$ is not all the integers but it varies over a finite subset of them only, which is determined by the spin length $s$. This is characteristic of finite-dimensional representations of spin systems while it does not occur for particle systems. The matrix elements of the other operators in Eq. (49) lead to expressions of the same structure.

There are two ways to study the expression (63). First, consider it as a quantum-mechanical statement in its own right. This means to give $\hbar$ its actual value and to let vary both pairs $(m_1,m_2')$ and $(k,l)$ over the finite range determined by the value of $s$. Within each $(2s+1)$-dimensional representation of the spin algebra, the modulus of $\langle\hat{\Delta}_{kl}^{-}\rangle$ will have some positive nonzero minimal value, $\Delta(s)$. Consequently, for sufficiently small values of $\varepsilon$, the expansion of the generator $\hat{u}_p$ in (37) is expected to converge because the terms $[\varepsilon/\Delta(s)]^p$ can be kept small. For spins of length $s$ the perturbed Hamiltonian $\hat{H}_\varepsilon$ is given by a finite-dimensional Hermitian matrix that guarantees the existence of a unitary transformation diagonalizing it. Therefore, the generic convergence of the construction should not come as a surprise (for possible technical difficulties, cf. [12]). For the present concept of integrability, however, it is essential that not one *specific* representation is studied but that the statements hold in an *algebraic* sense, or, equivalently, in *all* representations. The implications of this requirement will be made explicit now.

Imagine to have constructed the diagonalizing transformations in all representations. This set of matrices may either be the representations of one *single* algebraically defined operator $\hat{\mathscr{U}}_\varepsilon$ or not. In the latter case, the unitary transformations in the individual representations will not ''converge'' towards one specific unitary operator for large values of $s$ (since the value of $\hbar$ is kept fixed, this procedure is not identical to the classical limit to be discussed momentarily). In addition, for larger values of $s$ the number $\Delta(s)$ takes on smaller and smaller values, which requires the expansion parameter to be correspondingly smaller. If there is no *finite* value of $\varepsilon$ such that the perturbation series converges for all allowed values of $s$, i.e., algebraically, the perturbation $\widetilde{H}(\hat{\mathbf{S}},\varepsilon)$ renders the system nonintegrable. A strong decrease of the smallest occurring denominator $\Delta(s)$ as a function of $s$ has been observed numerically. If, however, the summation of the perturbation series for all $s$ does not require vanishing $\varepsilon$, one may expect an algebraic diagonalizing operator to exist; hence, the perturbation can be absorbed into an appropriate redefinition of the action operators. In classical mechanics, this convergence for finite $\varepsilon$ is known to result from appropriately decreasing numerators.

We turn now to the second way to study (63): in the semiclassical limit with $\hbar\sim 1/s$ and $s\to\infty$, one should recover the behavior of the classical frequency denominators from Eq. (63). Numerical tests make it plausible that, indeed, the value of $\Delta(s)$ decrease monotonically when larger values of $k$ and $l$ provide better and better approximations of the classical frequency ratio (the values of $\hbar m_1$ and $\hbar m_2'$ are kept fixed here, defining thus a specific ''torus''). An analytic study is not straightforward, even for the quadratically modified resonance condition associated with (63): the behavior of the last term is not easily controlled since $\hbar k^2$ and $\hbar l^2$ may have values of the order of $s$.

## VI. DISCUSSION

### A. Summary and outlook

For the sake of clarity, the main points of the development given in the previous pages are briefly summarized. Starting from the algebraic skeleton necessary to describe quantum (spin) systems, arguments for the existence of quantum-mechanical action and frequency operators in systems with a single degree of freedom have been put forward. When applying these concepts to systems with more degrees of freedom they lend themselves to a definition of quantum integrable systems. An algebraic version of perturbation theory of such systems has been formulated appropriate to absorb the effect of an added disturbance. Since this formulation respects (and exploits) the underlying Lie-algebraic structure, a tight analogy to classical Lie transforms is achieved. As a natural consequence, operator-valued analogs of the classical frequency denominators show up when constructing a unitary transformation that would diagonalize the Hamiltonian algebraically. In this way, the quantum-mechanical locus of the convergence problems known to exist in classical mechanics has been found, at least on a formal level. In an appropriate sense, the quantum-mechanical expressions for the denominators generalize the classical ones. The condition for a classical resonance to occur is, effectively, equivalent to a *linear* relation among the classical frequencies (associated with a ''plane'' in action space) whereas, in a given representation, the relevant quantum-mechanical relation turns out to be *nonlinear* (defining ''ellipsoids'' or other curved surfaces). Such structures have been observed in semiclassical treatments, for example, in the work by Berry and Tabor [13] who derive energy-level statistics for classically integrable quantum systems in the limit of small values for $\hbar$.

When scrutinizing the notion of quantum integrability the ultimate goal is to provide evidence for both, its usefulness and its consistency. Rigorously testable predictions of specific properties must result for quantum integrable (and nonintegrable) systems, just as the phase-space foliation of classically integrable systems flows from its classical counterpart. In our view, the major achievement of the present approach is to have boiled down the question of quantum integrability (and, *a fortiori*, of quantum chaos) to a *technical* problem, namely, to investigate the (convergence) properties of a perturbation series. Due to the *nonlinearities* in the quantum-mechanical expressions just mentioned, the behavior of the perturbation series is, from the present point of view, not obvious. In principle, there is no need for quantum systems to *exactly* parallel the properties of classically (non) integrable systems: the underlying unifying structure is

on an *algebraic* level but with the algebras being realized in different spaces, in phase space and in Hilbert space, respectively. In the semiclassical limit, however, one expects that the statements associated with the two realizations become comparable if appropriate tools such as Wigner functions are employed. The present formulation now calls for a detailed parallel investigation of the effects that a perturbation has on a classically integrable system and on its quantum counterpart.

Here is a brief sketch of a scenario being plausible in view of the present results which, however, has to be substantiated by further investigations. Focus on the fully quantum-mechanical regime, that is, fix the value of $\hbar$ and consider the behavior of the perturbation series in representations of variable dimension, $2s+1$. It is expected that the ''visibility'' of the perturbation will increase for dimensions with larger values of $s$. A vivid illustration of this effect has been reported for a system consisting of two coupled spins where a ''regular quantum web'' is gradually torn apart by a perturbation of increasing strength [14]. Related phenomena have been observed in particle systems by Bohigas, Tomsovic, and Ullmo [15]. In a study of the spin-boson model the observed ''resonance phenomena'' can be attributed to the presence of small denominators becoming more or less effective in representations of different dimensions [16]. An analytic study of these numerically observed effects in the vein of the present paper is under way [17]. In general, ''quantum resonances'' in a nonintegrable quantum system due to ever smaller denominators will become more and more pronounced if larger representations of the spin algebra are considered. The infinite-dimensional representation (not to be confused with the semiclassical limit) contains the most detailed structure, possibly leading to an actual divergence of the perturbation series.

### B. Related work

There is a large number of joints between earlier work and the present one that so far have been alluded to only occasionally. It is useful to dwell on them for a moment, to draw parallels and to point out differences.

The introduction of frequency operators (in the present terminology) provides a link to the most advanced papers of the ''old quantum mechanics.'' In 1925, Dirac [6] defined ''$q$ numbers,'' which would fulfill the fundamental commutation relations of position and momentum. Basic *algebraic* consequences are derived, partly by exploiting the analogy to the classical Poisson brackets. One section of the paper is devoted to ''multiply periodic systems'' characterized by the existence of ''uniformizing variables'' (which nowadays would be called action and angle operators) such that the Hamiltonian depends on the action operators only [cf. Eq. (3)]. In the terminology of the present work multiply periodic systems are thus recognized as quantum integrable ones. Assuming the action-angle operators to fulfill the same commutation relations as momentum and position—which is untenable due to the defectiveness of a phase operator [18]—Dirac introduced two different types of frequencies. The first one is supposed to govern the time evolution of the phase operator itself, whereas the second one is associated with the time derivative of the *exponentiated* phase operator. It turns out that the latter frequency operator is equivalent to the expression given in (20). Dirac also mentions its two possible versions reflecting the freedom of ordering in (18). For spin systems considered here, the operator $\hat{S}_+$ plays a role similar to the exponentiated angle operator.

Wentzel [19] continued Dirac's work by establishing a link between Heisenberg's matrix mechanics and the $q$ numbers. In particular, he wrote down expressions for quantum-mechanical frequencies similar to (20) being applicable to multiply periodic systems only. However, this line of reasoning seems to have come to an abrupt end by the advent of wave mechanics in 1926: the serious shortcoming of the earlier quantum theory to allow for quantization of multiply periodic systems only was removed by Schrödinger's equation, which is easily written down for particles subjected to arbitrary potentials.

Similarly, strong formal affinities to Heisenberg's formulation of perturbation theory [20] exist. This is easily understood if one recalls that before the introduction of Schrödinger's equation classical mechanics served much more than later as Ariadne's thread for quantum-mechanical developments. Still, Heisenberg's approach to treat perturbations and the widely used perturbation scheme of Rayleigh-Schrödinger [21] differ conceptually in an important way from the present one. Traditionally, *any* quantum system may serve as a starting point for perturbation theory, the only assumption being that its (necessarily periodic) solutions are known. In the approach developed here, the unperturbed system is assumed to be quantum integrable; hence, it (presumably) stems from a *restricted* class of systems, and the effect of the perturbation is to remove it from this class. In order to prove the KAM theorem, classical perturbation theory is developed relative to *integrable* systems: the fate of a torus under the perturbation is investigated, not its effect on an arbitrary periodic solution—which might happen to be an isolated periodic orbit of a nonintegrable system. KAM theory would not apply at all. It is hoped that by systematically moving away from *integrable* quantum systems generic properties will be seen to emerge for nonintegrable ones. As for a close-up of the relation between classical tori and Heisenberg's matrix mechanics which fits well into the scheme developed here, see the work by Greenberg, Klein, and Li [22].

Next, there are close ties to Birkhoff normal forms [1] and to the so-called ''algebraic quantization'' reviewed in [23]. The idea is to quantize integrable approximations to classically nonintegrable systems. Crehan [24] worked out quantum-mechanical normal forms in the spirit of Birkhoff and Gustavson, starting from the classical Hamiltonian function in the neighborhood of a point of stable equilibrium. Impressive agreement between exact quantum-mechanical solutions and the approximate ones has been obtained [25,26]. In contrast to these works, however, no recourse has been made to classical mechanics in the present approach.

Concerning the presence of the quantum equivalents of the small denominators, their occurrence has been noted already by Robnik [11] for particle systems (and by Graffi, cf. the introduction of [27]). Robnik pointed out that for small values of Planck's constant the classical denominators will be modified by terms of the order $\hbar$. In this way the resonance conditions are destroyed that govern the fate of an

individual classical torus, that is, its survival or destruction. Furthermore, it is conjectured that the series for the diagonaliting unitary transformation will converge almost always without possessing a classical limit. It is expected that in view of the exact expression (49) the effect of the denominators can be studied in more detail for spin systems.

Also, the understanding of clashes between the behavior of classical and quantum perturbation expansions may benefit from the present approach. It has been noted by Eckhardt [28] for a one-dimensional particle system that the convergence of a classical perturbation series is not automatically reflected in the convergence of the corresponding quantum perturbation series, as follows from a simple scaling argument.

In order to deal with issues of perturbation series for quantum systems a new setting has been provided by Bellissard and Vittot [27], whose work is based on the concept of noncommutative geometry. Their work is focussed on Lie-transform techniques for quantum-mechanical particle systems with respect to the classical limit. The aspect of integrability, seemingly, has not been addressed in detail. It is particularly important that estimates of the Nekhoroshev type become available that allow one to control the approximations for energy eigenvalues extremely well. For systems with one degree of freedom, the convergence of the perturbation series has been proven (cf. [29]). At present, the theory has been worked out for particle systems only while the transfer to spin systems is in preparation [30]. A common feature of many works in this area (cf. also [31]) is that the unperturbed systems considered are collections of harmonic oscillators. Having frequency operators at one's diposal, this restriction seems to be no longer necessary.

Finally, a review of the use of Lie-transform techniques and KAM-like results in quantum mechanics has been given by Jauslin [32] dealing, to a large extent, with externally driven systems.

## APPENDIX A: THE COMMUTATORS $[f(\hat{S}_z),\hat{S}_\pm^k]$

It will be shown by using the commutation relations of the spin operators that

$$[f(\hat{S}_z),\hat{S}_+^k]=\hat{S}_+^k[f(\hat{S}_z+k\hbar)-f(\hat{S}_z)]$$
$$=\hat{S}_+^k[\exp(k\hbar\partial_z)-1]f(\hat{S}_z), \tag{A1}$$

where $\partial_z$ is a shorthand for a (formal) derivative with respect to $\hat{S}_z$. The function $f(x)$ is assumed to have an expansion as a power series in $x$.

First, it is proved by induction that

$$[\hat{S}_z^n,\hat{S}_+]=\hat{S}_+[\exp(\hbar\partial_z)-1]\hat{S}_z^n. \tag{A2}$$

This relation holds for $n=1$,

$$[\hat{S}_z,\hat{S}_+]=\hat{S}_+[\exp(\hbar\partial_z)-1]\hat{S}_z=\hat{S}_+(\hat{S}_z+\hbar-\hat{S}_z)=\hbar\hat{S}_+. \tag{A3}$$

Equation (A2) is valid for $n+1$ if it is assumed to hold for $n$:

$$[\hat{S}_z^{n+1},\hat{S}_+]=[\hat{S}_z,\hat{S}_+]\hat{S}_z^n+\hat{S}_z[\hat{S}_z^n,\hat{S}_+]$$
$$=\hat{S}_+\{\hbar\hat{S}_z^n+(\hat{S}_z+\hbar)[\exp(\hbar\partial_z)-1]\hat{S}_z^n\}$$
$$=\hat{S}_+[\exp(\hbar\partial_z)-1]\hat{S}_z^{n+1}, \tag{A4}$$

since $(\hat{S}_z+\hbar)\exp(\hbar\partial_z)=\exp(\hbar\partial_z)\hat{S}_z$. Using $f(\hat{S}_z)=\sum_{n=0}^{\infty}f_n\hat{S}_z^n$ implies

$$[f(\hat{S}_z),\hat{S}_+]=\sum_{n=0}^{\infty}f_n[\hat{S}_z^n,\hat{S}_+]$$
$$=\hat{S}_+[\exp(\hbar\partial_z)-1]\sum_{n=0}^{\infty}f_n\hat{S}_z^n$$
$$=\hat{S}_+[\exp(\hbar\partial_z)-1]f(\hat{S}_z). \tag{A5}$$

Thus, Eq. (A3) holds for $k=1$, as is necessary for a proof by induction on $k$. The step from $k$ to $k+1$ reads

$$[f(\hat{S}_z),\hat{S}_+^{k+1}]=\hat{S}_+^k[f(\hat{S}_z),\hat{S}_+]+[f(\hat{S}_z),\hat{S}_+^k]\hat{S}_+$$
$$=\hat{S}_+^{k+1}\{[\exp(\hbar\partial_z)-1]$$
$$+[\exp(k\hbar\partial_z)-1]\exp(\hbar\partial_z)\}f(\hat{S}_z)$$
$$=\hat{S}_+^{k+1}\{\exp[(k+1)\hbar\partial_z]-1\}f(\hat{S}_z), \tag{A6}$$

where, in the second line, Eq. (A5) has been used in the form $f(\hat{S}_z)\hat{S}_+=\hat{S}_+\exp(\hbar\partial_z)f(\hat{S}_z)$, concluding the proof of (A1).

Relation (A1) can also be written as

$$f(\hat{S}_z)\hat{S}_+^k=\hat{S}_+^kf(\hat{S}_z+k\hbar)\quad\text{or}\quad f(\hat{S}_z-k\hbar)\hat{S}_+^k=\hat{S}_+^kf(\hat{S}_z); \tag{A7}$$

in words, the order of a function of $\hat{S}_z$ only and the $k$th power of the operator $\hat{S}_+$ may be exchanged if the argument of the function $f$ is shifted by an appropriate multiple of $\hbar$. Similar relations are obtained for the step-down operator by taking the Hermitian conjugate of Eqs. (A1) and (A7).

A proof of Eq. (A5) for *arbitrary* functions $f(\hat{S}_z)$ is easily given if one exploits the properties of the ladder operators in explicit representations. The action of the step-up operator is in all representations of the form

$$\hat{S}_+|m,s\rangle=c_m^s|m,s\rangle,\quad c_m^s=\sqrt{s(s+1)-m(m+1)}. \tag{A8}$$

Using $f(\hat{S}_z)|m,s\rangle=f(m\hbar)|m,s\rangle$, one obtains for all $|m,s\rangle$ that

$$f(\hat{S}_z)\hat{S}_+|m,s\rangle=c_m^sf((m+1)\hbar)|m+1,s\rangle \tag{A9}$$
$$=\hat{S}_+f((m+1)\hbar)|m+1,s\rangle$$
$$=\hat{S}_+f(\hat{S}_+\hbar)|m,s\rangle, \tag{A10}$$

implying that

$$f(\hat{S}_z)\hat{S}_+=\hat{S}_+f(\hat{S}_z+\hbar), \tag{A11}$$

which is equivalent to (A5). As before, induction on $k$ completes the proof of relation (A1).

### APPENDIX B: CLASSICAL PERTURBATION THEORY

Results of classical Lie-perturbation theory are collected; for easy comparison with the quantum-mechanical formulas an analogous notation is used. Consider a Hamiltonian $H(\mathbf{S},\varepsilon)=H_0(\mathbf{S}_z)+\widetilde{H}(\mathbf{S},\varepsilon)$, where $H_0(\mathbf{S}_z)$ is integrable and $\widetilde{H}(\mathbf{S},\varepsilon)$ is the perturbation. The goal is to remove the perturbation by introducing a new set of spin variables

$$\mathbf{S}'=\hat{T}\mathbf{S}, \tag{B1}$$

where the canonical transformation is implemented by the operator

$$\hat{T}=\exp(-\{u(\mathbf{S},\varepsilon),\cdot\}). \tag{B2}$$

The function $u(\mathbf{S},\varepsilon)$ is assumed to have an expansion in powers of $\varepsilon$, and $u(\mathbf{S},\varepsilon=0)=0$. When expanding the old and new Hamiltonian functions in powers of $\varepsilon$, the construction of the transformation $\hat{T}$ leads to a hierarchy of equations

$$\{H_0(\mathbf{S}_z),u_p(\mathbf{S}_\pm,\mathbf{S}_z)\}=R_p(\mathbf{S}_\pm,\mathbf{S}_z)-\mathscr{H}_p(\mathbf{S}_z)$$

$$p=0,1,2,\ldots, \tag{B3}$$

which is the classical counterpart of (39). They can be solved by an appropriate choice of the functions $u_p$ and $\mathscr{H}_p$.

If in classical mechanics the expansion of functions $F(\mathbf{S})$ is written in analogy to (C3) the solutions of (B3) are

$$\mathscr{H}_p(S_z)=R_{p,0}(S_z), \tag{B4}$$

$$u_p(S_\pm,S_z)=\sum_{k=1}^{\infty}\left(S_+^k\frac{R_{p,k}(S_z)}{i\omega_k(S_z)}-\frac{R_{p,k}^*(S_z)}{i\omega_k(S_z)}S_-^k\right). \tag{B5}$$

The expression for $u_p(S_\pm,S_z)$ can be simplified by using $\omega_k=k\omega$ from (13).

Similarly, the results for a two-spin system assume the form of the expansion (C6),

$$\mathscr{H}_p(\mathbf{S}_z)=R_{p,00}(\mathbf{S}_z), \tag{B6}$$

$$u_p(\mathbf{S}_\pm,\mathbf{S}_z)=\sum_{\substack{k,l=0\\(k,l)\neq(0,0)}}^{\infty}\left(S_{1+}^kS_{2+}^l\frac{R_{p,kl}^+(\mathbf{S}_z)}{i[\omega_k^{(1)}(\mathbf{S}_z)+\omega_l^{(2)}(\mathbf{S}_z)]}+S_{1+}^k\frac{R_{p,kl}^\pm(\mathbf{S}_z)}{i[\omega_k^{(1)}(\mathbf{S}_z)-\omega_l^{(1)}(\mathbf{S}_z)]}S_{2-}^l+\text{ c.c.}\right). \tag{B7}$$

### APPENDIX C: EXPANSION OF A FUNCTION $F(\hat{S}_\pm,\hat{S}_z)$

A convention for the expansion of functions of spin operators is established. For simplicity, the case of a single spin $\hat{\mathbf{S}}$ is considered first. Let $F(\hat{S}_\pm,\hat{S}_z)$ be expandable in powers of $\hat{S}_+$ and $\hat{S}_-$. Functions depending on $\hat{S}_z$ only are denoted by curly symbols $\mathscr{F}(\hat{S}_z)$. In general, $\hat{F}$ will consist of a sum of terms, each of which is of the form

$$\hat{S}_+^{n_{1+}}\hat{S}_-^{n_{1-}}\mathscr{F}_1(\hat{S}_z)\hat{S}_+^{n_{2+}}\hat{S}_-^{n_{2-}}\mathscr{F}_2(\hat{S}_z)\cdots. \tag{C1}$$

The exponents $n_{j,\pm}$ are integers greater than or equal to zero. Since the product $\hat{S}_+\hat{S}_-=g(\hat{S}_z)$ depends only on $\hat{S}_z$, one can write for arbitrary integers $n_\pm\geqslant 0$ that

$$\hat{S}_+^{n_+}\hat{S}_-^{n_-}=\begin{cases}\hat{S}_+^{n_+-n_-}\mathscr{F}_>(\hat{S}_z) & n_+>n_-\\ \mathscr{F}_=(\hat{S}_z) & \text{if}\quad n_+=n_-\\ \mathscr{F}_<(\hat{S}_z)\hat{S}_-^{n_--n_+} & n_+<n_-,\end{cases} \tag{C2}$$

by exchanging $g(\hat{S}_z)$ with $\hat{S}_\pm^k$ according to the rules (A7). Thus, expression (C1) can be cast into one of these forms if now $n_\pm$ are defined as the total number of $\hat{S}_\pm$ operators in (C1), $n_\pm=\Sigma_j n_{j\pm}$.

Collecting all terms in the expansion of $F(\hat{S}_\pm,\hat{S}_z)$ with the same number of $\hat{S}_+$ or $\hat{S}_-$, the operator $\hat{F}$ can be written as

$$F(\hat{S}_\pm,\hat{S}_z)=F_0(\hat{S}_z)+\sum_{k=1}^{\infty}[\hat{S}_+^kF_k^+(\hat{S}_z)+F_k^-(\hat{S}_z)\hat{S}_-^k], \tag{C3}$$

which will be considered as standard form. For the sake of generality, the index $k$ is assumed to run over all integers, while in a specific representation the sum in (C3) will run over $2s+1$ values only. If $\hat{F}$ is a Hermitian operator, then $\hat{F}_0$ is Hermitian and

$$F_k^+(\hat{S}_z)=[F_k^-(\hat{S}_z)]^\dagger. \tag{C4}$$

The generalization to two or more degrees of freedom is straightforward but the notation becomes more cumbersome. First consider a function $F(\hat{S}_{1\pm},\hat{S}_{1z},\hat{S}_{2\pm},\hat{S}_{2z})$ depending on the components of two spins $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$. As before, the function $F$ is assumed to have an expansion in powers of the spin components. Since the components of different spins commute, $\hat{F}$ can be brought to the form

$$\begin{aligned}F(\hat{S}_{1\pm},\hat{S}_{1z},\hat{S}_{2\pm},\hat{S}_{2z})&=F_{00}(\hat{S}_{1z},\hat{S}_{2z})+\sum_{\substack{k,l=0\\(k,l)\neq(0,0)}}^{\infty}\Big[\hat{S}_{1+}^k\hat{S}_{2+}^lF_{kl}^{++}(\hat{S}_{1z},\hat{S}_{2z})\\&+\hat{S}_{1+}^kF_{kl}^{+-}(\hat{S}_{1z},\hat{S}_{2z})\hat{S}_{2-}^l+\hat{S}_{2+}^lF_{kl}^{-+}(\hat{S}_{1z},\hat{S}_{2z})\hat{S}_{1-}^k\\&+F_{kl}^{--}(\hat{S}_{1z},\hat{S}_{2z})\hat{S}_{1-}^k\hat{S}_{2-}^l\Big].\end{aligned} \tag{C5}$$

If $\hat{F}$ is a Hermitian operator this expression simplifies to

$$F(\hat{\mathbf{S}}_1,\hat{\mathbf{S}}_2)=F_{00}(\hat{\mathbf{S}}_z)+\sum_{\substack{k,l=0\\(k,l)\neq(0,0)}}^{\infty}[\hat{S}_{1+}^k\hat{S}_{2+}^lF_{kl}^{++}(\hat{\mathbf{S}}_z)+\hat{S}_{1+}^kF_{kl}^{+-}(\hat{\mathbf{S}}_z)\hat{S}_{2-}^l+\text{ H.c.}], \tag{C6}$$

since, generalizing (C4)

$$\hat{F}_{kl}^{++}=(\hat{F}_{kl}^{--})^{\dagger},\quad \hat{F}_{kl}^{+-}=(\hat{F}_{kl}^{-+})^{\dagger}. \tag{C7}$$

Functions depending on the components of more than two spins can be expanded similarly. One gets one term depending only on the $z$ components and $2^N$ terms that contain the explicit dependence on the operators $\hat{S}_{j+}$ and $\hat{S}_{j-}$. A unique way of ordering would be, in an extension of the above, to throughout position the step-up operators $\hat{S}_{j+}$ on the left and their adjoints on the right of the middle part, which depends on the $z$ components only.


[1] A. J. Lichtenberg and M. A. Liebermann, *Regular and Stochastic Motion* (Springer, New York, 1983).
[2] *Chaos and Quantum Physics*, edited by M. J. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1991).
[3] St. Weigert and G. Müller, Chaos Solitons Fractals **5**, 1419 (1995).
[4] St. Weigert, Physica D **56**, 107 (1992).
[5] G. Falk, Z. Phys. **130**, 51 (1951); **131**, 470 (1952).
[6] P. A. M. Dirac, Proc. R. Soc. London **110**, 561 (1926).
[7] J. R. Cary, Phys. Rep. **79**, 131 (1981).
[8] I. Shavitt and L. T. Redmon, J. Chem. Phys. **73**, 5711 (1980).
[9] E. L. Sibert III, J. Chem. Phys. **88**, 4378 (1988).
[10] W. Thirring, *Lehrbuch der Mathematischen Physik, I* (Springer, New York, 1988).
[11] M. Robnik, J. Phys. A **19**, L841 (1986).
[12] H. R. Jauslin, M. Govin, and M. Cibils, in *Chaos—the interplay between stochastics and deterministic behaviour*, edited by P. Garbaczewski, M. Wolf, and A. Weron, Lecture Notes in Physics Vol. 457 (Springer, Berlin, 1995), p. 151.
[13] M. V. Berry and M. Tabor, Proc. R. Soc. London A **356**, 375 (1977).
[14] N. Srivastava and G. Müller, Z. Phys. B **81**, 137 (1990).
[15] O. Bohigas, S. Tomsovic, and D. Ullmo, Phys. Rep. **223**, 43 (1995).
[16] M. Cibils, Y. Cuche, and G. Müller, Z. Phys. B **97**, 569 (1995).
[17] G. Müller (private communication).
[18] R. G. Newton, Ann. Phys. (N.Y.) **124**, 327 (1980).
[19] G. Wentzel, Z. Phys. **37**, 80 (1926).
[20] W. Heisenberg, Z. Phys. **33**, 879 (1925).
[21] See, e.g., P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Vol. 2, Chap. IX.
[22] W. R. Greenberg, A. Klein, and C.-T. Li, Phys. Rev. Lett. **75**, 1244 (1995).
[23] L. E. Fried and G. S. Ezra, J. Phys. Chem. **92**, 3144 (1988).
[24] P. Crehan, J. Phys. A **23**, 5815 (1990).
[25] T. Uzer, D. W. Noid, and R. A. Marcus, J. Chem. Phys. **79**, 4412 (1983).
[26] D. Farelly, J. Chem. Phys. **85**, 2119 (1986).
[27] J. Bellissard and M. Vittot, Ann. Inst. Henri Poincaré **52**, 175 (1990).
[28] B. Eckhardt, J. Phys. A **19**, 2961 (1986).
[29] D. Bambusi, Nonlinearity **8**, 93 (1995).
[30] J. Bellissard (private communication).
[31] S. Graffi and T. Paul, Commun Math. Phys. **108**, 25 (1987).
[32] H. R. Jauslin, in *Computational Physics*, edited by P. L. Garrido and J. Marro (World Scientific, Singapore, 1993), p. 107.