Construction of Darboux coordinates and Poincaré-Birkhoff normal forms in noncanonical Hamiltonian systems

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Abstract. We demonstrate a general method to construct Darboux coordinates via normal form expansions in noncanonical Hamiltonian system obtained from e. g. a variational approach to quantum systems. The procedure serves as a tool to naturally extract canonical coordinates out of the variational parameters and at the same time to transform the energy functional into its Poincaré-Birkhoff normal form. The method is general in the sense that it is applicable for arbitrary degrees of freedom, in arbitrary orders of the local expansion, and it is independent of the precise form of the Hamilton operator. The method presented allows for the general and systematic investigation of quantum systems in the vicinity of fixed points, which e. g. correspond to ground, excited or transition states. Moreover, it directly allows to calculate classical and quantum reaction rates by applying transition state theory.

1. Introduction

It is at the core of physical sciences to describe and investigate the dynamics of systems. Depending on their nature, these can either be described by the Schrödinger equation in case of quantum mechanical systems, or e. g. in terms of Hamiltonian mechanics in case of a classical system. In both cases, a canonical structure of the dynamical equations [1,2] is inherent which is expressed in the existence of conjugate pairs of field operators $\hat{\psi}, \hat{\psi}^\dagger$ with infinite degrees of freedom or conjugate coordinates $\boldsymbol{q}, \boldsymbol{p}$ with a finite number of degrees of freedom. Both approaches serve as powerful frameworks to investigate a huge amount of different physical problems. In addition to the global dynamics of a physical system which can be determined by solving the corresponding equations of motion, its fixed points play a crucial role in many investigations: For example, fixed points which correspond to a (local) minimum of the Hamiltonian form (metastable) ground states of the system. Moreover, fixed points which are related to saddle points of the Hamiltonian are unstable, excited states. A special class of such unstable fixed points are rank-1 saddle points which possess exactly one unstable direction. These points are of special interest in dynamical systems, because they form bottlenecks in the underlying phase space which separate different regions therein. Considering a dynamical system, the transition from one to the other subregion of phase space is then mediated by the saddle point. Therefore, the latter determines the reaction dynamics between the different subregions which is the basic statement of transition state theory [3–19].

Beyond the fixed points of the system's dynamical equations themselves, their local properties are of high interest in many applications. For example, the local properties of a minimum of the Hamiltonian determine the physics of the system for small excitations from the ground state. Moreover, the local properties in the vicinity of a rank-1 saddle point or transition state determine the reaction dynamics and rates of the system.

For a detailed analysis of the local fixed point properties of a canonical Hamiltonian system a standard and powerful tool is its normal form expansion [15,20,21]. Especially in the field of reaction dynamics, the normal form Hamiltonian in the vicinity of rank-1 saddle points is important, because it provides a way of defining a normally hyperbolic invariant manifold [15, 18, 21–34] with which a nonrecrossing dividing surface between reactants and products in multi-degree-of-freedom systems can be constructed.

In Ref. [15], Waalkens *et al* describe this procedure in detail, of which our work will be a natural extension to *noncanonical* coordinates. We therefore give a brief overview of the method in the following: If the Hamiltonian H is given in terms of a set of canonical coordinates $\boldsymbol{q}, \boldsymbol{p}$ then its normal form can be constructed via the following expansion,

$$\tilde{H}(\boldsymbol{q},\boldsymbol{p}) = \sum_{j=0}^{\infty} \frac{1}{j!}\, \mathrm{ad}_W^j\, H(\boldsymbol{q},\boldsymbol{p})\,. \tag{1}$$

Here, W is an appropriate generating function and $\mathrm{ad}_W\, H = \{W, H\}$ is the adjoint operator that equals the definition of the Poisson bracket. Usually, the normal form Hamiltonian is required up to a certain polynomial order within a local expansion at a fixed point. Consequently, it is appropriate to regard, in general, expansions of all quantitues occurring in Eq. (1), i. e. the original Hamiltonian, the transformed one, and the generating function. This procedure has the advantage that the transformation in Eq. (1) can be applied order by order. Waalkens *et al* [15] describe in detail how these single steps are performed and how exactly the generating function W needs to be constructed through a homological equation in order to obtain the Poincaré-Birkhoff normal form of the Hamilton function (we refer the reader to this reference for more details). The final result is then, by construction, a Hamiltonian $H(\boldsymbol{J})$ which depends on the actions coordinates $\boldsymbol{J}$ all being constants of motion up to the respective order of the expansions.

With special regard to reactive systems, this normal form is of particular advantage, because – if J_1 corresponds to the reaction channel of the system, i. e. the unstable direction of a rank-1 saddle point – then a local, recrossing-free dividing surface is defined by $J_1 = 0$, The directional flux through the dividing surface at fixed energy E is then given by

$$f(E) = (2\pi)^{d-1}\, \mathcal{V}(E)\,, \tag{2}$$

where $\mathcal{V}(E)$ is the volume of actions $(J_2, \ldots, J_d)$ enclosed by the contour $H(0, J_2, \ldots, J_d) = E$ and the thermal reaction rate Γ at temperature $\beta = 1/k_{\mathrm{B}}T$ is obtained from the Boltzmann average of Eq. (2) which yields (cf. Ref. [35])

$$\Gamma = \frac{1}{2\pi\beta} \frac{\int \mathrm{d}J_2 \ldots \mathrm{d}J_d\, \exp\bigl(-\beta H(0, J_2, \ldots, J_d)\bigr)}{\int \mathrm{d}J_1' \ldots \mathrm{d}J_d'\, \exp\bigl(-\beta H'(J_1', \ldots, J_d')\bigr)}\,. \tag{3}$$

Here, H is the normal form at the transition state and H' that at the metastable ground state. In this context of reaction dynamics the importance of the knowledge

of a normal form Hamiltonian and, in order to be able to actually calculate reaction rates, an explicit construction scheme of the local action variables become obvious. We note that the work of Waalkens *et al* [15] goes even beyond this by also introducing how quantum reaction rates can be calculated within a formally equivalent procedure that merely requires a redefinition of the adjoint operator.

It is the purpose of this paper to extend the scheme of Waalkens *et al* [15] to the more general field of *noncanonical* Hamiltonian systems, as e. g. quantum mechanical wave packets whose dynamics is governed by the Schrödinger equation (see below). Therefore, we will describe in the following a quantum system within a variational approach, determine the respective dynamical equations by applying a time-dependent variational principle [36, 37], and show that it defines a general, *noncanonical* Hamiltonian system (see below for a precise definition). In such quantum systems, fixed points of the dynamical equations and their local properties have the same meaning for the quantum reaction dynamics as they have in classical systems. For a detailed analysis of the local properties, it is, therefore, desirable to obtain an analogue of the classical normal form also for the quantum system. However, the usual treatment (1) cannot be applied, because neither a classical Hamilton function $H(\boldsymbol{q}, \boldsymbol{p})$ in canonical coordinates nor such coordinates themselves are known.

Here, we present a method by which both the transformation of the variational approach as a noncanonical Hamiltonian system into its Poincaré-Birkhoff normal form and simultaneously the construction of canonical coordinates is obtained. The result of the transformations is, by construction, a set of canonical normal form coordinates. In the latter, the energy functional of the system will serve as a classical Hamilton function which has the advantageous property that it is directly formulated in action variables. If truncated at a certain order, the constructed Hamiltonian will serve as an approximation to the true quantum system which directly allows for the application of transition state theory and the evaluation of quantum reaction rates via Eqs. (2) and (3). In technical terms, the crucial difference between our procedure in noncanonical coordinates and the usual treatment in canonical ones is that we treat the dynamical equations as well as the energy functional separately. From the mathematical point of view, this brings with it that the generating function of the transformation and the corresponding operators require a different definition than in Eq. (1).

Our paper is organized as follows: In Sec. 2 we introduce a variational approach to quantum systems which defines a noncanonical Hamiltonian system for the variational parameters. Furthermore, we discuss its formal relation to classical canonical mechanics and some important fixed point properties of the linearised dynamical equations. In Sec. 3, the method to construct local canonical coordinates in the vicinity of the fixed point is introduced. Therefore, a symplectic basis formed by appropriately normalized eigenvectors of the linearised dynamical equations is used and higher-order terms of the expansions are treated via normal form transformations. As a key feature – and in contrast to the usual transformation (1) of canonical Hamiltonians – this procedure treats the dynamical equations and the energy functional separately. Moreover, the normal form expansions are carried out in two steps: First, its polynomial structure is generated using the nonresonant terms of the corresponding generating function (see below for the latters' definition). Second, the remaining resonant coefficients of the generating function which are free parameters are chosen in such a way that the dynamical equations as well as the energy functional in normal form coordinates fulfil canonical equations, i. e. the normal form coordinates are canonical ones by construction. We have written the paper such that the essential

steps that go beyond the work in Refs. [15,20] are presented in the 5 theorems presented in Sec. 3. In the appendix, we provide in addition both a numerical example of the presented procedure and an exemplary MATHEMATICA script code, in which the reader is welcome to execute the respective steps while reading the paper.

We note that it is not within the scope of this paper to deal with questions of existence and convergence of the objects made use of, but to present a scheme analogously to and beyond Ref. [15] by which canonical coordinates and the normal form can be constructed at the same time. The method developed in this paper presents the basis of e. g. the calculation of thermal decay rates of a metastable 1-dimensional potential as well as Bose-Einstein condensates with different kinds of interactions. Results using the leading order and including higher orders of the normal form expansion are presented in Refs. [38, 39] and [40–42], respectively.

2. Variational approach to quantum systems as a noncanonical Hamiltonian system

In this paper, we focus on quantum systems which are described by the Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\,\psi(\boldsymbol{r},t)=\hat{H}\psi(\boldsymbol{r},t)\,. \tag{4}$$

Here, $\psi(\boldsymbol{r},t)$ is the time-dependent wave function of the system and $\hat{H}$ is the Hamilton operator. As it is well known, there is a natural canonical structure inherent to this description. This becomes especially obvious, if one derives the Schrödinger equation in the framework of field theory from the Hamiltonian density

$$\mathcal{H}=\int \mathrm{d}^3r\;\psi^\dagger(\boldsymbol{r},t)\,\hat{H}\,\psi(\boldsymbol{r},t) \tag{5}$$

using the functional derivatives

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r},t)=\frac{\partial\mathcal{H}}{\partial\psi^\dagger(\boldsymbol{r},t)}\,,\qquad \mathrm{i}\hbar\frac{\partial}{\partial t}\psi^\dagger(\boldsymbol{r},t)=-\frac{\partial\mathcal{H}}{\partial\psi(\boldsymbol{r},t)}\,. \tag{6}$$

This description of a quantum system is very general, however, it is often not feasible in actual applications due to the field operator's infinite number of degrees of freedom.

One possible approach to reduce the system's number of degrees of freedom is its treatment within a variational approach. Therein, the Schrödinger equation (4) is solved approximately by replacing the original wave function $\psi(\boldsymbol{r},t)$ by a trial wave function

$$\psi(\boldsymbol{r},t)=\psi(\boldsymbol{r},\boldsymbol{z}(t))\,. \tag{7}$$

Here, $\boldsymbol{z}(t)=[z_1(t),z_2(t),\ldots,z_d(t)]^\mathsf{T}\in\mathbb{C}^d$ is a set of complex and time-dependent variational parameters, and the time evolution of the wave function is completely determined by that of the variational parameters. In the framework of the variational approach, expectation values of the system's observables, in general, become functions depending on the variational parameters $\boldsymbol{z}(t)$. In particular, the energy functional of the system is given by the expectation value of the Hamilton operator

$$E(\boldsymbol{z}(t))=\left\langle\psi(\boldsymbol{r},\boldsymbol{z}(t))\right|\hat{H}\left|\psi(\boldsymbol{r},\boldsymbol{z}(t))\right\rangle\,. \tag{8}$$

In order to describe the dynamics of the system in the Hilbert subspace which is spanned by the variational ansatz, we apply the Dirac-Frenkel-McLachlan variational

principle [36,37]. This claims to minimize the norm of the difference between the left- and the right-hand side of the Schrödinger equation (4),

$$I \equiv \|\mathrm{i}\phi - \hat{H}\psi\|^2 = \big\langle -\mathrm{i}\phi - \hat{H}\psi \big| \mathrm{i}\phi - \hat{H}\psi \big\rangle \stackrel{!}{=} \min. \tag{9}$$

Here, $\hbar = 1$ has been set, the arguments of the wave function ψ have been omitted for brevity, and also the time dependence of the variational parameters $\boldsymbol{z}$ will be dropped in the following. The quantity I is minimized with respect to ϕ and $\phi \equiv \dot{\psi}$ is set afterwards which means that the Schrödinger equation is solved within the Hilbert subspace of the variational ansatz with the least possible error. Since the approximate solution of the Schrödinger equation is intended to minimize the quantity I, the latter's variations must vanish,

$$\delta I = \big\langle -\mathrm{i}\,\delta\phi \big| \mathrm{i}\phi - \hat{H}\psi \big\rangle + \big\langle -\mathrm{i}\phi - \hat{H}\psi \big| \mathrm{i}\,\delta\phi \big\rangle \stackrel{!}{=} 0\,. \tag{10}$$

Because of Eq. (7), the time derivative of the trial wave function, $\phi = \dot{\psi}$, and its variation $\delta\phi$ yield

$$\phi = \sum_{m=1}^{d} \frac{\partial\psi}{\partial z_m}\,\dot{z}_m\,, \qquad \delta\phi = \sum_{n=1}^{d} \frac{\partial\psi}{\partial z_n}\,\delta\dot{z}_n\,, \tag{11}$$

so that one obtains

$$\delta I = \sum_{m,n=1}^{d} \left\langle \frac{\partial\psi}{\partial z_m} \middle| -\frac{\partial\psi}{\partial z_n}\dot{z}_n - \mathrm{i}\hat{H}\psi \right\rangle \delta\dot{z}_m^* + \left\langle -\frac{\partial\psi}{\partial z_n}\dot{z}_n + \mathrm{i}\hat{H}\psi \middle| \frac{\partial\psi}{\partial z_m} \right\rangle \delta\dot{z}_m \stackrel{!}{=} 0\,. \tag{12}$$

We now proceed from the complex variational parameters $\boldsymbol{z}$ to their real and imaginary parts

$$\boldsymbol{x} \equiv (\boldsymbol{z}^{\mathrm{r}}, \boldsymbol{z}^{\mathrm{i}})^{\mathsf{T}} \in \mathbb{R}^{2d}\,. \tag{13}$$

In this case, the variations with respect to the variational parameters in Eq. (12) are not independent, and both terms together result in the dynamical equations

$$\sum_{n=1}^{2d} \mathrm{Im}\left\langle \frac{\partial\psi}{\partial x_m} \middle| \frac{\partial\psi}{\partial x_n} \right\rangle \dot{x}_n = -\mathrm{Re}\left\langle \frac{\partial\psi}{\partial x_m} \middle| \hat{H}\psi \right\rangle \tag{14}$$

for the time evolution of each real variational parameter $m = 1, \ldots, 2d$. Using the property

$$\frac{\partial}{\partial\boldsymbol{x}} E(\boldsymbol{x}) = 2\,\mathrm{Re}\left\langle \frac{\partial\psi(\boldsymbol{x})}{\partial\boldsymbol{x}} \middle| \hat{H} \middle| \psi(\boldsymbol{x}) \right\rangle, \tag{15}$$

which directly follows from Eq. (8) with the replacement (13) and the definitions

$$K_{mn} \equiv 2\,\mathrm{Im}\left\langle \frac{\partial\psi}{\partial x_m} \middle| \frac{\partial\psi}{\partial x_n} \right\rangle, \tag{16a}$$

$$h_m \equiv 2\,\mathrm{Re}\left\langle \frac{\partial\psi}{\partial x_m} \middle| \hat{H}\psi \right\rangle, \tag{16b}$$

the dynamical equations (14) immediately take the form

$$K(\boldsymbol{x})\,\dot{\boldsymbol{x}} = -\frac{\partial E(\boldsymbol{x})}{\partial\boldsymbol{x}} \equiv -\boldsymbol{h}(\boldsymbol{x})\,, \tag{17}$$

which will be the basis of all considerations in this paper. We note that the matrix K with the entries (16a) is skew-symmetric by definition, because the imaginary part changes its sign under complex conjugation of the bracket. Therefore, K induces a symplectic geometry onto the space of variational parameters that can be expressed by the corresponding 2-form

$$\omega^2 = \sum_{\substack{m,n=1 \\ m<n}}^{2d} K_{mn}(\boldsymbol{x})\, \mathrm{d}x_m \wedge \mathrm{d}x_n \,. \tag{18}$$

This 2-form is nondegenerate if K is invertible which we will assume throughout this paper. Moreover, it is closed, i. e. its exterior derivative vanishes,

$$\mathrm{d}\omega^2 = \sum_{\substack{m,n,k=1 \\ m<n}}^{2d} \frac{\partial K_{mn}(\boldsymbol{x})}{\partial x_k}\, \mathrm{d}x_k \wedge \mathrm{d}x_m \wedge \mathrm{d}x_n = 0 \,, \tag{19}$$

because the single terms

$$\partial_{x_k} K_{mn} = \mathrm{Im} \left\langle \frac{\partial^2 \psi}{\partial x_k \partial x_m} \middle| \frac{\psi}{\partial x_n} \right\rangle - \mathrm{Im} \left\langle \frac{\partial^2 \psi}{\partial x_k \partial x_n} \middle| \frac{\psi}{\partial x_m} \right\rangle , \tag{20}$$

cancel out when it is summed over k, m, n. Under these conditions Darboux's theorem [43, 44] guarantees the existence of local canonical coordinates. In Sec. 3 we present a scheme by which such coordinates can actually be constructed via normal form expansions.

2.1. Relation to classical canonical Hamiltonian mechanics

The dynamical equations (17) are formally equivalent to Hamilton's equations in classical mechanics. To see this, let us consider a Hamiltonian system with d degrees of freedom, whose standard canonical coordinates $\boldsymbol{u} = (q_1, p_1, \ldots, q_d, p_d)^\mathsf{T}$, fulfil the Poisson brackets

$$\{q_i, p_j\} = \delta_{ij} \,, \quad \{q_i, q_j\} = 0 \,, \quad \{p_i, p_j\} = 0 \,. \tag{21}$$

The physics of this system is described by the Hamiltonian $H = H(\boldsymbol{u})$ and the dynamics of the system is then determined by Hamilton's equations

$$\mathcal{J}\dot{\boldsymbol{u}} = -\frac{\partial H(\boldsymbol{u})}{\partial \boldsymbol{u}} \,, \tag{22}$$

where, $\mathcal{J}$ is the standard symplectic matrix

$$\mathcal{J} \equiv \begin{pmatrix} \mathcal{J}_1 & & 0 \\ & \ddots & \\ 0 & & \mathcal{J}_1 \end{pmatrix} , \qquad \text{with} \qquad \mathcal{J}_1 \equiv \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{23}$$

The latter relates the Hamiltonian vector field $\dot{\boldsymbol{u}}$ to the derivative $\partial H/\partial \boldsymbol{u}$ of the Hamiltonian, and it induces a symplectic geometry on phase space.

In the dynamical equations (17), the time-derivative $\dot{\boldsymbol{x}}$ is also related to the gradient of the energy functional E via a skew-symmetric matrix, here K. The crucial

difference to Eq. (22) is that, because of its definition according to Eq. (16a), K has a more complicated structure than $\mathcal{J}$, in particular it generally depends on the variational parameters. As a consequence, the Poisson brackets (21) are not fulfilled for the variational parameters in the system (17) and, for this reason, we will refer to the latter as a *noncanonical* Hamiltonian system in this paper. The fact that the matrix K is not equal to $\mathcal{J}$ also leads to the fact that one can no longer identify certain pairs of "conjugate coordinates" x_i, x_j in variational space, because *all* the time-derivatives $\dot{x}_i, \dot{x}_j$ $(i, j = 1, \ldots, d)$ are, in general, coupled in a nontrivial way.

Both dynamical equations (17) and (22) have in common that they describe a *classical* dynamics. However, we emphasize that the classical dynamics (17) takes place in variational space and that this is an effective description of the fully quantized physical system that is described by the Schrödinger equation (4). Consequently, there is no need to take into account a further quantization of the variational parameters (including possible problems in context with their nature as noncanonical coordinates).

2.2. Local dynamical equations and their eigenvalue structure

As already mentioned in the introduction, we focus on the local dynamics of Eq. (17) in the vicinity of a fixed point. Thus, in the following, we consider local Taylor expansions of K and $\boldsymbol{h}$ at the fixed point up to any desired order $n_{\max}$,

$$\left(\sum_{n=0}^{n_{\max}-1} K_n(\boldsymbol{x}) \right) \dot{\boldsymbol{x}} = - \sum_{n=1}^{n_{\max}} \boldsymbol{h}_n(\boldsymbol{x}) \,, \tag{24}$$

where the matrix K and the vector $\boldsymbol{h}$ are expanded independently according to

$$K(\boldsymbol{x}) \approx \sum_{n=0}^{n_{\max}-1} K_n(\boldsymbol{x}) \,, \tag{25a}$$

$$\boldsymbol{h}(\boldsymbol{x}) \approx \sum_{n=1}^{n_{\max}} \boldsymbol{h}_n(\boldsymbol{x}) \,. \tag{25b}$$

Analogously, the energy functional is expanded as

$$E(\boldsymbol{x}) \approx \sum_{n=0}^{n_{\max}+1} E_n(\boldsymbol{x}) \,. \tag{26}$$

The terms K_n, $\boldsymbol{h}_n$, and E_n summarize all terms of the respective expansion which are homogeneous of degree n, and $\boldsymbol{h}_0 = 0$ vanishes because the expansion is performed at a fixed point. Alternatively, the expansion of the equations of motion (24) can be rewritten equivalently in the form

$$\dot{\boldsymbol{x}} = -K^{-1}(\boldsymbol{x})\, \boldsymbol{h}(\boldsymbol{x}) \approx \sum_{n=1}^{n_{\max}} \boldsymbol{f}_n(\boldsymbol{x}) \,, \tag{27}$$

where both K and $\boldsymbol{h}$ are combined on the same side of the equation and where $\boldsymbol{f}_n$ collects the terms of order n.

For the following considerations, the local eigenvalue structure of the dynamical equations at a fixed point $\dot{\boldsymbol{x}} = 0$ are of fundamental importance. These are determined by the linearised dynamical equations

$$K_0\, \dot{\boldsymbol{x}} = -\boldsymbol{h}_1(\boldsymbol{x}) = F\, \boldsymbol{x} \,, \tag{28}$$

where it is assumed that the fixed point is located at the origin $\boldsymbol{x} = 0$ for simplicity (this can always be achieved by a simple shift of the coordinates). K_0 is the zeroth-order expansion of the matrix K and $\boldsymbol{h}_1 = -F\boldsymbol{x}$ is the linearised vector $\boldsymbol{h}$ at the fixed point. Because K is skew-symmetric in general, this property of course also holds for its zeroth-order approximation. The matrix F is symmetric, because it is the negative Hessian matrix of the energy functional according to Eq. (17), $F_{mn} = -\partial^2 E/\partial x_m \partial x_n$. Consequently, the equations

$$K_0 = -K_0^{\mathsf{T}}\,, \qquad F = F^{\mathsf{T}} \tag{29}$$

hold. In order to obtain the eigenvalue spectrum of the linearised equations of motion, the first-order differential equation (28) is solved using the ansatz $\boldsymbol{x}(t) = \boldsymbol{v}\,\mathrm{e}^{\lambda t}$, where $\lambda \in \mathbb{C}$ is a complex parameter, and $\boldsymbol{v} \in \mathbb{C}^{2d}$ is a complex vector. Inserting this ansatz into Eq. (28), one obtains the generalized eigenvalue equation

$$F\,\boldsymbol{v} = \lambda K_0\,\boldsymbol{v}\,. \tag{30}$$

The eigenvalues λ are the roots of the characteristic polynomial $\chi(\lambda) = \det(F - \lambda K_0)$, and with the properties (29), it can easily be shown that the characteristic polynomial is an even function of λ, i.e. $\chi(\lambda) = \chi(-\lambda)$. Thus, if λ is a root of the characteristic polynomial, then also $-\lambda$ is a root, so that all the eigenvalues occur pairwise with different sign. Therefore, the eigenvalue spectrum of the linearised dynamical equations in the vicinity of a fixed point always exhibits the structure

$$\boldsymbol{\lambda}^{\pm} = (+\lambda_1, -\lambda_1, \ldots, +\lambda_d, -\lambda_d) \tag{31}$$

which will be of fundamental importance for the normal form expansions performed in the next Sec. 3.

3. Construction of canonical normal form coordinates

The knowledge of canonical coordinates is fundamental to many methods known from classical Hamiltonian mechanics and, beyond their existence, a central question is how these can be constructed. As the key result of this paper, a general method to construct canonical normal form coordinates will be presented in this section. As will be shown, this method has the advantage that it simultaneously yields both a procedure to extract canonical coordinates and a transformation of the system into its Poincaré-Birkhoff normal form. The procedure consists of the following three steps (see Fig. 1):

(i) In the first step, the expansions (25) and (26) are transformed via a linear change of coordinates to a symplectic basis which is defined by the eigenvectors of the linearised dynamical equations. The resulting diagonal coordinates are canonical ones in the first order of the expansions.

(ii) Successive Lie transforms are applied order by order to treat the higher-order corrections of the expansions. In the corresponding generating function two different types of terms will be distinguished, namely "nonresonant" and "resonant" coefficients (see below). The generation of the normal form structure will be performed via the nonresonant terms, and all of them are determined uniquely by the requirement that certain monomials of the dynamical equations

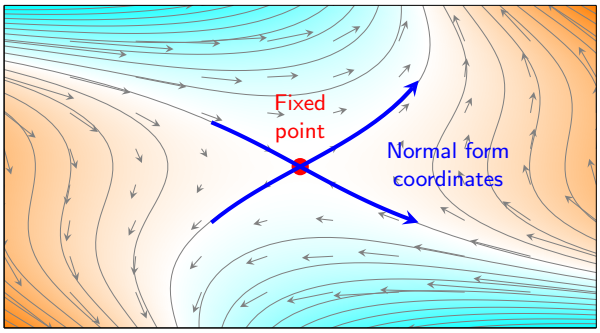

Figure 1. Schematic illustration of the normal form coordinates. The contour lines represent isosurfaces of the energy functional E and the arrows depict the vector field $\dot{\boldsymbol{x}}$ obtained by the dynamical equations (17). In the vicinity of a fixed point (red circle), the normal form coordinates define a local coordinate system whose origin is the fixed point.

shall be removed. Which of the terms remain after the Lie transforms is solely determined by a resonance condition depending on the eigenvalues, and because of their general structure (31), the normal form will exhibit a fundamental polynomial structure.

(iii) The normal form expansions leave the freedom to choose the resonant terms of the generating function. In the last step, these free parameters are chosen in a way that the dynamical equations and the energy functional fulfil canonical equations, i.e. the normal form coordinates are canonical ones by construction.

3.1. Symplectic basis

In order to "simplify" the system in its lowest order, it is sufficient to focus on the linearised dynamical equations (28), and therein the following theorem holds:

Theorem 1 (symplectic basis)**.** *There exists a symplectic basis, within which the linearized dynamical equations* (28) *can be transformed into a structure in which its left-hand side equals the standard symplectic matrix* $\mathcal{J}$ *in Eq.* (23) *and its right-hand side possesses a block structure containing the eigenvalues of the linearized equations of motion. Explicitely, there is a transformation matrix* T *with the properties*

$$T^{\mathsf{T}} K_0 T = \mathcal{J} \qquad \text{and} \qquad T^{\mathsf{T}} F T = \begin{pmatrix} 0 & \lambda_1 & & & \\ \lambda_1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & \lambda_d \\ & & & \lambda_d & 0 \end{pmatrix} . \tag{32}$$

Proof. A natural basis of this linearised system is spanned by its eigenvectors $\boldsymbol{v}_{2i-1}, \boldsymbol{v}_{2i}$. These are solutions of the generalized eigenvalue problem

$$F\,\boldsymbol{v}_{2i-1} = +\lambda_i\, K_0\, \boldsymbol{v}_{2i-1}\,, \tag{33a}$$

$$F\,\boldsymbol{v}_{2i} = -\lambda_i\, K_0\, \boldsymbol{v}_{2i}\,, \tag{33b}$$

where $i = 1, \ldots, d$. To obtain the desired form, we normalize the eigenvectors by

$$\langle \boldsymbol{v}_{2i-1}| K_0 |\boldsymbol{v}_{2i}\rangle = -\langle \boldsymbol{v}_{2i}| K_0 |\boldsymbol{v}_{2i-1}\rangle = 1\,, \tag{34a}$$

$$\langle \boldsymbol{v}_{2i-1}| F |\boldsymbol{v}_{2i}\rangle = \langle \boldsymbol{v}_{2i}| F |\boldsymbol{v}_{2i-1}\rangle = \lambda_i \tag{34b}$$

for all $i = 1, \ldots, d$. Combining the eigenvectors in the transformation matrix $T = (\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{2d})$, the choice (34) by construction guarantees the block structures where $\mathcal{J}$ is the standard symplectic matrix defined in Eq. (23). Consequently, the normalized eigenvectors define a symplectic basis and the coordinates are canonical ones concerning the linearised system. □

In order to regard the full, nonlinearised dynamical equations in this symplectic basis, the transformation $\boldsymbol{x} \to \boldsymbol{x}' = T^{-1}\boldsymbol{x}$ needs to be applied also to the higher-order terms. Emanating from Eq. (27) and omitting the prime, this linear change of coordinates transforms the dynamical equations into the form

$$\dot{\boldsymbol{x}} = T^{-1} \sum_{n=1}^{n_{\max}} \boldsymbol{f}_n(T\boldsymbol{x}) \equiv \boldsymbol{a}(\boldsymbol{x}) = \sum_{n=1}^{n_{\max}} \boldsymbol{a}_n(\boldsymbol{x})\,. \tag{35}$$

In the last step, the single expansion coefficients have been redefined by the coefficients $\boldsymbol{a}_n$ which collect the terms homogeneous of degree n. It is noted that, because the inverse matrix T^{-1} is used here instead of the transpose T^{T}, the linear term of Eq. (35) is diagonal by construction,

$$\boldsymbol{a}_1(\boldsymbol{x}) = (T^{-1}\,F\,T)\,\boldsymbol{x} = \begin{pmatrix} +\lambda_1 & & & & & \\ & -\lambda_1 & & & & \\ & & \ddots & & & \\ & & & +\lambda_d & & \\ & & & & -\lambda_d \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{2d-1} \\ x_{2d} \end{pmatrix}. \tag{36}$$

Note that the originally real vector field (27) is, in general, transformed into a complex one ($\boldsymbol{a}_n \in \mathbb{C}^{2d}$) by the diagonalisation, if the eigenvalue spectrum includes imaginary terms. Analogously to the dynamical equations, also the energy functional is expanded in the vicinity of the fixed point, and the linear transformation $\boldsymbol{x} \to \boldsymbol{x}' = T^{-1}\boldsymbol{x}$ is applied. This results in the scalar field

$$E(\boldsymbol{x}) = \sum_{n=0}^{n_{\max}+1} E_n(\boldsymbol{x})\,, \tag{37}$$

whose coefficients, again, become complex in general. The zeroth-order term E_0 is the fixed-point energy, the first-order of the expansion vanishes, $E_1 = 0$, and, with the normalization (34), the second-order term has the structure $E_2 = \sum_{i=1}^{d} \lambda_i\, x_{2i-1} x_{2i}$. Consequently, the energy functional (37) is in Poincaré-Birkhoff normal form up to the order $n = 2$.

3.2. Normal form transformations – nonresonant terms

The diagonalisation of the local dynamical equations as described in the previous section 3.1, simplifies their linear part in a way that it becomes diagonal. However, for the terms of higher order, a "simplification" cannot be achieved by this step. For

this purpose, a normal form expansion of the diagonalized dynamical equations (35) is performed in this section making use of successive Lie transforms. The general treatment of local dynamical systems and their normal forms has been described by Murdock [20] in detail. Here, it is applied to the $2d$-dimensional local dynamical equations (35) with their special eigenvalue structure (31).

In order to bring the local equations of motion into normal form, a nonlinear near-identity transformation

$$\boldsymbol{x} = \boldsymbol{\phi}_\varepsilon(\boldsymbol{y}) \tag{38}$$

is applied, which transforms from the "old" coordinates $\boldsymbol{x}$ to "new" ones $\boldsymbol{y}$, and which is differentiable in the new coordinates $\boldsymbol{y}$ as well as in the parameter ε. The latter serves as a continuous scaling parameter that is introduced in a way that for $\varepsilon = 0$ one obtains the identity transformation, while the finally desired transformation is obtained for $\varepsilon = 1$,

$$\boldsymbol{x} = \boldsymbol{\phi}_{\varepsilon=0}(\boldsymbol{y}) = \boldsymbol{y}\,, \tag{39a}$$

$$\boldsymbol{x} = \boldsymbol{\phi}_{\varepsilon=1}(\boldsymbol{y}) = \boldsymbol{\phi}(\boldsymbol{y})\,. \tag{39b}$$

Instead of providing the explicit function (38), the change of coordinates is defined implicitly, by the requirement that it is the solution of the differential equation

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}\varepsilon} = \boldsymbol{g}(\boldsymbol{x})\,, \tag{40}$$

with $\boldsymbol{g}$ being the generating function of the transformation. As it is shown in Ref. [20], the final change of variables (39b) transforms a vector field $\boldsymbol{a}$ defining the differential equation

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{a}(\boldsymbol{x}) \tag{41}$$

into a vector field $\boldsymbol{b}$ in the new coordinates $\boldsymbol{y}$ with

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{b}(\boldsymbol{y})\,. \tag{42}$$

The connection between the two vector fields is

$$\boldsymbol{b}(\boldsymbol{y}) = \sum_{j=0}^{\infty} \frac{1}{j!}\, \mathcal{L}_{\boldsymbol{g}}^{j} \boldsymbol{a}(\boldsymbol{x})\big|_{\boldsymbol{x}=\boldsymbol{y}}\,, \tag{43}$$

where $\mathcal{L}_{\boldsymbol{g}}$ is the *homological operator* acting on differentiable vector fields according to

$$\mathcal{L}_{\boldsymbol{g}} a_m(\boldsymbol{x}) \equiv \sum_{n=1}^{2d} \frac{\partial a_m(\boldsymbol{x})}{\partial x_n}\, g_n(\boldsymbol{x}) - \frac{\partial g_m(\boldsymbol{x})}{\partial x_n}\, a_n(\boldsymbol{x})\,. \tag{44}$$

Analogously, the same generating function transforms the energy functional according to

$$\tilde{E}(\boldsymbol{y}) = \sum_{j=0}^{\infty} \frac{1}{j!}\, \mathcal{D}_{\boldsymbol{g}}^{j} E(\boldsymbol{x})\big|_{\boldsymbol{x}=\boldsymbol{y}}\,. \tag{45}$$

Here, the *right-multiplication operator* $\mathcal{D}_{\boldsymbol{g}}$ is defined by

$$\mathcal{D}_{\boldsymbol{g}} E(\boldsymbol{x}) \equiv \frac{\partial E(\boldsymbol{x})}{\partial \boldsymbol{x}}\, \boldsymbol{g}(\boldsymbol{x})\,. \tag{46}$$

3.2.1. Transformation of multivariate polynomials As already mentioned above, the local dynamical equations as well as the energy functional are on hand in the form of a formal power series or local Taylor expansion, i.e. as a multivariate polynomial. Therefore, it is convenient to also define the generating function as a multivariate polynomial, so that the transformed fields will also be such ones. In the following, these polynomials are written as

$$\boldsymbol{a}(\boldsymbol{x}) = \sum_{n=1}^{n_{\max}} \boldsymbol{a}_n(\boldsymbol{x}) = \sum_{|\boldsymbol{m}|=1}^{n_{\max}} \boldsymbol{\alpha}_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}\,, \tag{47a}$$

$$\boldsymbol{b}(\boldsymbol{x}) = \sum_{n=1}^{n_{\max}} \boldsymbol{b}_n(\boldsymbol{x}) = \sum_{|\boldsymbol{m}|=1}^{n_{\max}} \boldsymbol{\beta}_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}\,, \tag{47b}$$

$$\boldsymbol{g}(\boldsymbol{x}) = \sum_{n=1}^{n_{\max}} \boldsymbol{g}_n(\boldsymbol{x}) = \sum_{|\boldsymbol{m}|=1}^{n_{\max}} \boldsymbol{\gamma}_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}\,, \tag{47c}$$

$$E(\boldsymbol{x}) = \sum_{n=0}^{n_{\max}+1} E_n(\boldsymbol{x}) = \sum_{|\boldsymbol{m}|=0}^{n_{\max}+1} \xi_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}\,, \tag{47d}$$

where $\boldsymbol{a}_n, \boldsymbol{b}_n, \boldsymbol{g}_n, E_n$ denote the terms of the respective series which are homogeneous of degree n, and $\boldsymbol{\alpha}_{\boldsymbol{m}}, \boldsymbol{\beta}_{\boldsymbol{m}}, \boldsymbol{\gamma}_{\boldsymbol{m}}, \xi_{\boldsymbol{m}}$ are the coefficients of the expansion. Furthermore, the multi-index notation

$$\boldsymbol{x}^{\boldsymbol{m}} = x_1^{m_1}\, x_2^{m_2}\, \ldots\, x_{2d}^{m_{2d}}\,, \tag{48a}$$

$$|\boldsymbol{m}| = m_1 + m_2 + \ldots + m_{2d} \tag{48b}$$

with the integer vector $\boldsymbol{m} \in \mathbb{N}_0^{2d}$ is used. The purpose of the following normal form transformation is that – for given expansion coefficients $\alpha_{\boldsymbol{m}k}$ and $\xi_{\boldsymbol{m}k}$ – the coefficients $\gamma_{\boldsymbol{m}k}$ of the generating function are chosen in such a way that as many as possible of the resulting coefficients $\beta_{\boldsymbol{m}k}$ vanish, and that they are connected to the energy functional via canonical equations.

Definition. *Define the set $\mathcal{M}$ of integer vectors by*

$$\mathcal{M} \equiv \left\{ \boldsymbol{m} \in \mathbb{N}^{2d} \,\middle|\, m_{2j-1} = m_{2j}\,;\, j = 1, 2, \ldots, d \right\}\,. \tag{49}$$

Then the transformed dynamical equation take the following form.

Theorem 2 (Polynomial structure of the transformed dynamical equations)**.** *If the eigenvalues λ_i of the linearized dynamical equations are pair-wise rationally independent (i.e. $\lambda_i/\lambda_j \notin \mathbb{Q}$, of all pairs of eigenvalues $i \neq j$), an appropriate generating function $\boldsymbol{g}$ transforms the vector field $\boldsymbol{a}$ into the general polynomial structure (cf. Table 1)*

$$b_{n(2i-1)} = \sum_{\substack{\boldsymbol{m}\in\mathcal{M},\\ |\boldsymbol{m}|=n+1,\\ \textit{nonneg.}}} \beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}\, \boldsymbol{x}^{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}]}\,, \tag{50a}$$

$$b_{n(2i)} = \sum_{\substack{\boldsymbol{m}\in\mathcal{M},\\ |\boldsymbol{m}|=n+1,\\ \textit{nonneg.}}} \beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)}\, \boldsymbol{x}^{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}]}\,. \tag{50b}$$

with $i = 1, 2, \ldots, d$. Here, the summation is carried out over the set (49) *and $\hat{\boldsymbol{e}}_{2i-1}$ as well as $\hat{\boldsymbol{e}}_{2i}$ are unit vectors. Moreover, the constraint "nonneg." in the summation denotes to add only those terms for which the indices $[\boldsymbol{m} - \hat{\boldsymbol{e}}_{2i}]$ and $[\boldsymbol{m} - \hat{\boldsymbol{e}}_{2i-1}]$ only have nonnegative entries, i. e. those $\boldsymbol{m} \in \mathcal{M}$ with $m_{2i-1} = m_{2i} = 0$ are not taken into account. An equivalent interpretation of this constraint is to set all terms $\beta_{\boldsymbol{m}k}$ to zero, if its index $\boldsymbol{m}$ possesses at least one negative entry.*

Proof. One can specifically transform the n-th order of the original vector field $\boldsymbol{a}_n$, if the generating function is chosen to be homogeneous of degree n,

$$\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{g}_n(\boldsymbol{x}) = \sum_{|\boldsymbol{m}|=n} \boldsymbol{\gamma}_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}\,. \tag{51}$$

Inserting the multivariate polynomials (47) with the constraint (51) for the generating function into Eq. (43), one obtains, after renaming $\boldsymbol{y}$ by $\boldsymbol{x}$, the homological equation

$$\boldsymbol{b}_n(\boldsymbol{x}) = \boldsymbol{a}_n(\boldsymbol{x}) + \mathcal{L}_{\boldsymbol{g}_n}\, \boldsymbol{a}_1(\boldsymbol{x}) \tag{52}$$

for the transformation of the monomials which are equal to the degree of the generating function. From this, the transformation of the single coefficients can be extracted. For the k-th component ($k = 1, 2, \ldots, 2d$) it reads

$$\beta_{\boldsymbol{m}k} = \alpha_{\boldsymbol{m}k} + \left(\lambda_k^{\pm} - \left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle\right) \gamma_{\boldsymbol{m}k}\,. \tag{53}$$

where $\left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle$ is the standard scalar product. One can see from Eq. (53) that a nonvanishing monomial ($\alpha_{\boldsymbol{m}k} \neq 0$) can be eliminated ($\beta_{\boldsymbol{m}k} = 0$) by the Lie transform with an appropriate choice of the generating function, if the eigenvalue $\lambda_k^{\pm}$ is "nonresonant", i. e. if

$$\lambda_k^{\pm} - \left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle \neq 0\,. \tag{54a}$$

Otherwise, if the condition of resonance

$$\lambda_k^{\pm} - \left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle = 0 \tag{54b}$$

is fulfilled, the respective term cannot be eliminated. The final polynomial structure of the normal form of the local dynamical equations is determined by the eigenvalues of the linearised equations of motion, because only monomials fulfilling Eq. (54b) remain after the Lie transforms. Moreover, due to the fact that these eigenvalues exhibit the general structure (31) of pairwise eigenvalues with different sign, the normal form also possesses a general polynomial structure. Denoting the entries of the integer vector by $\boldsymbol{m} = (m_1, m_2, \ldots, m_{2d})^{\mathsf{T}}$, the condition of resonance (54b) becomes ($i = 1, 2, \ldots, d$)

$$\left[\lambda_1(m_1 - m_2) + \lambda_2(m_3 - m_4) + \ldots + \lambda_d(m_{2d-1} - m_{2d})\right] = \pm\lambda_i\,, \tag{55}$$

where the upper sign is valid for $k = 2i - 1$ and the lower one for $k = 2i$. Assuming pair-wise rational independence of the eigenvalues, Eq. (55) is fulfilled if and only if

$$m_{2i-1} = m_{2i} \pm 1\,, \qquad (i = 1, 2, \ldots, d)\,, \tag{56a}$$

$$m_{2j-1} = m_{2j}\,, \qquad (j \neq i)\,. \tag{56b}$$

□

Table 1. Illustration of the fundamental polynomial structure of the dynamical equations (50) and the energy functional (58) for a system with $d = 2$ degrees of freedom. In normal form coordinates, there remain only terms with odd degree of the monomial in the equations of motion. Moreover, the exponents of the variables x_{2i-1}, x_{2i} in the respective component of the vector field differ by one and the terms x_{2j-1}, x_{2j} with $j \neq i$ (displayed in brackets) have the same exponent. By contrast, the energy functional only consists of monomials with even degree and all variables x_{2j-1}, x_{2j} occur in products. The extension of this structure to $d > 2$ degrees of freedom is straightforward. In this case, additional terms $(x_5x_6), (x_7x_8), \ldots$ occur in the expansions.

	Degree n of the monomial						
Field	0	1	2	3	4	5	6
$\dot{x}_1$	–	x_1	–	$x_1^2x_2^1(x_3x_4)^0$ $x_1^1x_2^0(x_3x_4)^1$	–	$x_1^3x_2^2(x_3x_4)^0$ $x_1^2x_2^1(x_3x_4)^1$ $x_1^1x_2^0(x_3x_4)^2$	–
$\dot{x}_2$	–	x_2	–	$x_1^1x_2^2(x_3x_4)^0$ $x_1^0x_2^1(x_3x_4)^1$	–	$x_1^2x_2^3(x_3x_4)^0$ $x_1^1x_2^2(x_3x_4)^1$ $x_1^0x_2^1(x_3x_4)^2$	–
$\dot{x}_3$	–	x_3	–	$x_3^2x_4^1(x_1x_2)^0$ $x_3^1x_4^0(x_1x_2)^1$	–	$x_3^3x_4^2(x_1x_2)^0$ $x_3^2x_4^1(x_1x_2)^1$ $x_3^1x_4^0(x_1x_2)^2$	–
$\dot{x}_4$	–	x_4	–	$x_3^1x_4^2(x_1x_2)^0$ $x_3^0x_4^1(x_1x_2)^1$	–	$x_3^2x_4^3(x_1x_2)^0$ $x_3^1x_4^2(x_1x_2)^1$ $x_3^0x_4^1(x_1x_2)^2$	–
E	const.	–	$(x_1x_2)^1$ $(x_3x_4)^1$	–	$(x_1x_2)^2(x_3x_4)^0$ $(x_1x_2)^1(x_3x_4)^1$ $(x_1x_2)^0(x_3x_4)^2$	–	$(x_1x_2)^3(x_3x_4)^0$ $(x_1x_2)^2(x_3x_4)^1$ $(x_1x_2)^1(x_3x_4)^2$ $(x_1x_2)^0(x_3x_4)^3$

Definition. *In the following, monomials $\boldsymbol{x}^{\boldsymbol{m}}$ whose integer vector $\boldsymbol{m}$ fulfils Eq.* (54a) *are referred to as "nonresonant monomials" and those fulfilling Eq.* (54b) *are called "resonant monomials". Analogously, their coefficients are referred to as nonresonant and resonant coefficients, respectively.*

Definition. *The vector field $\boldsymbol{a}$ is said to be in normal form with respect to its linear part $\boldsymbol{a}_1$, if it only contains monomials fulfilling Eq.* (54b).

Concluding, in normal form coordinates, the variables x_{2i-1}, x_{2i} in the respective component of the dynamical equations occur with exponents which differ exactly by one, while the terms x_{2j-1}, x_{2j} with $j \neq i$ have the same exponent (cf. Table 1). Note that all monomials remaining in Eqs. (50) are of odd degree. All terms of even degree have been eliminated completely by the Lie transforms, because the condition of resonance (54b) cannot be fulfilled, if $|\boldsymbol{m}|$ is even.

3.2.2. Determination of the generating function to eliminate the nonresonant terms After having discussed the general structure of the normal form, its actual calculation is presented in this section. The calculation will be carried out order by order, i. e. the orders $n = 2, 3, 4, \ldots$ are treated successively. It is assumed that the system is already in normal form up to the order $n - 1$. Then, a generating function $\boldsymbol{g}_n$ is constructed to transform the n-th order of the equations of motion.

As already mentioned above, the coefficients $\gamma_{\boldsymbol{m}k}$ of the generating function which are nonresonant, i. e. Eq. (54a) is valid, can be chosen in such a way that the corresponding term $\alpha_{\boldsymbol{m}k}$ of the original expansion is eliminated. Such nonresonant coefficients occur in every order of the expansion. In particular, the generating function of each even degree n only consists of nonresonant coefficients. The determination of the nonresonant coefficients $\gamma_{\boldsymbol{m}k}$ of the generating function is straightforward. Since their purpose is to eliminate the original term $\alpha_{\boldsymbol{m}k}$, they are uniquely determined by Eq. (53). Requiring $\beta_{\boldsymbol{m}k} = 0$ and solving for the coefficient of the generating function (51), one obtains

$$\gamma_{\boldsymbol{m}k} = \begin{cases} \dfrac{\alpha_{\boldsymbol{m}k}}{\left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle - \lambda_k^{\pm}}, & \text{if } \lambda_k^{\pm} - \left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle \neq 0\,, \\ c_{\boldsymbol{m}k}\,, & \text{else.} \end{cases} \tag{57}$$

The choice in the first line guarantees the elimination of the term $\alpha_{\boldsymbol{m}k}$ in the nonresonant case. All coefficients $c_{\boldsymbol{m}k}$ related to the resonant terms are free parameters, which do not change the $\beta_{\boldsymbol{m}k}$ of the order $|\boldsymbol{m}| = n$. For simplicity these terms are set to $c_{\boldsymbol{m}k} = 0$ in the transformations of the nonresonant coefficients and their final determination will be treated separately (see Sec. 3.3).

Theorem 3 (Polynomial structure of the transformed energy functional)**.** *The application of the generating function* $\boldsymbol{g}$ *with coefficients fulfilling Eq.* (57) *to the energy functional, transforms the latter into the general polynomial structure (cf. Table 1)*

$$E_{n+1}(\boldsymbol{x}) = \sum_{\substack{\boldsymbol{m} \in \mathcal{M} \\ |\boldsymbol{m}| = n+1}} \xi_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}\,. \tag{58}$$

Proof. As already mentioned in Sec. 2, the symplectic 2-form (18) is skew-symmetric, nondegenerate, and closed. Therefore, Darboux' theorem guarantees the existence of canonical coordinates fulfilling the relation (22). Any polynomial structure differing from Eq. (58) would result in terms that have no relation in the corresponding dynamical equations (50) and would, therefore, violate Darboux' theorem. □

3.3. Normal form transformations – resonant terms

In normal form coordinates the dynamical equations (50) and the energy functional (58) naturally exhibit a polynomial structure that allows for the identification of the normal form coordinates as canonical ones according to the canonical equation

$$\boldsymbol{b}_n(\boldsymbol{x}) = \mathcal{J}\, \frac{\partial}{\partial \boldsymbol{x}}\, E_{n+1}(\boldsymbol{x}) \tag{59}$$

with the energy functional acting as Hamiltonian. Equation (59) is valid in each order n, if the coefficients $\beta_{\boldsymbol{m}k}$ and $\xi_{\boldsymbol{m}}$ in Eqs. (50) and (58) fulfil the conditions

$$m_{2i}\xi_{\boldsymbol{m}} = \beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}\,, \tag{60a}$$

$$\beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)} = -\beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)}\,, \tag{60b}$$

$$\frac{\beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}}{m_{2i}} = \frac{\beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2j}](2j-1)}}{m_{2j}} \tag{60c}$$

for all $i, j = 1, 2, \ldots, d$ $(i \neq j)$ and $\boldsymbol{m} \in \mathcal{M}$ with $|\boldsymbol{m}| = n + 1$. Here, Eq. (60a) is the requirement that the coefficients of the dynamical equations and those of the energy functional are connected via derivatives according to Eqs. (59). The sign structure of the symplectic matrix $\mathcal{J}$ is taken into account by Eq. (60b) for each pair x_{2i-1}, x_{2i} of "conjugate coordinates", and Eq. (60c) considers the fact that terms in the expansion of *different* pairs x_{2i-1}, x_{2i} and x_{2j-1}, x_{2j} $(i \neq j)$ result from the *same* term of the energy functional.

As a consequence of the normal form expansion together with the general eigenvalue structure (31), Eq. (60b) is fulfilled after the Lie transforms have been applied as discussed in Sec. 3.2. However, the conditions (60a) and (60c) are *not* fulfilled, in general. This is due to the fact that – although the polynomial structure of the expansions is uniquely determined by the eigenvalue structure – the explicit normal form, i.e. the coefficients of the expansion, are not unique. The reason is that the resonant coefficients $c_{\boldsymbol{m}k}$ of the generating function in Eq. (57) are free, and that the choice to set them zero does not guarantee the fulfilment of all Eqs. (60). Therefore, further steps are necessary in order to guarantee that the latter are valid, and these steps are presented in the following.

We emphasize that it is precisely this treatment of the resonant terms of the generating function which is the difference between the usual normal form procedure of canonical Hamiltonians and the transformation of the noncanonical system: If the coordinates had been canonical at the beginning, the choice $c_{\boldsymbol{m}k} = 0$ in Eq. (57) would have kept this property. Vice versa, we will use an appropriate choice $c_{\boldsymbol{m}k} \neq 0$ in the following to generate canonical coordinates.

3.3.1. Particular choice of the resonant generating function and the corresponding transformations Resonant terms occur in every odd order $n = 3, 5, 7, \ldots$ of the generating function (51), and a fundamental property of them is the fact that they do not affect the polynomial structure of the expansions, but they only modify their coefficients. Vice versa, this property can be used in order to guarantee the fulfilment of the canonical equations (60) by a suitable choice of the resonant terms as it will be demonstrated in the following. For this purpose, it is investigated in detail in this section how a resonant generating function of degree n transforms the next-higher order terms of the dynamical equations as well as the energy functional. Finally, Eqs. (60) will serve as conditional equations for the determination of the resonant coefficients.

In a resonant generating function of degree n, there occur coefficients $\gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}$ and $\gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)}$ with $\boldsymbol{m} \in \mathcal{M}$ and $|\boldsymbol{m}| = n+1$, i.e. there is exactly one term corresponding to each of the monomials remaining in the dynamical equations (50). In order to guarantee that Eqs. (60) hold for the whole expansion, it will be sufficient only to consider the terms $\gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}$ and to set $\gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)} = 0$ for simplicity. With this choice, the resonant generating function homogeneous of degree n has the form

$$g_{n(2i-1)}(\boldsymbol{x}) = \sum_{\substack{\boldsymbol{m}\in\mathcal{M},\\ |\boldsymbol{m}|=n+1,\\ \text{nonneg.}}} \gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}\, \boldsymbol{x}^{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}]}\,, \tag{61a}$$

$$g_{n(2i)}(\boldsymbol{x}) = 0\,. \tag{61b}$$

It is easily verified from Eq. (46) that the j-fold application $\mathcal{D}^j_{\boldsymbol{g}_n} E_k$ of the right-

multiplication operator with a generating function homogeneous of degree n onto the part of the energy functional of degree k results in a polynomial homogeneous of degree $k + j(n-1)$. Furthermore, the lowest order which is affected in Eq. (45) is $n+1$. Consequently, there are two cases which contribute to the order $n+1$ of the transformed field, namely those with $k + j(n-1) \stackrel{!}{=} n+1$. On the one hand, this is the contribution $k = n+1$ and $j = 0$, on the other hand it is $k = 2$ and $j = 1$, so that the precise transformation reads

$$\tilde{E}_{n+1}(\boldsymbol{x}) = E_{n+1}(\boldsymbol{x}) + \mathcal{D}_{\boldsymbol{g}_n} E_2(\boldsymbol{x})\,, \tag{62}$$

where $\tilde{E}_{n+1} = \sum_{|\boldsymbol{m}|=n+1} \tilde{\xi}_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}$ is the transformed field. Inserting the expansions (47) into Eq. (62), and using the fact that the second order of the energy functional has the form $E_2 = \sum_{i=1}^{d} \lambda_i\, x_{2i-1}\, x_{2i}$ in normal form coordinates, Eq. (62) can directly be reformulated in terms of the energy functional's coefficients:

$$\tilde{\xi}_{\boldsymbol{m}} = \xi_{\boldsymbol{m}} + \sum_{\substack{i=1,\\ \text{nonneg.}}}^{d} \lambda_i\, \gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)}\,. \tag{63}$$

Analogously, the effect of a resonant generating function onto the dynamical equations can be investigated. If the latter are already in their normal form (50), there are only odd degrees of the expansion $\boldsymbol{b}_1, \boldsymbol{b}_3, \boldsymbol{b}_5, \ldots$ left as discussed above. By definition, the first-order term $\boldsymbol{b}_1$ containing the eigenvalues does not contribute to the Lie operator for a resonant generating function, i. e. $\mathcal{L}_{\boldsymbol{g}_n} \boldsymbol{b}_1 = 0$. This identity directly follows from Eq. (53), because the resonant coefficients are always multiplied by zero. Therefore, the lowest-order term which leads to a contribution of the Lie operator is the term $\boldsymbol{b}_3$. From Eq. (43) it follows that the lowest-order term which is modified by a resonant generating function of degree n together with $\boldsymbol{b}_3$ is the order $n+2$ of the dynamical equations,

$$\tilde{\boldsymbol{b}}_{n+2}(\boldsymbol{x}) = \boldsymbol{b}_{n+2}(\boldsymbol{x}) + \mathcal{L}_{\boldsymbol{g}_n} \boldsymbol{b}_3(\boldsymbol{x})\,. \tag{64}$$

Multiple applications of the Lie operator as well as higher-order terms $\boldsymbol{b}_n$ with $n > 3$ lead to higher-order corrections and do not need to be considered here. Analogously to the energy functional, this transformation can be rewritten directly in terms of the vector field's coefficients. After a short calculation, one obtains

$$\tilde{\beta}_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)} = \beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)} + \sigma_{\boldsymbol{m}(2i-1)}\,, \tag{65a}$$

$$\tilde{\beta}_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)} = \beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)} + \sigma_{\boldsymbol{m}(2i)} \tag{65b}$$

with the quantities

$$\begin{aligned}\sigma_{\boldsymbol{m}(2i-1)} \equiv \sum_{\substack{\boldsymbol{m}''\in\mathcal{M},\\ |\boldsymbol{m}''|=4,\\ \text{nonneg.}}} \Bigg[& -(m''_{2i}-1)\,\beta_{[\boldsymbol{m}''-\hat{\boldsymbol{e}}_{2i-1}](2i)}\,\gamma_{[\boldsymbol{m}-\boldsymbol{m}''+\hat{\boldsymbol{e}}_{2i-1}](2i-1)} \\ & + \sum_{\substack{i'=1\\ i'\neq i}}^{d} m''_{2i'} \Big(\beta_{[\boldsymbol{m}''-\hat{\boldsymbol{e}}_{2i}](2i-1)}\,\gamma_{[\boldsymbol{m}-\boldsymbol{m}''+\hat{\boldsymbol{e}}_{2i'-1}](2i'-1)} \\ & \qquad -\beta_{[\boldsymbol{m}''-\hat{\boldsymbol{e}}_{2i'}](2i'-1)}\,\gamma_{[\boldsymbol{m}-\boldsymbol{m}''+\hat{\boldsymbol{e}}_{2i'-1}+\hat{\boldsymbol{e}}_{2i'}-\hat{\boldsymbol{e}}_{2i}](2i-1)} \\ & \qquad -\beta_{[\boldsymbol{m}''-\hat{\boldsymbol{e}}_{2i'-1}](2i')}\,\gamma_{[\boldsymbol{m}-\boldsymbol{m}''+\hat{\boldsymbol{e}}_{2i'-1}+\hat{\boldsymbol{e}}_{2i'}-\hat{\boldsymbol{e}}_{2i}](2i-1)}\Big)\Bigg]\,,\end{aligned} \tag{66a}$$

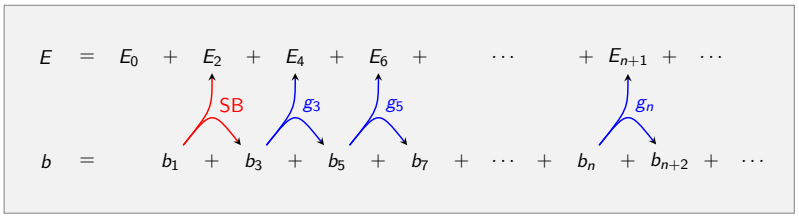

Figure 2. Scheme of the procedure to determine the resonant coefficients of the generating function. In each order $n \geq 3$, it is assumed that the term $\boldsymbol{b}_n$ of the dynamical equations fulfils Eqs. (60b) and (60c). Then, the resonant coefficients of the generating function are determined using the part E_{n+1} of the energy functional and the next-higher order term $\boldsymbol{b}_{n+2}$ of the equations of motion (blue). The resonant generating function is constructed in a way that $\boldsymbol{b}_n$ as well as E_{n+1} are connected via the canonical equation (59) and that Eqs. (60b) and (60c) are valid for the term $\boldsymbol{b}_{n+2}$. The whole procedure is applied successively for the orders $n = 3, 5, 7, \ldots$ Note that the same conditions are fulfilled automatically for the terms $\boldsymbol{b}_1$, E_2, and $\boldsymbol{b}_3$, if the symplectic basis (SB; red) is made use of as discussed in Sec. 3.1.

$$\sigma_{\boldsymbol{m}(2i)} \equiv \sum_{\substack{\boldsymbol{m}''\in\mathcal{M},\\ |\boldsymbol{m}''|=4,\\ \text{nonneg.}}} \Bigg[(m''_{2i}-1)\,\beta_{[\boldsymbol{m}''-\hat{\boldsymbol{e}}_{2i-1}](2i)}\,\gamma_{[\boldsymbol{m}-\boldsymbol{m}''+\hat{\boldsymbol{e}}_{2i-1}](2i-1)} + \sum_{\substack{i'=1\\ i'\neq i}}^{d} m''_{2i'}\,\beta_{[\boldsymbol{m}''-\hat{\boldsymbol{e}}_{2i-1}](2i)}\,\gamma_{[\boldsymbol{m}-\boldsymbol{m}''+\hat{\boldsymbol{e}}_{2i'-1}](2i'-1)} \Bigg] . \tag{66b}$$

It is emphasized that $\sigma_{\boldsymbol{m}(2i-1)}$ and $\sigma_{\boldsymbol{m}(2i)}$ depend on the resonant coefficients $\gamma_{\boldsymbol{m}k}$ *linearly* and that only the third-order coefficients $\beta_{\boldsymbol{m}k}$ occur therein.

3.3.2. Determination of the generating function's resonant coefficients As already mentioned above, the resonant coefficients of each generating function are free parameters, in the sense that they do neither change the polynomial structure of the dynamical equations nor that of the energy functional. However, they do modify the coefficients of the respective expansions.

Theorem 4 (Choice of the resonant generating function)**.** *The choice of the resonant coefficients of the generating function according to*

$$\gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i-1}](2i)} = 0 \tag{67a}$$

$$\sum_{\substack{i=1\\ \text{nonneg.}}}^{d} \lambda_i \gamma_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)} = \tilde{\xi}_{\boldsymbol{m}} - \xi_{\boldsymbol{m}}\,, \tag{67b}$$

$$m_{2j}\,\sigma_{\boldsymbol{m}(2i-1)} - m_{2i}\,\sigma_{\boldsymbol{m}(2j-1)} = m_{2i}\,\beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2j}](2j-1)} - m_{2j}\,\beta_{[\boldsymbol{m}-\hat{\boldsymbol{e}}_{2i}](2i-1)} \tag{67c}$$

guarantees that all the conditions of integration (60) *are fulfilled, i. e. the final set of coordinates are standard canonical coordinates.*

Proof. The proof works as follows (see Fig. 2):

(i) It is assumed that Eqs. (60b) and (60c) are fulfilled for $|\boldsymbol{m}| = n+1$, i.e. the respective term of the dynamical equations can be written as a symplectic gradient

$$\boldsymbol{b}_n(\boldsymbol{x}) = \mathcal{J}\frac{\partial}{\partial \boldsymbol{x}}\tilde{E}_{n+1}(\boldsymbol{x}) \tag{68}$$

with a scalar function $\tilde{E}_{n+1} = \sum_{|\boldsymbol{m}|=n+1} \tilde{\xi}_{\boldsymbol{m}}\, \boldsymbol{x}^{\boldsymbol{m}}$. Note that the latter does not need to be identical to the energy functional, $\tilde{E}_{n+1} \neq E_{n+1}$.

(ii) Replacing $\beta_{\boldsymbol{m}k} \to \tilde{\beta}_{\boldsymbol{m}k}$ and $\xi_{\boldsymbol{m}} \to \tilde{\xi}_{\boldsymbol{m}}$, Eq. (60a) with $|\boldsymbol{m}| = n+1$ as well as (60c) with $|\boldsymbol{m}| = n+2$ are used as conditional equations for the determination of the resonant coefficients of the order n. These equations form a linear system of equations with the resonant coefficients being the variables.

(iii) By construction of step (ii), the assumption in step (i) is fulfilled in the next-higher order $n+2$. Therefore, the procedure can be repeated successively for the orders $n = 3, 5, 7, \ldots$

After having calculated the term $\tilde{E}_{n+1}$ in step (i), the system of equations in step (ii) can be set up by inserting Eqs. (63) and (65) into the Eqs. (60a) and (60c) after having replaced $\beta_{\boldsymbol{m}k} \to \tilde{\beta}_{\boldsymbol{m}k}$ and $\xi_{\boldsymbol{m}} \to \tilde{\xi}_{\boldsymbol{m}}$.

Equation (67b) must hold for all $|\boldsymbol{m}| = n+1$ and Eq. (67c) for all $|\boldsymbol{m}| = n+2$ as well as $i, j = 1, \ldots, d$ with $i \neq j$. Equations (67) are written in a way that all terms which depend on the resonant coefficients $\gamma_{\boldsymbol{m}k}$ occur on the left-hand side, while the right-hand side is independent of these terms. Because of the fact that the resonant coefficients enter Eqs. (67) linearly according to Eqs. (66), they form a linear system of equations which can formally be written as

$$\mathcal{A}\,\mathcal{G} = \mathcal{B}\,. \tag{69}$$

Here, the matrix $\mathcal{A}$ and the vector $\mathcal{B}$ are both determined by the known quantities $\beta_{\boldsymbol{m}k}$, λ_i, $\xi_{\boldsymbol{m}}$, $\tilde{\xi}_{\boldsymbol{m}}$, and m_k. All the unknown terms, i.e. the resonant coefficients $\gamma_{\boldsymbol{m}k}$, are collected in the vector $\mathcal{G}$. The number of the resonant coefficients is, in general, smaller than the number of equations, so that the system (69) is overdetermined. However, it is guaranteed by Darboux's theorem that there exists a solution, because otherwise the latter would be violated and it would not be possible to construct canonical coordinates. □

We note that it is appropriate to solve Eq. (69) via a least-square fit $\|\mathcal{A}\mathcal{G} - \mathcal{B}\| \stackrel{!}{=} \min$. The minimum of this fit must be zero because of Darboux's theorem, and its actual value in a numerical implementation is a measure of success of the procedure. After the resonant coefficients of a certain degree n have been determined as the solutions of Eq. (69), the corresponding transformation needs to be applied to the full expansion, i.e. Eqs. (43) and (45) must be evaluated.

3.4. Canonical torus structure of the noncanonical Hamiltonian system

After the normal form expansion has been applied as discussed in Secs. 3.2 and 3.3, the normal form coordinates are canonical ones by construction. The expansions fulfil the canonical equations (59) in every order n with the energy functional acting as Hamiltonian

$$H = E(\boldsymbol{x})\,. \tag{70}$$

Theorem 5 (Final structure of the normal form Hamiltonian)**.** *In the final set of coordinates, the products $x_{2i-1}x_{2i}$ are constants of motion and the transformed energy functional is dierctly given in terms of action variables $\boldsymbol{J}$,*

$$H = E(\boldsymbol{J}) = \sum_{n=0}^{m} E_n(\boldsymbol{J})\,. \tag{71}$$

Proof. Because of the summation over $\boldsymbol{m} \in \mathcal{M}$ in Eq. (58), this Hamiltonian only consists of monomials

$$\boldsymbol{x}^{\boldsymbol{m}}\big|_{\boldsymbol{m}\in\mathcal{M}} = \prod_{i=1}^{d}(x_{2i-1}x_{2i})^{m_{2i}} \equiv \prod_{i=1}^{d}(q_i\,p_i)^{m_{2i}}\,, \tag{72}$$

where the normal form coordinates can be interpreted pairwise as standard canonical coordinates $q_i \equiv x_{2i-1}$ and $p_i \equiv x_{2i}$ in the last step. Moreover, these products directly define action variables

$$J_i \equiv \begin{cases} q_i p_i\,, & \lambda_i = \kappa_i \quad (\kappa_i \in \mathbb{R})\,, \\ \mathrm{i}q_i p_i\,, & \lambda_i = \mathrm{i}\omega_i \quad (\omega_i \in \mathbb{R})\,, \end{cases} \tag{73}$$

where the imaginary unit in the definition compensates the respective contribution of each purely imaginary eigenvalue. If all the action variables correspond to stable oscillations of the system, and denoting the corresponding angle variables by φ_i, the dynamical equations are

$$\dot{\varphi}_i = \quad \frac{\partial H(\boldsymbol{J})}{\partial J_i} \equiv \omega_i(\boldsymbol{J})\,, \tag{74a}$$

$$\dot{J}_i = -\frac{\partial H(\boldsymbol{J})}{\partial \varphi_i} = 0\,, \tag{74b}$$

where $\omega_i(\boldsymbol{J})$ are the characteristic frequencies of the system. These have the solution

$$\varphi_i(t) = \omega_i t + \varphi_i(0)\,, \tag{75a}$$

$$J_i(t) = \text{const.} \tag{75b}$$

□

In normal form coordinates, the dynamics of the system is restricted to a d-dimensional torus $\mathcal{T}^d$ if all eigenvalues are purely imaginary. If k of the actions (73) correspond to real eigenvalues, then the dynamics takes place on a manifold with the structure $\mathcal{T}^{d-k} \times \mathbb{R}^k$. As already mentioned above, an important case in the field of reaction dynamics in variational space is that of rank-1 saddle points ($k = 1$). These form transition states where the reaction channel is given by the unstable direction of the saddle. If the normal form Hamiltonian (71) has been constructed at such a point the corresponding quantum reaction rate is directly given by Eqs. (2) and (3).

We finally note that our procedure basically also applies if the original coordinates are canonical ones and in this case, the procedure presented here merges the treatment already described by Waalkens *et al* [15]. Technically, this is expressed in the relation that, for canonical coordinates, the generating function W in Eq. (1) is a special case of the generator $\boldsymbol{g}$. The precise relation between the respective generating functions is then $\boldsymbol{g}(\boldsymbol{x}) = \mathcal{J} \times [\partial W(\boldsymbol{x})/\partial \boldsymbol{x}]$ in which all resonant terms $\gamma_{\boldsymbol{m}i}$ in Eq. (67) are identically zero.

3.5. Implementation

The procedure to construct local normal form Hamiltonians in action-angle variables presented above has the advantage that it can step-by-step be implemented using symbolic computations. In the appendix, we provide both an exemplary code in the script language MATHEMATICA which allows for the constructive application of the symbolic computation scheme in arbitrary normal form orders m and for arbitrary degrees of freedom d as well as the intermediate numerical results of the procedure. As input, the code uses the definitions of the matrix K, the vector $\boldsymbol{h}$ in Eqs. (16) and the energy functional (8), as well as the values of the respective degrees of freedom and the desired normal form order. The output is the normal form Hamiltonian (71) in action-angle coordinates. This general numerical implementation allows for practical applications of the procedure, such as e. g. the calculation of thermal decay rates in Bose-Einstein condensates in Refs. [38–42].

4. Conclusion and outlook

In this paper, we have demonstrated a general method to construct local, canonical coordinates in the vicinity of a fixed point of a noncanonical Hamiltonian system via normal form expansions. The method allows for the general and systematic investigation of e. g. quantum systems which are described within a variational approach. It is applicable for systems with arbitrary degrees of freedom, in arbitrary order of the local expansion, it is independent of the precise form of the Hamilton operator, and it can be implemented in symbolic computations step by step.

Extensions and generalizations of the procedure will be necessary in case of zero-eigenvalues [$\lambda_i = 0$ in Eq. (31)], degenerate ones or in case of higher-order resonances $\left(\left\langle \boldsymbol{m}, \boldsymbol{\lambda}^{\pm} \right\rangle = \lambda_k^{\pm}\right)$. This would allow one to construct the system's canonical normal form also in situations with strong mode coupling of the different degrees of freedom. Further reductions of the constructed normal form Hamiltonian can be performed e. g. using the methods of hypernormal forms and spectral sequences [45–49] which can also be used in case of zero-eigenvalues of the linearised system.

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Appendix A. Numerical example

In this appendix, a numerical example of the normal form procedure discussed in the present paper is presented. In the following, both an exemplary MATHEMATICA script code as well as important intermediate results of the calculations are shown.

The system considered is a BEC with additional $1/r$-interaction which has already been discussed in detail in Ref. [41], and it is described within a variational approach

(7) consisting of $N_\mathrm{g} = 2$ coupled Gaussian wave functions,

$$\psi(\boldsymbol{r},t) = \sum_{k=1}^{N_\mathrm{g}} g_k(\boldsymbol{r},t) \quad \text{with} \quad g_k = \mathrm{e}^{-a_k r^2 + \gamma_k} \,. \tag{A.1}$$

A detailed description of the variational approach's application is also given in Ref. [41], so that we concentrate in the following on the normal form procedure. Note further that we set the physical parameters in Ref. [41] to $\gamma_\mathrm{trap}^2 = 2.5 \times 10^{-4}$ and $a = -0.99$.

A MATHEMATICA script can be set up as follows: In a first step, the global parameters for the number N_g of coupled Gaussian wave functions, the number of degrees of freedom d, the physical parameters $a, \gamma_\mathrm{trap}^2$ in the GPE as well as the maximum normal form order n_max are set:

```
Ng      = 2;
d       = 2Ng-1;
a       = -0.99;
γtrap2  = 2.5×10^-4;
nmax    = 7;
```

Furthermore, the following commands are defined for the use in the subsequent script code:

```
x     = ToExpression["x" <> ToString[#]] &/@ Range[2d];
y     = ToExpression["y" <> ToString[#]] &/@ Range[2d];
m     = ToExpression["m" <> ToString[#]] &/@ Range[2d];

ytox  = ToExpression["y" <> ToString[#] <> "→x" <>
        ToString[#]] &/@ Range[2d];
xtoy  = ToExpression["x" <> ToString[#] <> "→y" <>
        ToString[#]] &/@ Range[2d];
xoddtozero = ToExpression["x" <> ToString[2#-1] <>
             "→0"] &/@ Range[d];
meventoodd = ToExpression["m" <> ToString[2#] <> "→m" <>
             ToString[2#-1]] &/@ Range[d];
xtoj  = ToExpression["x" <> ToString[2#-1] <> "→j" <>
        ToString[#] <> "/x" <> ToString[2#]] &/@ Range[d];
z     = ToExpression["{a" <> ToString[#] <> ",γ" <>
        ToString[#] <> "}"] &/@ Range[Ng]/.γ1→0
pwr[x_, m_] := Product[x[[i]]^m[[i]], {i,2d}];
```

In order to evaluate the expectation values (8) of the single contributions of the Hamilton operator, it is appropriate to define the auxiliary functions

```
i0[{a_,γ_}] := (π/a) Sqrt[π/a] Exp[-γ];
i2[{a_,γ_}] := (3π/(2a^2)) Sqrt[π/a] Exp[-γ];
im[{a_,γ_}] := π Sqrt[π/a] Exp[-γ];
```

with which the norm of the wave function and the normalized expectation values (8) can be evaluated as follows:

```
ξ[k_,l_] := z[[k]] + ComplexExpand[Conjugate[z[[l]]]];
ξ[i_,j_,k_,l_] := z[[i]] + ComplexExpand[Conjugate[z[[j]]]] +
                  z[[k]] + ComplexExpand[Conjugate[z[[l]]]];

N2    = Sum[ i0[ξ[k,l]] , {k,Ng}, {l,Ng}];
```

```
Ekin  = Sum[ 6z[[k,1]] i0[ξ[k,1]] - 4z[[k,1]]^2 i2[ξ[k,1]]
           , {k,Ng}, {l,Ng}] / N2;

Etrap = γtrap2 Sum[ i2[ξ[k,1]] , {k,Ng}, {l,Ng}] / N2;

Ec    = 8πa / N2^2
        Sum[ i0[ξ[i,j,k,l]], {i,Ng}, {j,Ng}, {k,Ng}, {l,Ng}];

Emon  = -4π Sum[ im[ξ[i,j,k,l]] / (ξ[i,j][[1]] ξ[k,l][[1]])
                , {i,Ng}, {j,Ng}, {k,Ng}, {l,Ng}] / N2^2;
```

Therewith, the energy functional and the vector $\boldsymbol{h}$ in Eq. (16b) can be obtained by

```
Emf = Ekin + Eext + (Ec + Emon)/2;
h   = D[Emf, {Delete[Flatten[z], 2]}];
```

With an appropriate set of initial values `z0`, a root search yields the fixed point of the dynamical equations, and the fixed point energy is obtained by inserting the parameters into the energy functional:

```
fp   = FindRoot[h, z0];
emf0 = emf/.fp
```

For the above given physical parameters, one fixed point is

$$\texttt{a1} = \texttt{0.0631758}\,, \qquad \texttt{a2} = \texttt{0.215522}\,, \qquad \gamma\texttt{2} = \texttt{-0.481071}\,. \tag{A.2}$$

The normalization of the wave function at this fixed point is explicitly taken into account in the script by dividing the expectation values by `N2`. The fixed point corresponds to the ground state and it has an energy of

$$\texttt{emf0} = \texttt{-0.137356}\,. \tag{A.3}$$

After the fixed point has been determined it is shifted to the origin of the coordinate system:

```
yrel = ToExpression["y" <> ToString[2#-1] <> "+Iy" <>
       ToString[2#]] &/@Range[d];
yrel = Partition[Insert[yrel,0,2] ,2];
z2   = z + ϵ yrel /.fp;
z1   = z2 /.ytox;
```

Here, `z1` and `z2` are two independent sets of local coordinates at the fixed point. In the next step, the TDVP is set up in these local coordinates:

```
ξ[k_,l_] := z1[[k]] + ComplexExpand[Conjugate[z1[[l]]]];
ξ[i_,j_,k_,l_] := z1[[i]] + ComplexExpand[Conjugate[z1[[j]]]] +
                  z1[[k]] + ComplexExpand[Conjugate[z1[[l]]]];

N2    = Sum[ i0[ξ[k,l]] , {k,Ng}, {l,Ng}] // Simplify;

Ekin  = Sum[ 6z1[[k,1]] i0[ξ[k,l]] - 4z1[[k,1]]^2 i2[ξ[k,l]]
           , {k,Ng}, {l,Ng}] / N2;

Etrap = γ2 Sum[ i2[ξ[k,l]] , {k,Ng}, {l,Ng}] / N2;
```

```
Ec    = 8πa / N2^2
        Sum[ i0[ξ[i,j,k,l]] , {i,Ng}, {j,Ng}, {k,Ng}, {l,Ng}];

Emon  = -4π Sum[ im[ξ[i,j,k,l]] / (ξ[i,j] ξ[k,l])
                , {i,Ng}, {j,Ng}, {k,Ng}, {l,Ng}] / N2^2;
```

Therewith, the energy functional, the matrix K, as well as the vector $\boldsymbol{h}$ can be defined in local coordinates at the fixed point, and they are expanded up to the order $n_{\max}$:

```
(* Matrix K *)
S    = Simplify[Sum[ i0[(z1[[k]] +
       ComplexExpand[Conjugate[z2[[l]]]])] , {k,Ng}, {l,Ng}]];
Si   =  D[S, {x}] /.ytox;
Sj   =  D[S, {y}] /.ytox;
dnx  = -D[N2,{x}] / (2 Sqrt[N2]^3);
term = 2 Expand[(D[S,{x},{y}] /.ytox) / (N2 ϵ^2) +
       ( Outer[Times, Si/ϵ, dnx/ϵ] +
         Outer[Times, dnx/ϵ, Sj/ϵ] ) / Sqrt[N2]];

kcoef      = Table[0, {nmax}];
kcoef[[1]] = ComplexExpand[Im[Expand[term /.ϵ→0]]];

Do[ term       = D[term, ϵ]/(n-1);
    kcoef[[n]] = ComplexExpand[Im[Expand[term /.ϵ→0]]]
  , {n, 2, nmax}]

(* Vector h *)
hcoef = Table[0, {nmax}];
term  = D[Ekin + Etrap + (Ec + Emon)/2, ϵ];

Do[ term       = D[term, ϵ]/(n+1);
    hcoef[[n]] = ComplexExpand[Re[Expand[
                 -D[term /.ϵ→0, {x}]]]]
  , {n, nmax}];

(* Energy functional Emf *)
emfcoef = Table[0, {nmax-2}];
term    = D[Ekin + Etrap + (Ec + Emon)/2, ϵ];

Do[ term         = D[term, ϵ]/(n+1);
    emfcoef[[n]] = Expand[term /. ϵ→0]
  , {n, nmax-2}];

(* Increase precision *)
kcoef   = SetPrecision[kcoef   // Chop, 50];
hcoef   = SetPrecision[hcoef   // Chop, 50];
emfcoef = SetPrecision[emfcoef // Chop, 50];
```

Up to this point, the script is adapted to the special physical system of a BEC with $1/r$-interaction. The following script code, however, is independent of the system which is investigated. Only the structure of some do-loops has to be adapted if calculations are performed with $d \neq 3$ degrees of freedom.

Appendix A.1. Diagonalization and symplectic basis

After the steps performed above, the local expansions of the matrix K, the vector $\boldsymbol{h}$ and the energy functional E are known, and the single terms of the expansion are orderwise stored in the quantities `kcoef`, `hcoef`, and `emfcoef`. Consequently, the transformations can be applied as described in Secs. 3.1 to 3.3. As explained in Sec. 3.1, the first step of the transformations is to diagonalize the system with respect to its linearized part. Therefore, the latter's eigenvalues and -vectors are required which can be obtained the following way:

```
k0    = kcoef[[1]];
k0inv = Inverse[k0];

Do[ kcoef[[i]] = k0inv.kcoef[[i]] // Expand;
    hcoef[[i]] = k0inv.hcoef[[i]] // Expand
  , {i,nmax}];

ktmp = kcoef;
htmp = hcoef;

Do[
    Do[ ktmp[[i+j]] = ktmp[[i+j]] -
                      kcoef[[i]].ktmp[[1+j]] // Expand
      , {j,0,nmax-i}];

    Do[ htmp[[i+j]] = htmp[[i+j]] -
                      kcoef[[i]].htmp[[1+j]] // Expand
      , {j,0,nmax-i}];

    kcoef = ktmp;
    hcoef = htmp

  , {i,2,nmax}];

(* Eigenvalues and -vectors *)
Jac = D[hcoef[[1]], {x}];
λ   = Eigenvalues[Jac] // Chop;
T   = Eigenvectors[Jac] // Chop;
```

For the above mentioned parameters, the eigenvalues are

$$\lambda = \{\pm 1.87399\mathrm{i},\ \pm 0.855197\mathrm{i},\ \pm 0.182227\mathrm{i}\} \tag{A.4}$$

and they possess the structure (31). The matrix `T` contains the eigenvectors of the linearized dynamical equations, whose symplectic normalization (34) can be carried out as follows:

```
tk0tt = T.k0.Transpose[T] // Chop;
Do[ T[[i]] = T[[i]] / tk0tt[[i-1,i]] , {i,2,2d,2}];
jmat = T.k0.Transpose[T] // Chop;
```

Finally, the transformation of the dynamical equations and the energy functional to the symplectic basis is obtained by

```
emfcoef = Collect[emfcoef /.xtoy, y];
```

```
hcoef    = Collect[hcoef    /.xtoy, y];

ttx      = Transpose[T].x;
ytottx   = ToExpression[ "y" <> ToString[#] <> "→ttx[[" <>
           ToString[#] <> "]]" & /@ Range[2 d]];

emfcoef = emfcoef /. ytottx // Expand;
hcoef    = hcoef    /. ytottx // Expand;
ttinv    = Inverse[Transpose[T]];

Do[ hcoef[[i]] = ttinv.hcoef[[i]] // Expand // Chop, {i,nmax}];
```

After this transformation to the symplectic basis, the dynamical equations have the diagonal linear term

$$\texttt{hcoef[[1]]} = \begin{pmatrix} \texttt{+1.87399i x1} \\ \texttt{-1.87399i x2} \\ \texttt{+0.855197i x3} \\ \texttt{-0.855197i x4} \\ \texttt{+0.182227i x5} \\ \texttt{-0.182227i x6} \end{pmatrix}, \tag{A.5}$$

whose entries are the eigenvalues (A.4) and the quadratic order of the energy functional is

$$\texttt{emfcoef[[1]]} = \texttt{1.87399i x1 x2 + 0.855197i x3 x4 + 0.182227i x5 x6}\,. \tag{A.6}$$

At this point, it is obvious that the coordinates `x1,x2,x3,x4,x5,x6` are pairwise canonical up to this order of the expansion. It is noted that the higher-order terms `hcoef[[i]]` and `hcoef[[i]]` with `i>1` have not been simplified by this step. In general, they still contain all possible monomials, and because of the huge amount of terms, they are not shown here.

Appendix A.2. Lie transforms for truncated expansions

As discussed in Sec. 3.2, these higher-order terms are simplified via a normal form expansion, which is performed order by order (`n=1,2,3,...`). Since the dynamical equations are on hand as truncated Taylor expansions (47), the number of applications of the Lie operator in Eq. (43) and the right-multiplication operator in Eq. (45) can be limited. In addition, it is appropriate to apply the operators to the different orders of the expansions separately. For a generating function $\boldsymbol{g}_n$ of degree n, the corresponding transformations (43) and (45) then read

$$\sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{L}_{\boldsymbol{g}_n}^j \boldsymbol{a}(\boldsymbol{x}) = \sum_{k=1}^{n_{\max}} \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{L}_{\boldsymbol{g}_n}^j \boldsymbol{a}_k(\boldsymbol{x}) \quad \longrightarrow \quad \sum_{k=1}^{n_{\max}} \sum_{j=0}^{j_{\max}} \frac{1}{j!} \mathcal{L}_{\boldsymbol{g}_n}^j \boldsymbol{a}_k(\boldsymbol{x})\,, \tag{A.7a}$$

$$\sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{D}_{\boldsymbol{g}_n}^j E(\boldsymbol{x}) = \sum_{k=0}^{n_{\max}+1} \sum_{j=0}^{\infty} \frac{1}{j!} \mathcal{D}_{\boldsymbol{g}_n}^j E_k(\boldsymbol{x}) \quad \longrightarrow \quad \sum_{k=0}^{n_{\max}+1} \sum_{j=0}^{j_{\max}} \frac{1}{j!} \mathcal{D}_{\boldsymbol{g}_n}^j E_k(\boldsymbol{x})\,, \tag{A.7b}$$

where the limit of the summation over j has been reset to $j_{\max}$ in the respective last steps.

Both the expressions $\mathcal{L}_{\boldsymbol{g}_n}^j \boldsymbol{a}_k(\boldsymbol{x})$ and $\mathcal{D}_{\boldsymbol{g}_n}^j E_k(\boldsymbol{x})$ occurring on the right-hand side of Eqs. (A.7) are of the order $k + j(n-1)$. Thus, if one focuses only on the l-th order of

the transformed field, there will only contribute such terms for which $k+j(n-1) \stackrel{!}{=} l$. Consequently, it is sufficient to apply the operators no more than

$$j_{\max} = \left\lfloor \frac{l-k}{n-1} \right\rfloor \tag{A.8}$$

times, where $\lfloor \cdot \rfloor$ denotes the integer part of its argument.

Moreover, it is numerically appropriate not to apply the operators $\mathcal{L}^j_{\boldsymbol{g}_n}$ and $\mathcal{D}^j_{\boldsymbol{g}_n}$ several times and to add the respective terms afterwards, as the formal transformations in Eqs. (A.7) suggest, but to calculate the transformation via the Horner-like scheme

$$\sum_{j=0}^{j_{\max}} \tfrac{1}{j!} \mathcal{L}^j_{\boldsymbol{g}_n} \boldsymbol{a}_k(\boldsymbol{x}) = \boldsymbol{a}_k(\boldsymbol{x}) + \mathcal{L}_{\boldsymbol{g}_n} \left(\boldsymbol{a}_k(\boldsymbol{x}) + \tfrac{1}{2} \mathcal{L}_{\boldsymbol{g}_n} \left(\boldsymbol{a}_k(\boldsymbol{x}) + \ldots \left(\boldsymbol{a}_k(\boldsymbol{x}) + \tfrac{1}{j_{\max}} \mathcal{L}_{\boldsymbol{g}_n} \boldsymbol{a}_k(\boldsymbol{x}) \right) \right) \right), \tag{A.9a}$$

$$\sum_{j=0}^{j_{\max}} \tfrac{1}{j!} \mathcal{D}^j_{\boldsymbol{g}_n} E_k(\boldsymbol{x}) = E_k(\boldsymbol{x}) + \mathcal{D}_{\boldsymbol{g}_n} \left(E_k(\boldsymbol{x}) + \tfrac{1}{2} \mathcal{D}_{\boldsymbol{g}_n} \left(E_k(\boldsymbol{x}) + \ldots \left(E_k(\boldsymbol{x}) + \tfrac{1}{j_{\max}} \mathcal{D}_{\boldsymbol{g}_n} E_k(\boldsymbol{x}) \right) \right) \right), \tag{A.9b}$$

where the maximum value of $j_{\max}$ is determined by Eq. (A.8). For each order, the generating function is first constructed according to Eq. (57). Second, for each generating function, the corresponding transformations (43) and (45) are evaluated:

```
m1 = n - Sum[m[[i]], {i, 2, 2d}];

Do[ (* Construction of the generating function *)
    g = Table[0, {2d}];

    Do[ term = pwr[x, m];

        Do[ nen = λ.m - λ[[i]];

            If[ Abs[nen] > 10^(-10) ,
                g[[i]] = g[[i]] +
                Coefficient[hcoef[[n, i]], term]/nen term; ]

          , {i,2d}]

      (* The range of the loop is adapted to d=3 *)
      , {m6, 0, n}
      , {m5, 0, n - m6}
      , {m4, 0, n - m6 - m5}
      , {m3, 0, n - m6 - m5 - m4}
      , {m2, 0, n - m6 - m5 - m4 - m3}];

  (* Transformation of the dynamical equations *)
  g1   = Transpose[D[g, {x}]] // Expand;
  jmax = Floor[(nmax-1)/(n-1)];
  len  = nmax - (n-1)*jmax;
  b    = hcoef;
  lg   = Table[0, {nmax}];
```

```
  Do[ lg[[n;;n+len-1]] = (D[b[[1;;len]],{x}].g -
                          b[[1;;len]].g1) / (jmax+1-j);
      b = lg + hcoef // Expand;
      len = len + n - 1
    , {j, jmax}];

  (* Transformation of the energy functional *)
  If[jmax > 0, {hcoef = b; hcoef[[n]] = hcoef[[n]] // Chop}];
  jmax = Floor[(nmax-3)/(n-1)];
  len  = nmax - 2 - (n-1)*jmax;
  b    = emfcoef;
  lg   = Table[0, {nmax-2}];

  Do[ lg[[n;;n+len-1]] = (D[b[[1;;len]], {x}].g) / (jmax+1-j);
      b = lg + emfcoef // Expand;
      len = len + n - 1
    , {j, jmax}];

  If[jmax > 0, {emfcoef = b; emfcoef[[n]]
                = If[OddQ[n], Chop[emfcoef[[n]],10^(-8)],0]}];

, {n, 2, nmax}];
```

The normal form transformations in this step have removed all terms of the dynamical equations of even order and the odd-order terms of the energy functional, i.e.

$$\texttt{hcoef[[2]]} = \texttt{hcoef[[4]]} = \texttt{hcoef[[6]]} = 0\,, \tag{A.10a}$$

$$\texttt{emfcoef[[2]]} = \texttt{emfcoef[[4]]} = \texttt{emfcoef[[6]]} = 0\,. \tag{A.10b}$$

The first-order terms of the dynamical equations and the second-order terms of the energy functional have been left unchanged. The next-higher order corrections read

$$\texttt{hcoef[[3]]} = \begin{pmatrix} 420.512\,x1^2x2 + 68.8326\,x1\,x3\,x4 - 3.2175\,x1\,x5\,x6 \\ -420.512\,x1\,x2^2 - 68.8326\,x2\,x3\,x4 + 3.2175\,x2\,x5\,x6 \\ 68.8326\,x1\,x2\,x3 + 47.0488\,x3^2\,x4 - 0.972187\,x3\,x5\,x6 \\ -68.8326\,x1\,x2\,x4 - 47.0488\,x3\,x4^2 + 0.972187\,x4\,x5\,x6 \\ -3.2175\,x1\,x2\,x5 - 0.972187\,x3\,x4\,x5 + 0.712752\,x5^2\,x6 \\ 3.2175\,x1\,x2\,x6 + 0.972187\,x3\,x4\,x6 - 0.712752\,x5\,x6^2 \end{pmatrix} \tag{A.11}$$

in the dynamical equations and

$$\begin{aligned} \texttt{emfcoef[[3]]} = &- 394.668\,x1^2\,x2^2 + 348.835\,x1\,x2\,x3\,x4 \\ &- 9.43647\,x3^2\,x4^2 - 25.7015\,x1\,x2\,x5\,x6 \\ &- 8.61906\,x3\,x4\,x5\,x6 - 0.148958\,x5^2\,x6^2 \end{aligned} \tag{A.12}$$

in the energy functional, which both possess the polynomial structures (50) and (58). The same polynomial structure is also present in the higher-order terms, but they are not shown because of the large number of monomials.

Appendix A.3. Determination of the resonant coefficients

Obviously, the third-order terms (A.11) fulfill the conditions of integrability (60b) and (60c). However, they are not connected to the fourth-order term (A.12) via Eq. (60a).

In order to achieve the fulfillment of the canonical equation, the transformation using the resonant terms of the generating function is applied as discussed in Sec. 3.3. As an alternative to its explicit evaluation, the system of equations (69) is here set up by evaluating the term $\mathcal{L}_{\boldsymbol{g}_n}\boldsymbol{b}_3$ instead of calculating each component (67) separately. For this purpose, the resonant terms in the generating function are labeled c_i and they are treated as free parameters in the Lie transform.

In order to determine the resonant coefficients of a generating function, the linear system of equations (69) must be solved. As already discussed in Sec. 3.3, this system is overdetermined, but it is guaranteed by Darboux's theorem that a solution exists. However, because of numerical errors, one may be prevented from finding an *exact* solution of the equations. Therefore, an appropriate way to find the resonant coefficients is to apply a least-square fit

$$\|\mathcal{A}\,\mathcal{G} - \mathcal{B}\|^2 \stackrel{!}{=} \min. \tag{A.13}$$

to the system of equations (69). It is emphasized that Eq. (A.13) is *not* an approximation to the solution of the resonant coefficients, because its minimum value must be (numerically) zero. The least-square fit is rather a suitable method to solve the overdetermined system of equations.

```
hint = Table[0, {nmax}]; n = 1;
hint[[n]] = Expand[Sum[Integrate[
            hcoef[[n,2i-1]] /.xoddtozero[[1;;i-1]],x[[2i]]]
            , {i, d}]];

Do[ hint[[n]] = Expand[Sum[Integrate[ hcoef[[n,2i-1]]
                /.xoddtozero[[1;;i-1]],x[[2i]]] , {i,d}]];

    hdiff = hint[[n]] - emfcoef[[n]];
    nc    = d Binomial[d + (n-3)/2, d-1];
    noe1  = Binomial[d + (n-1)/2, d-1];

    (* Generating function with free parameters *)
    c     = ToExpression["c" <> ToString[#]] & /@ Range[nc];
    g = 0; cnt = 0; eqcnt = 0; n1h = (n+1)/2;
    eq = Table[1, {noe1}];
    m1 = n1h - Sum[m[[i]], {i,3,2d,2}];

    Do[ eqcnt = eqcnt + 1;

        Do[ If[ m[[i]] > 0, {cnt = cnt + 1;
                eq[[eqcnt]] = eq[[eqcnt]] - c[[cnt]];
                term = pwr[x, m /. meventoodd];
                g = g + c[[cnt]] Coefficient[hdiff, term]
                term/x[[i]]/λ[[i]] UnitVector[2d, i+1]}
              ]
          , {i,1,2d,2}]

      (* The range of the loop is adapted to d=3 *)
      , {m5, 0, n1h}
      , {m3, 0, n1h - m5}];

  (* Transformation induced by the generating function *)
```

```
g1   = Transpose[D[g,{x}]];
htmp = hcoef[[n+2]] + D[hcoef[[3]],{x}].g - hcoef[[3]].g1;
n3h  = (n+3)/2;
m1   = n3h - Sum[m[[i]], {i,3,2d,2}];

Do[ term = pwr[x, m /. meventoodd];

    Do[ If[m[[i]] > 0,

        Do[ If[ m[[j]] > 0, {
            eqcnt = eqcnt + 1; AppendTo[eq, Expand[
            Coefficient[htmp[[i]], term/x[[i+1]]]/m[[i]] -
            Coefficient[htmp[[j]], term/x[[j+1]]]/m[[j]]]]}]
          , {j,i+2,2d,2}] ]
      , {i,1,2d-2,2}]

  , {m5, 0, n3h}
  , {m3, 0, n3h - m5}];

(* Determination the resonant coefficients *)
cmat = D[eq, {c}];
b    = -eq /.Table[c[[i]] → 0, {i,nc}];
c    = LeastSquares[cmat, b];
crep = ToExpression[ "c" <> ToString[#] <> "→c[[" <>
       ToString[#] <> "]]" & /@ Range[nc]];
g    = g /. crep;
g1   = Transpose[D[g, {x}]];

(* Transformation of the dynamical equations *)
jmax = Floor[(nmax-1)/(n-1)];
len  = nmax - (n-1)*jmax;
b    = hcoef;
lg   = Table[0, {nmax}];

Do[ lg[[n;;n+len-1]] = (D[b[[1;;len]],{x}].g -
                        b[[1;;len]].g1)/(jmax+1-j);
    b = lg + hcoef // Expand;
    len = len + n - 1
  , {j, jmax}];

If[jmax > 0, hcoef = b];

(* Transformation of the energy functional *)
jmax = Floor[(nmax-3)/(n-1)];
len  = nmax - 2 - (n-1)*jmax;
b    = emfcoef;
lg   = Table[0, {nmax-2}];

Do[ lg[[n;;n+len-1]] = (D[b[[1;;len]],{x}].g)/(jmax+1-j);
    b   = lg + emfcoef // Expand;
    len = len + n - 1
  , {j, jmax}];
```

```
    If[jmax > 0, emfcoef = b]

  , {n,3,nmax-2,2}];
```

The resonant coefficients of the generating function do only need to be determined up to the order $n_{\max}-2$. This guarantees the fulfillment of the conditions of integrability in the order $n_{\max}-1$, so that the energy functional in order $n_{\max}$ is obtained by a simple integration of the dynamical equations:

```
n = nmax;
hint[[n]] = Expand[Sum[Integrate[
            hcoef[[n,2i-1]] /.xoddtozero[[1;;i-1]],
            x[[2i]]], {i,d}]];

(* Definition of action valiables *)
jfac = Table[1, {nd}];
jvar = Table[i, {nd}];
Do[ If[Chop[Abs[Im[λ[[2i-1]]]]] > 10^-10,
       {jfac[[i]] = I, jvar[[i]] = j}]
  , {i, 1, nd}]
actionvar= ToExpression[ "j" <> ToString[#] <> "→" <>
           ToString[jvar[[#]]] <> ToString[#] <> "/" <>
           ToString[jfac[[#]]]] & /@ Range[nd]

H = hint /.xtoj /.actionvar;
```

The last step takes into account the definition of the action variables (73) and it guarantees that the integrated Hamiltonian is real. In order to keep the information, which variables correspond to real (unstable) and imaginary (stable) eigenvalues, the coordinates are labeled "i" in the former and "j" in the latter case.

Finally, the canonical equations are fulfilled in every order of the expansion by construction, and the local Hamiltonian in action coordinates orderwise consists of the terms

$$\texttt{H[[1]]} = \texttt{1.87399 j1 + 0.855197 j2 + 0.182227 j3}\,, \tag{A.14a}$$

$$\begin{aligned}\texttt{H[[3]]} = {}& \texttt{- 210.256 j1}^2 \texttt{ - 68.8326 j1 j2 - 23.5244 j2}^2 \\ & \texttt{+ 3.2175 j1 j3 + 0.972187 j2 j3 - 0.356376 j3}^2\,,\end{aligned} \tag{A.14b}$$

$$\begin{aligned}\texttt{H[[5]]} = {}& \texttt{37771.3 j1}^3 \texttt{ + 20967.8 j1}^2\texttt{ j2 - 10084.8 j1 j2}^2 \\ & \texttt{+ 861.764 j2}^3 \texttt{ - 1195.23 j1}^2\texttt{ j3 - 1505.82 j1 j2 j3} \\ & \texttt{- 104.915 j2}^2\texttt{ j3 + 118.681 j1 j3}^2 \texttt{ + 48.8141 j2 j3}^2 \\ & \texttt{- 2.74901 j3}^3\,,\end{aligned} \tag{A.14c}$$

$$\begin{aligned}\texttt{H[[7]]} = {}& \texttt{- 9.61439}\times 10^6\,\texttt{j1}^4 \texttt{ + 3.27764}\times 10^7\,\texttt{j1}^3\texttt{ j2 - 2.97357}\times 10^7\,\texttt{j1}^2\texttt{ j2}^2 \\ & \texttt{+ 3.79731}\times 10^6\,\texttt{j1 j2}^3 \texttt{ - 138082. j2}^4 \texttt{ + 315564. j1}^3\texttt{ j3} \\ & \texttt{+ 3.49666}\times 10^6\,\texttt{j1}^2\texttt{ j2 j3 - 1.45983}\times 10^6\,\texttt{j1 j2}^2\texttt{ j3} \\ & \texttt{+ 39551.6 j2}^3\texttt{ j3 - 56668.5 j1}^2\texttt{ j3}^2 \texttt{ - 70531.1 j1 j2 j3}^2 \\ & \texttt{- 1471.93 j2}^2\texttt{ j3}^2 \texttt{ + 3042.69 j1 j3}^3 \texttt{ + 1240.61 j2 j3}^3 \texttt{ - 62.99 j3}^4\,.\end{aligned} \tag{A.14d}$$

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