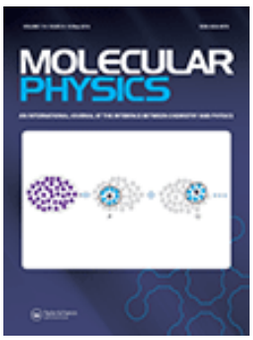

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General framework for constraints in molecular dynamics simulations

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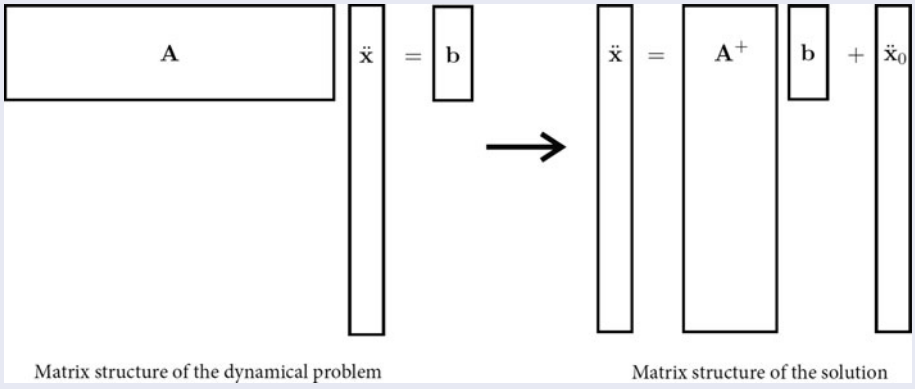
ABSTRACT

The article presents a theoretical framework for molecular dynamics simulations of complex systems subject to any combination of holonomic and non-holonomic constraints. Using the concept of constrained inverse matrices both the particle accelerations and the associated constraint forces can be determined from given external forces and kinematical conditions. The formalism enables in particular the construction of explicit kinematical conditions which lead to the well-known Nosé–Hoover type equations of motion for the simulation of non-standard molecular dynamics ensembles. Illustrations are given for a few examples and an outline is presented for a numerical implementation of the method.



Matrix structure of the dynamical problem — Matrix structure of the solution

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1. Introduction

Since many years, classical molecular dynamics (MD) simulations are an indispensable tool for the investigation of structural and dynamical properties of condensed matter systems. Starting with the pioneering MD simulations by Rahman and Verlet [1,2], the simulated systems rapidly evolved from simple liquids to polymers and biomolecular systems [3,4]. In this context, constraints were an important methodological concept to develop the field of MD simulations. A standard application is the replacement of fast intramolecular vibrations by bond constraints, which enables the use of larger time steps for the iterative integration of the Newtonian equations of motion [5,6]. New routes for the application of MD simulations were opened by conceiving constraints for the simulation of rare events [7,8] and for the simulation of many particle systems in non-equilibrium conditions [9,10]. Thermodynamic constraints, which have been conceived to simulate non-standard MD ensembles, such as the canonical and the isobaric-isothermal ensemble, play here a special role since they are not defined through explicit kinematical conditions, but by coupling the physical system to an external heat and/or pressure reservoir. The method is usually referred to as 'extended systems approach' [11–13]. For this reason, the construction of equations of motion for systems which are subjected to a combination of thermodynamic and 'normal' constraints remains a difficult task. An example is the simulation of semi-rigid polymers in the isobaric or isobaric-isothermal ensemble, where the bond constraints interfere with the scaling of the simulation box which is used to adapt the pressure. The corresponding equations of motions can be derived within the extended systems approach [14,15], but their

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construction is quite involved since one has to consider constrained Hamiltonian systems [16,17].

In this paper it is shown that explicit non-holonomic kinematical conditions corresponding to thermodynamic constraints can be derived within an existing theory of constrained many particle systems [18,19], enabling a quasi-automatised derivation of the equations of motion of multi-constrained dynamical systems as well as the handling of redundant and inconsistent constraints. The numerical implementation of the novel method is outlined.

2. General framework

2.1. Newton's equations of motion

In the following we consider N point-like particles, representing typically atoms or pseudo-atoms whose positions are described by three Cartesian coordinates, x, y, z. The $3N$-dimensional column vector $\boldsymbol{x}$ contains the ensemble of all these coordinates:[1]

$$\boldsymbol{x} = (x_1, y_1, z_1, \ldots, x_N, y_N, z_N)^T. \tag{1}$$

The unconstrained dynamics of the system is described by Newton's equations of motion,

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}, \dot{\boldsymbol{x}}, t), \tag{2}$$

where the external forces, $\boldsymbol{f}$, are arbitrary and may depend on the particle positions, velocities, and explicitly on time. The mass matrix $\boldsymbol{M}$ has diagonal form

$$\boldsymbol{M} = \mathrm{diag}(m_1, m_1, m_1, \ldots, m_N, m_N, m_N), \tag{3}$$

with $m_k > 0$ $(k = 1, \ldots N)$ being the masses of the particles.

2.2. Constraints

The mechanical system is now considered to be subject to constraints which are grouped into

(1) n_h holonomic constraints of the form

$$f_j(\boldsymbol{x}(t), t) \equiv 0, \quad j = 1, \ldots, n_h, \tag{4}$$

(2) n_{nh} non-holonomic constraints of the form

$$g_k(\boldsymbol{x}(t), \dot{\boldsymbol{x}}(t), t) \equiv 0, \quad k = 1, \ldots, n_{nh}. \tag{5}$$

By differentiating Equation (4) twice and Equation (5) once with respect to time, one obtains in total a set of $n_c = n_h + n_{nh}$ linear equations to be satisfied by the $3N$ components of the acceleration vector, $\ddot{\boldsymbol{x}}$ (the argument t is omitted):

$$\boldsymbol{A}(\boldsymbol{x}, \dot{\boldsymbol{x}}, t) \cdot \ddot{\boldsymbol{x}} = \boldsymbol{b}(\boldsymbol{x}, \dot{\boldsymbol{x}}, t). \tag{6}$$

Since the number of constraints must be smaller than the number of degrees of freedom, i.e. $n_c < 3N$, Equation (6) defines an underdetermined system of linear equations for the accelerations (Figure 1(a)). If a solution exists, it defines the set of all possible accelerations which are compatible with the imposed constraints.

The condition for the existence of a solution of Equation (6) and the solution itself can be conveniently expressed in terms of the generalised inverse of $\boldsymbol{A}$ [20], whose definition and properties are briefly resumed in the appendix. Multiplying Equation (6) from the left with $\boldsymbol{A} \cdot \boldsymbol{A}^+$ and using the Moore–Penrose condition (A2) leads to

$$\boldsymbol{A} \cdot \boldsymbol{A}^+ \cdot \boldsymbol{b} = \boldsymbol{b}, \tag{7}$$

which is a *consistency condition* for the imposed constraints. This condition is trivially fulfilled if $\boldsymbol{b} = \boldsymbol{0}$ and if $\boldsymbol{A} \cdot \boldsymbol{A}^+ = \boldsymbol{1}_{n_c \times n_c}$, which holds if $\boldsymbol{A}$ has full rank. Given that Equation (7) is true, Equation (6) has an infinite number of solutions of the form (Figure 1(b)),

$$\ddot{\boldsymbol{x}} = \boldsymbol{A}^+ \cdot \boldsymbol{b} + \ddot{\boldsymbol{x}}_0, \tag{8}$$

where $\ddot{\boldsymbol{x}}_0 \in \mathbb{R}^{3N}$ is an arbitrary vector in the null space of $\boldsymbol{A}$,

$$\boldsymbol{A} \cdot \ddot{\boldsymbol{x}}_0 = \boldsymbol{0}. \tag{9}$$

The dimension of this null space defines the number of degrees of freedom of the dynamical system:

$$f = 3N - \mathrm{rank}(\boldsymbol{A}). \tag{10}$$

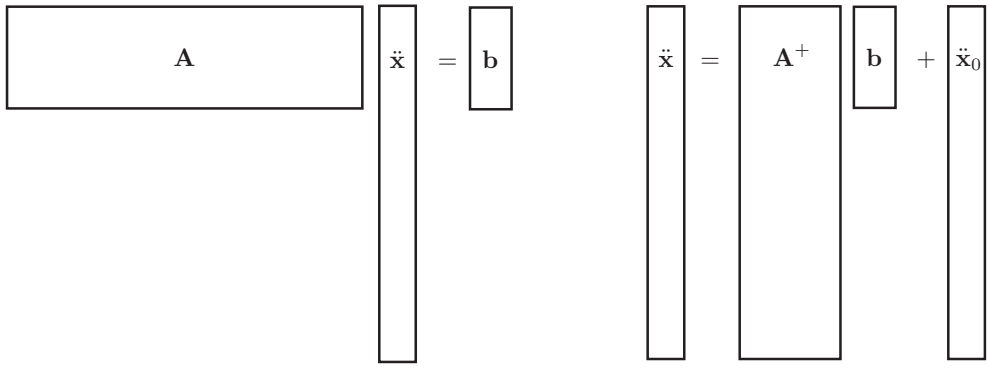
The number of degrees of freedom is not necessarily constant since $\boldsymbol{A}$ varies with time and its rank may vary too.

It is worthwhile noting that Expression (8) is also the solution of the least squares problem,

$$\|\boldsymbol{A} \cdot \ddot{\boldsymbol{x}} - \boldsymbol{b}\|^2 = \mathrm{Min}, \tag{11}$$

which may be considered instead of Equation (6) if the consistency condition (7) is *not* fulfilled. In this case, the resulting acceleration vector $\ddot{\boldsymbol{x}}$ minimises the inconsistencies in the constraints in a least square sense:

$$\left\|\boldsymbol{A} \cdot \boldsymbol{A}^+ \cdot \boldsymbol{b} - \boldsymbol{b}\right\|^2 = \mathrm{Min}. \tag{12}$$



(a) Matrix structure of Eq. (6).

(b) Matrix structure of the solution of Eq (6).

Figure 1. Linear acceleration constraints. (a) Matrix structure of Equation (6) and (b) matrix structure of the solution of Equation (6).

In the following, the null space of $\boldsymbol{A}$ will be denoted as $\mathcal{N}(\boldsymbol{A})$ and its orthogonal complement, the row space of $\boldsymbol{A}$, as $\mathcal{R}(\boldsymbol{A})$. It follows from the Moore–Penrose conditions (A1) and (A3) that

$$\boldsymbol{P} = \mathbf{1} - \boldsymbol{A}^{+} \cdot \boldsymbol{A}, \tag{13}$$

$$\boldsymbol{Q} = \boldsymbol{A}^{+} \cdot \boldsymbol{A}, \tag{14}$$

are orthogonal projectors on $\mathcal{N}(\boldsymbol{A})$ and $\mathcal{R}(\boldsymbol{A})$, respectively, and that

$$\boldsymbol{P} \cdot \ddot{\boldsymbol{x}} = \ddot{\boldsymbol{x}}_0, \tag{15}$$

$$\boldsymbol{Q} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{A}^{+} \cdot \boldsymbol{b}. \tag{16}$$

Equation (8) is thus an orthogonal decomposition of the acceleration vector into its components in $\mathcal{N}(\boldsymbol{A})$ and $\mathcal{R}(\boldsymbol{A})$, respectively.

2.3. Equations of motion for constrained systems

2.3.1. General form

The standard form of the equations of motion for a classical dynamical system is

$$\ddot{\boldsymbol{x}}(t) = \boldsymbol{a}(\boldsymbol{x}, \dot{\boldsymbol{x}}, t) \tag{17}$$

which expresses that, for a given time, the particle accelerations are uniquely determined by the positions and velocities. This is not so in constrained systems, where the particle accelerations are partially determined by the imposed constraints. Equation (8) may, in fact, be considered as a partially defined equation of motion, where the influence of the external forces still needs to be determined. This point will be discussed in the following.

2.3.2. Possibly rank deficient matrices A and M

If the decomposition (8) of the acceleration vector is inserted into Newton's equations of motion (2), the latter will in general not hold since the external force vector $\boldsymbol{f}$ on the r.h.s of Equation (2) is arbitrary, but the vector $\boldsymbol{M} \cdot \ddot{\boldsymbol{x}}$ on the l.h.s. is not if constraints are imposed. It follows, in fact, from Equation (8) that $\ddot{\boldsymbol{x}}$ is composed of a fixed component $\boldsymbol{A}^{+} \cdot \boldsymbol{b}$, which is determined by the positions and velocities of all or some particles of the dynamical system, and a component $\ddot{\boldsymbol{x}}_0$, which is constrained to the null space of $\boldsymbol{A}$. Therefore, Newton's equations of motion must be supplemented by appropriate constraint forces,

$$\boldsymbol{M} \cdot (\underbrace{\boldsymbol{A}^{+} \cdot \boldsymbol{b} + \ddot{\boldsymbol{x}}_0}_{\ddot{\boldsymbol{x}}}) = \boldsymbol{f} + \boldsymbol{z}, \tag{18}$$

which are comprised in the vector $\boldsymbol{z}$. Formally,Equation (18) is a linear set of $3N$ equations for *two* vector variables, $\ddot{\boldsymbol{x}}_0$ and $\boldsymbol{z}$. A necessary and sufficient condition for the existence of a solution is

$$\boldsymbol{z} \perp \ddot{\boldsymbol{x}}_0 \Leftrightarrow \boldsymbol{z} \in \mathcal{R}(\boldsymbol{A}), \tag{19}$$

and its explicit form has been discussed by Bott and Duffin in the context of linear network theory [21]. Following their line of thinking, we define the matrix

$$\boldsymbol{G} = \boldsymbol{M} \cdot \boldsymbol{P} + \boldsymbol{Q} \tag{20}$$

and the vector

$$\boldsymbol{h} = \boldsymbol{f} - \boldsymbol{M} \cdot \boldsymbol{A}^{+} \cdot \boldsymbol{b}, \tag{21}$$

which define a normal system of linear equations,

$$\boldsymbol{G} \cdot \boldsymbol{u} = \boldsymbol{h}, \tag{22}$$

from which $\ddot{\boldsymbol{x}}_0$ and $\boldsymbol{z}$ are computed in two steps:

(1) Solve the system of linear equations (22) for $\boldsymbol{u}$, formally

$$\boldsymbol{u} = \boldsymbol{G}^{-1} \cdot \boldsymbol{h}, \quad \text{where} \quad \det(\boldsymbol{G}) \neq 0. \tag{23}$$

The determinant of $\boldsymbol{G}$ is the *discriminant* of $\boldsymbol{M}$ in $\mathcal{N}(\boldsymbol{A})$.

(2) Extract $\ddot{\boldsymbol{x}}_0$ and $\boldsymbol{z}$ by projection,

$$\ddot{\boldsymbol{x}}_0 = \boldsymbol{P} \cdot \boldsymbol{u}, \tag{24}$$

$$\boldsymbol{z} = -\boldsymbol{Q} \cdot \boldsymbol{u}. \tag{25}$$

With Equations (8) and (24) we obtain the most general form for the equations of motion:

$$\ddot{\boldsymbol{x}} = \underbrace{\boldsymbol{P} \cdot \boldsymbol{u} + \boldsymbol{A}^{+} \cdot \boldsymbol{b}}_{a(x,\dot{x},t)}. \tag{26}$$

These equations of motion even hold for possibly rank-deficient matrices $\boldsymbol{A}$ and $\boldsymbol{M}$, as long as $\det(\boldsymbol{G}) \neq 0$. In physical terms this means that there may be redundant constraints and some particles may have vanishing masses. At a first glance, particles with zero mass may seem unphysical, but such objects can be used to define force centres in partially rigid molecules where forces can act, but which do not contribute to the inertial properties of the molecule. A well-known example is the classical ST2 model for water [22], where the force centres represent electron pairs.

2.3.3. Full rank matrices A and M

We consider now the special situation where the matrices $\boldsymbol{A}$ and $\boldsymbol{M}$ have full rank. In this case the constraint forces can be analytically computed, which yields insight into their physical meaning. Referring to Equation (19), the constraint force vector $\boldsymbol{z}$ can be expressed by the row vectors of the matrix $\boldsymbol{A}$:

$$\boldsymbol{z} = \boldsymbol{A}^{T} \cdot \boldsymbol{\lambda}. \tag{27}$$

Here, $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_{n_c})^T$ is a yet unknown column vector whose components ('Lagrange parameters') define the strength of the different contributions to the constraint forces. Inserting Equation (27) into the general form (18) of the equations of motion and multiplying from the left with $\boldsymbol{A} \cdot \boldsymbol{M}^{-1}$ leads to a system of linear equations for the components of $\boldsymbol{\lambda}$:

$$\left(\boldsymbol{A} \cdot \boldsymbol{M}^{-1} \cdot \boldsymbol{A}^{T}\right) \cdot \boldsymbol{\lambda} = \boldsymbol{b} - \boldsymbol{A} \cdot \boldsymbol{M}^{-1} \cdot \boldsymbol{f}. \tag{28}$$

One uses here that $\boldsymbol{A} \cdot \ddot{\boldsymbol{x}}_0 = \boldsymbol{0}$ and that $\boldsymbol{A} \cdot \boldsymbol{A}^{+} = \boldsymbol{1}_{n_c \times n_c}$ since $\boldsymbol{A}$ has full rank. Since $\boldsymbol{M}$ has full rank, too, it follows that $\det(\boldsymbol{A} \cdot \boldsymbol{M}^{-1} \cdot \boldsymbol{A}^{T}) \neq 0$ and (28) thus has a unique solution which determines the constraint forces. The canonical form of the equations of motion, in which all quantities on the r.h.s. are then known, reads

$$\ddot{\boldsymbol{x}} = \underbrace{\boldsymbol{M}^{-1} \cdot \left(\boldsymbol{f} + \boldsymbol{A}^{T} \cdot \boldsymbol{\lambda}\right)}_{a(x,\dot{x},t)}. \tag{29}$$

2.4. Gauß' principle of least constraint

The determination of the acceleration vector described in Section 2.3 can be formulated as a minimum principle for the accelerations. On account of Equation (8) all possible variations of the acceleration vector $\ddot{\boldsymbol{x}}$ which are compatible with the imposed constraints are in the null space of $\boldsymbol{A}$:

$$\boldsymbol{\delta}\ddot{\boldsymbol{x}} = \boldsymbol{\delta}(\boldsymbol{A}^{+} \cdot \boldsymbol{b} + \ddot{\boldsymbol{x}}_0) = \boldsymbol{\delta}\ddot{\boldsymbol{x}}_0 \in \mathcal{N}(\boldsymbol{A}).$$

The above relation holds since only $\ddot{\boldsymbol{x}}_0$ can be varied and since $\ddot{\boldsymbol{x}}_0 \in \mathcal{N}(\boldsymbol{A})$ implies that $\boldsymbol{\delta}\ddot{\boldsymbol{x}}_0 \in \mathcal{N}(\boldsymbol{A})$. Since $\boldsymbol{z} \in \mathcal{R}(\boldsymbol{A})$ is in the orthogonal subspace, it follows that

$$\underbrace{(\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} - \boldsymbol{f})}_{\boldsymbol{z}} \cdot \boldsymbol{\delta}\ddot{\boldsymbol{x}} = 0. \tag{30}$$

This relation can be considered as necessary condition for

$$g(\ddot{\boldsymbol{x}}) \equiv \frac{1}{2}\, \ddot{\boldsymbol{x}} \cdot \boldsymbol{M} \cdot \ddot{\boldsymbol{x}} - \ddot{\boldsymbol{x}} \cdot \boldsymbol{f} = \text{Min}, \ \text{ subject to } \boldsymbol{A} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{b}, \tag{31}$$

which can be written in the form of Gauß' principle of least constraint [23–25]:

$$G(\ddot{\boldsymbol{x}}) = \frac{1}{2} \|\boldsymbol{M}^{-1/2} \cdot \boldsymbol{z}\|^2 = \text{Min}, \ \text{ subject to } \boldsymbol{A} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{b}. \tag{32}$$

One uses here that $\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} - \boldsymbol{f} = \boldsymbol{z}$ and that $G(\ddot{\boldsymbol{x}})$ and $g(\ddot{\boldsymbol{x}})$ differ only by the constant term $\boldsymbol{f}^{T} \cdot \boldsymbol{M}^{-1} \cdot \boldsymbol{f}/2$. The equivalence of Equations (31) and (32) requires, of course, that $\det(\boldsymbol{M}) \neq 0$, i.e. that all masses are non-zero.

3. Analytical examples

Based on the equations of motion derived in Section 2.3.3, a few analytical examples will be discussed in the following. They illustrate in particular how the simulation of non-standard MD ensembles can be enforced through explicit non-holonomic constraints.

3.1. Rigid diatomic molecule

We consider first a rigid diatomic molecule with equal atomic masses as the simplest example for a holonomic geometrical constraint. Defining $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ to be the positions of the two atoms and $\boldsymbol{x}_{12} \equiv \boldsymbol{x}_1 - \boldsymbol{x}_2$, the constraint reads

$$|\boldsymbol{x}_{12}(t)|^2 - d_{12}^2 = 0, \tag{33}$$

where d_{12} is the prescribed bond length. Double differentiation of Equation (33) with respect to time leads then to $\boldsymbol{x}_{12}^T \cdot \ddot{\boldsymbol{x}}_{12} = -|\dot{\boldsymbol{x}}_{12}|^2$, which may be written as $\boldsymbol{A} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{b}$ (cf. Equation (6)), with

$$\boldsymbol{A} = (\boldsymbol{x}_{12}^T, -\boldsymbol{x}_{12}^T) \quad \text{and} \quad \boldsymbol{b} \equiv b = -|\dot{\boldsymbol{x}}_{12}|^2. \tag{34}$$

Note that $\boldsymbol{A} \in \mathbb{R}^{1\times 3N}$ is here a row vector and $\boldsymbol{b} \equiv b \in \mathbb{R}^{1\times 1}$ is a scalar. It follows then from Equation (28) that the equation for the one Lagrange parameter λ takes the form

$$\frac{2d_{12}^2}{m}\lambda = -|\dot{\boldsymbol{x}}_{12}|^2 - \frac{1}{m}\boldsymbol{x}_{12}^T \cdot \boldsymbol{f}_{12},$$

where $|\boldsymbol{x}_{12}|^2 = d_{12}^2$. With $\boldsymbol{f}_{12} = \boldsymbol{f}_1 - \boldsymbol{f}_2$ and $\boldsymbol{n}_{12} = \boldsymbol{x}_{12}/d_{12}$, the equation of motion becomes

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{f} - \frac{m|\dot{\boldsymbol{x}}_{12}|^2}{2d_{12}^2}\begin{pmatrix} \boldsymbol{x}_{12} \\ -\boldsymbol{x}_{12} \end{pmatrix} - \frac{1}{2}\begin{pmatrix} (\boldsymbol{n}_{12}^T \cdot \boldsymbol{f}_{12})\boldsymbol{n}_{12} \\ -(\boldsymbol{n}_{12}^T \cdot \boldsymbol{f}_{12})\boldsymbol{n}_{12} \end{pmatrix}. \tag{35}$$

The constraint forces acting on the individual atoms are each split into a component compensating for the centrifugal forces and a component compensating for forces acting along the bond. Their sum vanishes, and therefore the centre-of-mass motion is determined by the sum of forces $\boldsymbol{f}_1$ and $\boldsymbol{f}_2$, which act on particles 1 and 2, respectively.

3.2. Isokinetic ensemble

A simple illustration for a non-holonomic constraint is the 'isokinetic ensemble', where the kinetic energy is forced to have a prescribed value:

$$\frac{1}{2}\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}} = \frac{3Nk_BT}{2}. \tag{36}$$

This example was considered by Hoover [26] and is treated here to prepare for the construction of non-holonomic constraints for the canonical ensemble. Differentiation of Equation (36) with respect to time leads to the linear acceleration constraint,

$$\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \ddot{\boldsymbol{x}} = 0, \tag{37}$$

where $\boldsymbol{M}$ is symmetric. Comparing to Equation (6), the matrix $\boldsymbol{A}$ and the vector $\boldsymbol{b}$ here take the form

$$\boldsymbol{A} = \dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \quad \text{and} \quad \boldsymbol{b} \equiv b = 0. \tag{38}$$

Using that $\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}} = 3Nk_BT$, it follows from Equation (28) that $3Nk_BT\,\lambda = -\boldsymbol{A} \cdot \boldsymbol{M}^{-1} \cdot \boldsymbol{f} = -\dot{\boldsymbol{x}}^T \cdot \boldsymbol{f}$. The resulting equation of motion

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{f}(t) \underbrace{- \left(\frac{\dot{\boldsymbol{x}}^T \cdot \boldsymbol{f}(t)}{3Nk_BT} \right) \boldsymbol{M} \cdot \dot{\boldsymbol{x}}}_{\boldsymbol{z}(t)}, \tag{39}$$

shows that the constraint force has the form of a friction force depending linearly on velocity. In contrast to the friction constant in purely dissipative systems, the factor $\dot{\boldsymbol{x}}^T \cdot \boldsymbol{f}(t)/(3Nk_BT)$ can be positive or negative. The constraint force represents effectively a controller which maintains a desired kinetic energy. It is important to be aware that the kinetic energy is not steered towards that value and for this reason condition (36) must be initially fulfilled, such that $\boldsymbol{z}(0) = \boldsymbol{0}$.

3.3. Canonical ensemble – Nosé–Hoover thermostat

We now consider a system of particles in thermodynamic equilibrium, which is coupled to an external heat bath. Here the corresponding kinematic condition is not given, but is to be constructed on the basis of given equations of motion. The latter have been derived by Nosé and Hoover [12,13] using the extended systems approach:

$$\dot{\boldsymbol{x}} = \boldsymbol{M}^{-1} \cdot \boldsymbol{p}, \tag{40}$$

$$\dot{\boldsymbol{p}} = \boldsymbol{f} - \xi(t)\,\boldsymbol{p}, \tag{41}$$

$$\dot{\xi}(t) = \frac{1}{Q}\left(2E_{\text{kin}}(t) - 3Nk_BT\right). \tag{42}$$

Here, Q plays the role of a mass which determines the characteristic reaction time of the thermostat. Writing the above equations of motion in Newtonian form,

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{f} \underbrace{-\xi(t)\,\boldsymbol{M} \cdot \dot{\boldsymbol{x}}}_{\boldsymbol{z}(t)}, \tag{43}$$

shows that the thermostat corresponding to the canonical ensemble is realised by a constraint force which has again the form of a friction force, $\boldsymbol{z} = -\xi(t)\,\boldsymbol{M} \cdot \dot{\boldsymbol{x}}$.

Comparing this expression to the general form (27) of the constraint forces shows that $\boldsymbol{A} = \dot{\boldsymbol{x}}^T \cdot \boldsymbol{M}$ and that the single Lagrange parameter is given by $\lambda = -\xi(t)$. Insertion into Equation (28) yields $\boldsymbol{b} \equiv b = -\xi(t)\,\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}} + \dot{\boldsymbol{x}}^T \cdot \boldsymbol{f}$. The *NVT*-ensemble thus corresponds to the linear acceleration constraint:

$$\underbrace{\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M}}_{A} \cdot \ddot{\boldsymbol{x}} = \underbrace{-\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}}\,\xi(t) + \dot{\boldsymbol{x}}^T \cdot \boldsymbol{f}}_{b}. \tag{44}$$

In case the forces can be derived from a potential, $\boldsymbol{f} = -\partial U/\partial \boldsymbol{x}$, Equation (44) is of the form

$$\frac{d}{dt}\big(E_{\mathrm{kin}}(t) + U(\boldsymbol{x}(t))\big) = -2\xi(t) E_{\mathrm{kin}}(t), \tag{45}$$

where $E_{\mathrm{kin}}(t) = \dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}}/2$ is the kinetic energy of the system. Expressing the inertial parameter as $Q = 3Nk_BT\tau_{NH}^2$, where τ_{NH} defines a time scale, it follows from Equation (42) and the initial condition $\xi(0) = 0$ that

$$\xi(t) = \frac{1}{\tau_{NH}^2} \int_0^t d\tau \left[\frac{2E_{\mathrm{kin}}(\tau)}{3Nk_BT} - 1\right]. \tag{46}$$

Note that $\xi(0) = 0$ implies that $\boldsymbol{z}(0) = \boldsymbol{0}$, which guarantees that the imposed constraint is initially fulfilled. Expression (46) shows that τ_{NH} is the reaction time of the temperature controller. The friction coefficient ξ vanishes for $\tau_{NH} \to \infty$ and Equation (45) expresses that the initial total energy is constant. Since the total energy of a Hamiltonian system is automatically conserved, the corresponding constraint force must be zero, which is indeed the case, since $\boldsymbol{z} \propto \xi(t)$. Any kinematical condition for a dynamical system which leads to a vanishing constraint force expresses, in fact, a conservation law.

3.4. Berendsen thermostat

If Equation (46) is replaced by

$$\xi(t) = \gamma\left(\frac{2E_{\mathrm{kin}}(t)}{3Nk_BT} - 1\right), \tag{47}$$

where γ has dimension 1/time, one obtains the equations of motion for the Berendsen thermostat [27]. This thermostat is widely used, in particular for the simulation of biomolecular systems, but it does not correspond to a proper thermodynamic ensemble. From a technical point of view, the Berendsen thermostat acts as a proportional controller, whereas the Nosé–Hoover thermostat acts as an integral controller. As for the previous thermostats, the Berendsen thermostat is represented by constraint force of the form $\boldsymbol{z} = -\xi(t)\,\boldsymbol{M} \cdot \dot{\boldsymbol{x}}$ and $\boldsymbol{z} = \boldsymbol{0}$ must be fulfilled to guarantee that the system is initially on the constraint surface. Therefore, one must require that $\xi(0) = 0$.

3.5. Isobaric-isoenthalpic ensemble – Anderson barostat

Another important thermodynamic constraint is the simulation of a molecular system in the isobaric-isoenthalpic ensemble, where the pressure fluctuates about a prescribed value. As in the preceding example, we wish to derive the corresponding non-holonomic constraint from given equations of motion. These equations of motion have been first derived by Andersen [11],

$$\dot{\boldsymbol{x}} = \boldsymbol{M}^{-1} \cdot \boldsymbol{p} + \frac{\dot{V}}{3V}\boldsymbol{x}, \tag{48}$$

$$\dot{\boldsymbol{p}} = \boldsymbol{f} - \frac{\dot{V}}{3V}\boldsymbol{p}, \tag{49}$$

$$\mu\ddot{V}(t) = P_{\mathrm{ext}} - \frac{1}{3V}\left(\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}} + \boldsymbol{x}^T \cdot \boldsymbol{f}\right), \tag{50}$$

where P_{ext} is the external pressure on the system, V is the volume of the simulation box, which here is assumed to be cubic, and μ is the 'mass' of the barostat ('piston'). The equations of motion are again first transformed into Newtonian form in order to extract the constraint forces corresponding to the *NPH*-ensemble. Solving Equation (48) for $\boldsymbol{p}$ and inserting the result into Equation (49) leads to

$$\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} = \boldsymbol{f} + \lambda(t)\boldsymbol{M} \cdot \boldsymbol{x}, \tag{51}$$

where the parameter $\lambda(t)$ is given by

$$\lambda(t) = \frac{\ddot{L}(t)}{L(t)}, \quad \text{with} \quad L(t) = V(t)^{1/3}. \tag{52}$$

The constraint force here has the form

$$\boldsymbol{z} = \lambda(t)\boldsymbol{M} \cdot \boldsymbol{x}, \tag{53}$$

and comparison with Equation (27) shows that $\boldsymbol{A} = \boldsymbol{x}^T \cdot \boldsymbol{M}$. From the general equation (28) for the Lagrange parameters one obtains $\boldsymbol{b} \equiv b = (\boldsymbol{x}^T \cdot \boldsymbol{M} \cdot \boldsymbol{x})\lambda(t) + \boldsymbol{x}^T \cdot \boldsymbol{f}$, and the corresponding linear acceleration constraint describing the *NPH*-ensemble reads

$$\underbrace{\boldsymbol{x}^T \cdot \boldsymbol{M}}_{\boldsymbol{A}} \cdot \ddot{\boldsymbol{x}} = \underbrace{(\boldsymbol{x}^T \cdot \boldsymbol{M} \cdot \boldsymbol{x})\lambda(t) + \boldsymbol{x}^T \cdot \boldsymbol{f}}_{\boldsymbol{b}}. \tag{54}$$

Noting that $\boldsymbol{M} \cdot \ddot{\boldsymbol{x}} - \boldsymbol{f} = \boldsymbol{z}$, the above constraint corresponds to imposing a particular form for the virial of the

constraint forces:

$$\boldsymbol{x}^T \cdot \boldsymbol{z} = (\boldsymbol{x}^T \cdot \boldsymbol{M} \cdot \boldsymbol{x})\lambda(t). \tag{55}$$

The Lagrange parameter λ can be determined from Equations (50) and (52),

$$\lambda(t) = -\frac{2}{9}\left(\frac{d\ln V}{dt}\right)^2 + \frac{1}{3\mu V}\left(P_{\text{ext}} - \frac{1}{3V}\left(\dot{\boldsymbol{x}}^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}} + \boldsymbol{x}^T \cdot \boldsymbol{f}\right)\right), \tag{56}$$

where $V(t)$ is the solution of Equation (50). The initial conditions must be chosen such that $\lambda(0) = 0$, i.e. $\dot{V}(0) = 0$ and $V(0) = V_0$, where $P_{\text{ext}}V_0 = (\dot{\boldsymbol{x}}(0)^T \cdot \boldsymbol{M} \cdot \dot{\boldsymbol{x}}(0) + \boldsymbol{x}(0)^T \cdot \boldsymbol{f}(0))/3$.

4. Numerical solution of the Bott–Duffin problem

Until now, the construction of explicit equations of motion for constrained dynamical systems has been treated on a purely formal level. In the following it will be shown how this problem can be solved numerically. The central point is to use the singular value decomposition (SVD) [28] of a given $n_c \times 3N$ matrix $\boldsymbol{A}$. The SVD can be very efficiently computed with linear algebra libraries, such as LAPACK [29].

4.1. Bases for $\mathcal{N}(A)$ and $\mathcal{R}(A)$

Concrete representations for the basis vectors spanning the null space of matrix $\boldsymbol{A}$ may be obtained from its SVD,

$$\boldsymbol{A} = \boldsymbol{U} \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{V}^T, \tag{57}$$

$$\boldsymbol{\Sigma} = (\boldsymbol{\sigma}, \boldsymbol{0}), \quad \text{with} \quad \boldsymbol{\sigma} = \text{diag}(\sigma_1, \ldots \sigma_r, 0, \ldots, 0). \tag{58}$$

Here, $\boldsymbol{U}$ and $\boldsymbol{V}$ are orthogonal matrices of dimensions $n_c \times n_c$ and $3N \times 3N$, respectively, and $\boldsymbol{\Sigma}$ is a rectangular diagonal matrix of dimensions $n_c \times 3N$ which contains the $r \equiv \text{rank}(\boldsymbol{A})$ strictly positive singular values of $\boldsymbol{A}$. Now let $\boldsymbol{p}$ be an arbitrary vector in the null space of $\boldsymbol{A}$, such that $\boldsymbol{U} \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{V}^T \cdot \boldsymbol{p} = \boldsymbol{0}$. Defining the coordinate transform $\tilde{\boldsymbol{p}} \equiv \boldsymbol{V}^T \cdot \boldsymbol{p}$, it follows from the special form of $\boldsymbol{\Sigma}$ that $\tilde{\boldsymbol{p}} = (0, \ldots, 0, \tilde{p}_{r+1}, \ldots, \tilde{p}_{3N})^T$. Therefore, $\boldsymbol{p} = \boldsymbol{V} \cdot \tilde{\boldsymbol{p}}$ has the form

$$\boldsymbol{p} = \sum_{k=r+1}^{3N} \tilde{p}_k \boldsymbol{v}_k \in \mathcal{N}(\boldsymbol{A}).$$

where $\boldsymbol{v}_k$ are the column vectors of $\boldsymbol{V}$. Similarly any vector $\boldsymbol{q} \in \mathcal{R}(\boldsymbol{A})$ can be represented as

$$\boldsymbol{q} = \sum_{k=1}^{r} \tilde{q}_k \boldsymbol{v}_k \in \mathcal{R}(\boldsymbol{A}),$$

where $\tilde{q}_1, \ldots, \tilde{q}_r$ are the only non-zero components of $\tilde{\boldsymbol{q}} = \boldsymbol{V}^T \cdot \boldsymbol{q} = (\tilde{q}_1, \ldots, \tilde{q}_r, 0, \ldots, 0)^T$. Projectors on $\mathcal{N}(\boldsymbol{A})$ and $\mathcal{R}(\boldsymbol{A})$ are readily constructed with the SVD of the generalised inverse of $\boldsymbol{A}$,

$$\boldsymbol{A}^+ = \boldsymbol{V} \cdot \boldsymbol{\Sigma}^+ \cdot \boldsymbol{U}^T, \tag{59}$$

$$\boldsymbol{\Sigma}^+ = \begin{pmatrix} \boldsymbol{\sigma}^+ \\ \boldsymbol{0} \end{pmatrix}, \quad \text{with } \boldsymbol{\sigma}^+ = \text{diag}(\sigma_1^{-1}, \ldots \sigma_r^{-1}, 0, \ldots, 0). \tag{60}$$

Inserting the SVDs of $\boldsymbol{A}$ and $\boldsymbol{A}^+$ into Expressions (13) and (14) shows that the matrix $\boldsymbol{V}$ generates a transformation to a coordinate system in which the projectors $\boldsymbol{P}$ and $\boldsymbol{Q}$ are diagonal:

$$\boldsymbol{P} = \boldsymbol{V} \cdot \tilde{\boldsymbol{P}} \cdot \boldsymbol{V}^T, \qquad \tilde{\boldsymbol{P}} = \begin{pmatrix} \boldsymbol{0}_{r\times r} & \boldsymbol{0}_{r\times f} \\ \boldsymbol{0}_{f\times r} & \boldsymbol{1}_{f\times f} \end{pmatrix}, \tag{61}$$

$$\boldsymbol{Q} = \boldsymbol{V} \cdot \tilde{\boldsymbol{Q}} \cdot \boldsymbol{V}^T, \qquad \tilde{\boldsymbol{Q}} = \begin{pmatrix} \boldsymbol{1}_{r\times r} & \boldsymbol{0}_{r\times f} \\ \boldsymbol{0}_{f\times r} & \boldsymbol{0}_{f\times f} \end{pmatrix}. \tag{62}$$

4.2. Bott–Duffin problem

The matrix structure of the Bott–Duffin problem (22) takes a particularly simple form if it is transformed into the coordinate system in which the projectors $\boldsymbol{P}$ and $\boldsymbol{Q}$ are diagonal. One obtains

$$\underbrace{\left(\begin{array}{ccc|ccc} 1 & \ldots & 0 & \tilde{M}_{1,r+1} & \ldots & \tilde{M}_{1,3N} \\ \vdots & \ddots & \vdots & \vdots & & \vdots \\ 0 & \ldots & 1 & \tilde{M}_{r,r+1} & \ldots & \tilde{M}_{r,3N} \\ \hline 0 & \ldots & 0 & \tilde{M}_{r+1,r+1} & \ldots & \tilde{M}_{r+1,3N} \\ \vdots & \ddots & \vdots & \vdots & & \vdots \\ 0 & \ldots & 0 & \tilde{M}_{3N,r+1} & \ldots & \tilde{M}_{3N,3N} \end{array}\right)}_{\tilde{\boldsymbol{G}}} \cdot \underbrace{\left(\begin{array}{c} -\tilde{z}_1 \\ \vdots \\ -\tilde{z}_r \\ \hline \ddot{\tilde{x}}_{0,1} \\ \vdots \\ \ddot{\tilde{x}}_{0,f} \end{array}\right)}_{\tilde{\boldsymbol{u}}} = \underbrace{\left(\begin{array}{c} \tilde{h}_1 \\ \vdots \\ \tilde{h}_r \\ \hline \tilde{h}_{r+1} \\ \vdots \\ \tilde{h}_{3N} \end{array}\right)}_{\tilde{\boldsymbol{h}}}, \tag{63}$$

where

$$\begin{aligned} \tilde{\boldsymbol{G}} &= \boldsymbol{V}^T \cdot \boldsymbol{G} \cdot \boldsymbol{V} = \tilde{\boldsymbol{M}} \cdot \tilde{\boldsymbol{P}} + \tilde{\boldsymbol{Q}}, \\ \tilde{\boldsymbol{M}} &= \boldsymbol{V}^T \cdot \boldsymbol{M} \cdot \boldsymbol{V}, \\ \tilde{\boldsymbol{u}} &= \boldsymbol{V}^T \cdot \boldsymbol{u}, \\ \tilde{\boldsymbol{h}} &= \boldsymbol{V}^T \cdot \boldsymbol{h} = \tilde{\boldsymbol{f}} - \tilde{\boldsymbol{M}} \cdot \boldsymbol{\Sigma}^+ \cdot \boldsymbol{U}^T \cdot \boldsymbol{b}. \end{aligned}$$

The definition (21) of the vector $\boldsymbol{h}$ has here been used in combination with the explicit form (59) for the generalised inverse of $\boldsymbol{A}$ and the definition $\tilde{\boldsymbol{f}} = \boldsymbol{V}^T \cdot \boldsymbol{f}$. The block triangular structure of $\tilde{\boldsymbol{G}}$ enables the successive calculation of the f components of $\ddot{\tilde{\boldsymbol{x}}}$ and of the $r \equiv \mathrm{rank}(\boldsymbol{A})$ components of $\tilde{\boldsymbol{z}}$. Partitioning Equation (63) in the form

$$\begin{pmatrix} \mathbf{1} & \tilde{\boldsymbol{G}}_{rf} \\ \mathbf{0} & \tilde{\boldsymbol{G}}_{ff} \end{pmatrix} \cdot \begin{pmatrix} \tilde{\boldsymbol{u}}_r \\ \tilde{\boldsymbol{u}}_f \end{pmatrix} = \begin{pmatrix} \tilde{\boldsymbol{h}}_r \\ \tilde{\boldsymbol{h}}_f \end{pmatrix}, \tag{64}$$

yields

$$\tilde{\boldsymbol{u}}_f = \tilde{\boldsymbol{G}}_{ff}^{-1} \cdot \tilde{\boldsymbol{h}}_f, \quad \text{where} \quad \det\left(\tilde{\boldsymbol{G}}_{ff}\right) \neq 0, \tag{65}$$

$$\tilde{\boldsymbol{u}}_r = \tilde{\boldsymbol{h}}_r - \tilde{\boldsymbol{G}}_{rf} \cdot \tilde{\boldsymbol{u}}_f. \tag{66}$$

Note that $\det(\tilde{\boldsymbol{G}}_{ff}) = \det(\boldsymbol{G})$, such that the conditions for the solvability of Equations (22) and (64) are equivalent. The $3N$-dimensional vectors $\ddot{\boldsymbol{x}}$ and $\boldsymbol{z}$ are finally obtained through (compare Equations (24) and (25))

$$\ddot{\boldsymbol{x}}_0 = \boldsymbol{V} \cdot \begin{pmatrix} \mathbf{0} \\ \tilde{\boldsymbol{u}}_f \end{pmatrix} = \sum_{k=r+1}^{3N} \tilde{u}_k \boldsymbol{v}_k, \tag{67}$$

$$\boldsymbol{z} = \boldsymbol{V} \cdot \begin{pmatrix} -\tilde{\boldsymbol{u}}_r \\ \mathbf{0} \end{pmatrix} = -\sum_{k=1}^{r} \tilde{u}_k \boldsymbol{v}_k, \tag{68}$$

where $r \equiv \mathrm{rank}(\boldsymbol{A})$ and $\boldsymbol{v}_k$ are the column vectors of $\boldsymbol{V}$.

5. Conclusion and outlook

The theory of constrained dynamical many body systems which has been presented in this paper has the following key features:

- It is based on the concepts of linear algebra and leads to a transparent explanation of Gauß' principle of least constraint, which is itself based on D'Alembert's principle of virtual displacements.
- Any type of holonomic and non-holonomic constraint can be handled, as long as the resulting constraints for the particle acceleration are linear functions of the accelerations.
- It permits the construction of explicit non-holonomic constraints corresponding to thermodynamic constraints.
- Redundant constraint and massless force centres can be handled.

It is crucial to realise that the equation motions are correct from a theoretical point of view. As mentioned previously, this implies in particular that the constraints are just maintained and there is no mechanism steering the system back to the surface in phase space on which it is supposed to stay. Numerical errors will thus inevitably lead to violation of the imposed constraints if they are not corrected for. This is well known for geometrical constraints and was actually the reason to develop the SHAKE-algorithm [5]. In the theoretical framework for constraints presented here such and similar correction algorithms can be effectively added 'on top' of a standard MD integrator since the underlying equations of motions are correct from a theoretical point of view.

A numerically challenging point is the calculation of the SVD of the matrix $\boldsymbol{A}$ (see Equation (57)), which must be performed at any time step of the MD simulation under consideration. The computational complexity for an $m \times n$ matrix is $O\{4mn^2+8mn^2+9n^3\}$ if no special features of $\boldsymbol{A}$, such as sparseness or a special block structure are used [28]. If $\boldsymbol{A}$ has for example block form, the computational costs can be drastically reduced by breaking the SVD down to a series of SVDs for smaller matrices. Such a situation occurs for example if geometrical constraints are imposed in a solvent of many small molecules, such as water. The numerical efficiency of the SVD of the $\boldsymbol{A}$-matrix still needs to be explored in detail in order to develop efficient integration algorithms which implement the theory presented here. There is in particular a large bulk of literature on the SVD of very large matrices and corresponding work on our side is in progress.

Note

1. The symbol T denotes a transposition.

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Appendix. Generalised inverses

A1 Definition

For any matrix $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ exists a generalised inverse $\boldsymbol{A}^+ \in \mathbb{R}^{n\times m}$ which is uniquely defined by the Moore–Penrose conditions:

$$\boldsymbol{A}^+ \cdot \boldsymbol{A} \cdot \boldsymbol{A}^+ = \boldsymbol{A}^+ \tag{A1}$$

$$\boldsymbol{A} \cdot \boldsymbol{A}^+ \cdot \boldsymbol{A} = \boldsymbol{A}, \tag{A2}$$

$$(\boldsymbol{A}^+ \cdot \boldsymbol{A})^\dagger = \boldsymbol{A}^+ \cdot \boldsymbol{A}, \tag{A3}$$

$$(\boldsymbol{A} \cdot \boldsymbol{A}^+)^\dagger = \boldsymbol{A} \cdot \boldsymbol{A}^+. \tag{A4}$$

The above relations define the projector matrices,

$$\boldsymbol{P}_{\text{row}} = \boldsymbol{A}^+ \cdot \boldsymbol{A} \in \mathbb{R}^{n\times n}, \tag{A5}$$

$$\boldsymbol{P}_{\text{col}} = \boldsymbol{A} \cdot \boldsymbol{A}^+ \in \mathbb{R}^{m\times m}, \tag{A6}$$

which fulfill the general projector relations $\boldsymbol{P}^2 = \boldsymbol{P}$ and $\boldsymbol{P}^\dagger = \boldsymbol{P}$ and which project, respectively, on the row and column space of $\boldsymbol{A}$ (column and row space of $\boldsymbol{A}^+$). If $\boldsymbol{A}$ has full rank, its generalised inverse is given by

$$\boldsymbol{A}^+ = \begin{cases} \boldsymbol{A}^\dagger \cdot (\boldsymbol{A} \cdot \boldsymbol{A}^\dagger)^{-1} & \text{if } m < n, \\ (\boldsymbol{A}^\dagger \cdot \boldsymbol{A})^{-1} \cdot \boldsymbol{A}^\dagger & \text{if } m \geq n. \end{cases} \tag{A7}$$

For a full rank square matrix $\boldsymbol{A}$, the generalised inverse reduces to the normal inverse, $\boldsymbol{A}^+ = \boldsymbol{A}^{-1}$.

A2 Singular value decomposition

The numerical calculation of generalised inverse matrices is efficiently performed by singular value decomposition (SVD). The SVD of an arbitrary complex $m \times n$ matrix $\boldsymbol{A}$ reads

$$\boldsymbol{A} = \boldsymbol{U} \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{V}^\dagger, \tag{A8}$$

where $\boldsymbol{U}$ and $\boldsymbol{V}$ are hermitian $m \times m$ and $n \times n$ matrices, respectively. The $m \times n$ matrix $\boldsymbol{\Sigma}$ has the form

$$\boldsymbol{\Sigma} = \begin{cases} (\boldsymbol{\sigma}, \boldsymbol{0}) & \text{if} \quad m \leq n, \\ \begin{pmatrix} \boldsymbol{\sigma} \\ \boldsymbol{0} \end{pmatrix} & \text{if} \quad m > n, \end{cases} \quad \text{where}$$
$$\boldsymbol{\sigma} = \text{diag}(\sigma_1, \ldots \sigma_r, 0, \ldots, 0) \tag{A9}$$

is a diagonal matrix of dimension $r \times r$, with

$$r \equiv \text{rank}(\boldsymbol{A}) \leq \min(m, n). \tag{A10}$$

The elements σ_k on the diagonal of $\boldsymbol{\sigma}$ are the singular values of $\boldsymbol{A}$ and they fulfill $\sigma_k > 0$ $(k = 1, \ldots, r)$. With these prerequisites, the generalised inverse of $\boldsymbol{A}$ is given by

$$\boldsymbol{A}^+ = \boldsymbol{V} \cdot \boldsymbol{\Sigma}^+ \cdot \boldsymbol{U}^\dagger, \tag{A11}$$

where

$$\boldsymbol{\Sigma}^{+} = \boldsymbol{\Sigma}^{T}\left(\left\{\sigma_k^{-1}\right\}\right). \tag{A12}$$

Since $\boldsymbol{U}$ and $\boldsymbol{V}$ are hermitian matrices, it follows from (A8) and (A11) that

$$\boldsymbol{P}_{\mathrm{row}} = \boldsymbol{V} \cdot \boldsymbol{\Sigma}^{+} \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{V}^{\dagger}, \tag{A13}$$

$$\boldsymbol{P}_{\mathrm{col}} = \boldsymbol{U} \cdot \boldsymbol{\Sigma} \cdot \boldsymbol{\Sigma}^{\dagger} \cdot \boldsymbol{U}^{\dagger}. \tag{A14}$$

Noting that

$$\boldsymbol{\Sigma}^{+} \cdot \boldsymbol{\Sigma} = \begin{pmatrix} \mathbf{1}_{r\times r} & \mathbf{0}_{r\times(n-r)} \\ \mathbf{0}_{(n-r)\times r} & \mathbf{0}_{(n-r)\times(n-r)} \end{pmatrix} \equiv \tilde{\boldsymbol{P}}_{\mathrm{row}}, \tag{A15}$$

$$\boldsymbol{\Sigma} \cdot \boldsymbol{\Sigma}^{+} = \begin{pmatrix} \mathbf{1}_{r\times r} & \mathbf{0}_{r\times(m-r)} \\ \mathbf{0}_{(m-r)\times r} & \mathbf{0}_{(m-r)\times(m-r)} \end{pmatrix} \equiv \tilde{\boldsymbol{P}}_{\mathrm{col}}, \tag{A16}$$

the matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ describe thus transformations to coordinate systems in which the projectors $\boldsymbol{P}_{\mathrm{col}}$ and $\boldsymbol{P}_{\mathrm{row}}$, respectively, are diagonal.