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J. Phys. A: Math. Gen. 39 (2006) 7383-7409

doi:10.1088/0305-4470/39/23/015

# **Optimized lower bounds for** *N***-body Hamiltonians**

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Received 4 January 2006 Published 23 May 2006 Online at stacks.iop.org/JPhysA/39/7383

#### Abstract

Generalizing a method used previously for three-body, four-body and very recently for five-body systems, we derive a lower bound for the ground state energy of an *N*-body Hamiltonian, with arbitrary *N*. Because the expression of the lower bound obtained in this way depends on a number of parameters, we obtain in fact a family of lower bounds, a lower bound for each set of values of these parameters. The best of these is of course obtained by maximizing over these parameters and is correspondingly named optimized lower bound. The set of values of the parameters corresponding to the optimized lower bound satisfy a number of relations, named universal dynamical constraints, which result from the application of a dynamical principle and are independent of the particular form of the potential. For N = 3, 4, 5, they can be worked out in the most general case. For N = 6 up, they can be worked out only for particular mass configurations. Furthermore, the optimized lower bound proves to be saturated in the harmonic oscillator case.

PACS number: 03.65.-w

#### 1. Introduction

The *N*-body problems are very complicated. Even the most simple of them, that is, the onebody problem in a central potential or the two-body problem in the case of a translationally and rotationally invariant potential, are exactly solvable only in a very limited number of cases. The complexity of the problem grows rapidly with the number of particles *N*. Even the numerical resolution, very simple in the case of one-body and two-body problems under the conditions mentioned above, gets complicated quickly as the number of particles grows, requiring thereby considerable calculational facilities. An alternative to numerical computations is to focus oneself on exact results. Among these, exact lower bounds for *N*-body Hamiltonians occupy

0305-4470/06/237383+27\$30.00 © 2006 IOP Publishing Ltd Printed in the UK

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a particular place. Our goal here is to derive lower bounds for the ground state energies of *N*-body systems in the case of non-relativistic kinematics and translationally invariant two-body forces, i.e., for systems described by Hamiltonians of the form

$$H = \sum_{i=1}^{N} \frac{1}{2m_i} p_i^2 + \sum_{i< j=1}^{N} V^{(ij)}(r_{ij}),$$
(1)

where  $m_i$ ,  $r_i$ ,  $p_i$  stand, respectively, for the mass, the position and the linear momentum of the *i*th particle.  $r_{ij} := r_i - r_j$ ,  $i \neq j = 1, 2, ..., N$ . It will be noted that the potential  $V^{(ij)}$  from which the two-body force is derived may depend on the two involved particles. Our procedure will generalize to arbitrary N optimized lower bounds obtained previously for three-body [1] and four-body [2–5] cases.

Our work may have applications in various areas of physics and even in quantum chemistry. We can by no means pretend to be exhaustive here. In the following, let us simply cite some possible applications in the two domains of nuclear and particle physics. In the framework of the so-called potential models of hadronic spectroscopy, baryons are considered as three-quark bound states and the hypothetical multi-quark states, also called exotic hadrons, are treated as bound states of more than three quarks and/or anti-quarks [6, 7]. To determine the ground state energy of such hadrons, one often has recourse to variational calculations, such as systematic expansions on correlated Gaussians [8]. Such computations provide us with an upper bound for the ground state energy. If we want this upper bound to be accurate, i.e., close to the exact ground state energy, one must include many terms in the variational calculations. This results in involved computations. On the other hand, our procedure described hereafter provides one with an accurate lower bound for the ground state energy. Combining the upper and lower bounds would result in a framing of the ground state energy. Furthermore in the case of exotic hadrons, one deals with the important issue of stability. In other words, one has to examine whether multi-quark states are relatively stable or spontaneously decay via a super-allowed mechanism into ordinary hadrons, by a simple rearrangement of quarks and/or anti-quarks [6, 7, 9]. To this end, one has to compare the ground state energy of the multi-quark state under study with those of its possible dissociation thresholds. One then concludes that the multi-quark state is stable or unstable according to whether the ground state energy of the multi-quark is lower than the energies of all its dissociation thresholds or not. Here the lower bound obtained by our procedure may have a twofold interest: it gives a relatively accurate approximation to the ground state energy of the multi-quark state and, in addition, if it proves that such a lower bound is greater than one of the multi-quark dissociation thresholds, one immediately concludes that the multi-quark state is unstable. Nearly the same situation occurs for exotic molecules with bosonic constituents [10]. The same central issue of stability is addressed. The only important difference with the multi-quark states case is the mechanism of binding. To be more precise, exotic molecules are bound by electromagnetic forces whereas multi-quark states are bound by strong forces. This results in the case of a systematic expansion on correlated Gaussians in a slower convergence of the computations as compared with the multi-quark case (it is a known general feature of the method of systematic expansion on correlated Gaussians that it works better for smooth than for singular potentials [2], as it is the case for the Coulombic potential, responsible for the binding of exotic molecules). All we have said for multi-quark states can be repeated word by word for exotic molecules with bosonic constituents. Another possible application of our procedure is to the so-called borromean systems [11], i.e., bound systems with no bound subsystems, which are seen in nuclear physics. For those systems it is the kinetic energy decomposition, which is (as we will show below) the starting point of our procedure, that serves to obtain sufficient conditions for the nonexistence of borromean systems.

## 2. Optimized lower bound

Our starting point will be the following decomposition,

$$\sum_{i=1}^{N} \frac{1}{2m_i} p_i^2 = \left(\sum_{j=1}^{N} b_j p_j\right) \left(\sum_{i=1}^{N} p_i\right) + \sum_{i< j=1}^{N} a_{ij} p_{ij}^2,$$
(2)

of the kinetic part of the Hamiltonian involving the parameters  $b_j$ , j = 1, ..., N, and the necessary positive parameters  $a_{ij}$ , i < j = 1, 2, ..., N.  $p_{ij}$  is a linear combination of the various momenta  $p_k$ ,

$$p_{ij} = \sum_{k=1}^{N} \frac{x_{ij,k}}{2} p_k,$$
(3)

with the coefficients  $x_{ij,k}$  of the linear combination chosen such that  $r_{ij}$  and  $p_{ij}$  are conjugate variables of one another, that is, satisfying canonical commutation relations

$$[r_{ij,k}, p_{ij,\ell}] = i\hbar \delta_{k,\ell} \qquad k, \ell = 1, 2, 3,$$
(4)

where  $r_{ij,k}$  and  $p_{ij,\ell}$  stand, respectively, for the kth component of  $r_{ij}$  and the  $\ell$ th component of  $p_{ij}$ . Replacing the momenta  $p_{ij}$  by their expressions, (3), (2) can be rewritten as

$$\sum_{i=1}^{N} \frac{1}{2m_i} \boldsymbol{p}_i^2 = \left(\sum_{j=1}^{N} b_j \boldsymbol{p}_j\right) \left(\sum_{i=1}^{N} \boldsymbol{p}_i\right) + \sum_{i< j=1}^{N} \frac{a_{ij}}{4} \left(\sum_{k=1}^{N} x_{ij,k} \boldsymbol{p}_k\right)^2.$$
(5)

It will be remarked that the parameters  $b_j$ ,  $a_{ij}$  and  $x_{ij,k}$  are constrained by relations obtained by identifying both sides of (5). More precisely, the identification of the left-hand side of (5)with its right-hand side provides N + N(N-1)/2 constraints. If one remarks that the number of  $b_j$  is N and the number of  $a_{ij}$  is N(N-1)/2, these constraints may be used to eliminate  $b_i$  and  $a_{ij}$  in favour of  $x_{ij,k}$ . From now on,  $b_j$  and  $a_{ij}$  are considered as implicit functions of  $x_{ij,k}$ . We may, without loss of generality, take  $x_{ij,i}$  equal to 1 by a redefinition of  $a_{ij}$  and of  $x_{ij,k}$  for  $k \neq i = 1, 2, ..., N$ . Then imposing the canonical commutation relations (4) one ends with  $x_{ij,j} = -1$ . The decomposition of the Hamiltonian (1) corresponding to (5) is

$$H = \left(\sum_{j=1}^{N} b_j p_j\right) \left(\sum_{i=1}^{N} p_i\right) + \sum_{i< j=1}^{N} \left(\frac{a_{ij}}{4} \left(\sum_{k=1}^{N} x_{ij,k} p_k\right)^2 + V_{(ij)}(r_{ij})\right).$$
(6)

Let  $|\Psi\rangle$  be the normalized ground state of the system and E the corresponding energy. We have

$$E = \langle \Psi | H | \Psi \rangle$$
  
=  $\langle \Psi | \left( \sum_{j=1}^{N} b_j p_j \right) \left( \sum_{i=1}^{N} p_i \right) | \Psi \rangle + \sum_{i< j=1}^{N} \langle \Psi | \left( \frac{a_{ij}}{4} \left( \sum_{k=1}^{N} x_{ij,k} p_k \right)^2 + V^{(ij)}(r_{ij}) \right) | \Psi \rangle.$  (7)  
Since the ground state  $|\Psi\rangle$  is invariant under translation, then

Since the ground state  $|\Psi\rangle$  is invariant under translation, then

$$\left(\sum_{i=1}^{N} p_{i}\right) |\Psi\rangle = \mathbf{0},\tag{8}$$

and thus the contribution of the first term on the right-hand side of (7) vanishes. The following results:

$$E = \sum_{i < j=1}^{N} \langle \Psi | \left( \frac{a_{ij}}{4} \left( \sum_{k=1}^{N} x_{ij,k} \boldsymbol{p}_k \right)^2 + V^{(ij)}(\boldsymbol{r}_{ij}) \right) | \Psi \rangle.$$
(9)

But, by virtue of the variational principle,

$$\langle \Psi | \left( \frac{a_{ij}}{4} \left( \sum_{k=1}^{N} x_{ij,k} \boldsymbol{p}_k \right)^2 + V^{(ij)}(\boldsymbol{r}_{ij}) \right) | \Psi \rangle \ge E_{ij}^{(2)}[a_{ij}(x_{kl,m})], \tag{10}$$

where  $E_{ij}^{(2)}[a_{ij}(x_{kl,m})]$  stands for the ground state energy of the two-particle Hamiltonian

$$H_{ij}^{(2)}[a_{ij}(x_{kl,m})] = \frac{a_{ij}}{4} \left( \sum_{k=1}^{N} x_{ij,k} \boldsymbol{p}_k \right)^2 + V^{(ij)}(\boldsymbol{r}_{ij}).$$
(11)

It follows that

$$E \ge \sum_{i
(12)$$

Thus one obtains a family of lower bounds for E, a lower bound

$$\sum_{i< j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{kl,m})],$$
(13)

for each set of values of the parameters  $x_{kl,m}$ . The best of these bounds corresponds obviously to those values of  $x_{kl,m}$  which maximize  $\sum_{i< j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{kl,m})]$ . The following is called the optimized lower bound:

$$E_{\text{olb}} := \max_{x_{kl,m}} \sum_{i< j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{kl,m})].$$
(14)

#### 3. Universal dynamical constraints

Before pursuing, we find it convenient to introduce the following notation:

$$L_N := \frac{N(N-1)}{2}, \qquad C_N := \frac{N(N-1)(N-2)}{2}, \qquad R_N := \frac{N(N-1)}{2} - 1 = L_N - 1.$$
(15)

When  $\sum_{i< j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{kl,m})]$  reaches its maximum with respect to  $x_{kl,m}$ , all the derivatives with respect to  $x_{kl,m}$  must vanish, that is,

$$\sum_{i
(16)$$

Since  $\partial E_{ij}^{(2)}/\partial a_{ij}$  are not all zero, the  $L_N \times C_N$  matrix  $\mathbf{\tilde{B}}$  with matrix elements  $\partial a_{ij}/\partial x_{kl,m}$ , where ij and kl, m correspond, respectively, to the line and column indices, must be of rank  $R_N$  at most. This means that every  $L_N \times L_N$  matrix extracted from the matrix  $\mathbf{\tilde{B}}$ , by selecting  $L_N$  of its columns, must be of determinant zero. Requiring the matrix  $\mathbf{\tilde{B}}$  to be of rank  $R_N$  at most will result in  $C_N - R_N$  relations between the values of the  $C_N$  parameters when the optimized lower bound is reached. These relations will be referred to hereafter as universal dynamical constraints, universal because they have the nice property to be independent of the particular form of the potential, and dynamical since they result from the application of a dynamical principle, i.e., the variational principle. Let us now look for the explicit expressions of  $a_{ij}$  as functions of  $x_{kl,m}$ . Identifying both sides of (5) gives

$$b_k + \sum_{i< j=1}^N \frac{x_{ij,k}^2}{4} a_{ij} = \frac{1}{2m_k},$$
(17)

for the terms in  $p_k^2$  and

$$b_k + b_\ell + \sum_{i< j=1}^N \frac{x_{ij,k} x_{ij,\ell}}{2} a_{ij} = 0,$$
(18)

for the terms in  $p_k \cdot p_\ell$ ,  $k \neq \ell = 1, 2, ..., N$ . Combining equations (17) and (18), one obtains a set of  $L_N$  linear equations with  $L_N$  unknowns  $a_{ij}$ , and  $C_N$  parameters  $x_{ij,k}$ ,

$$\sum_{k=j=1}^{N} \tilde{C}_{ij,k\ell} a_{k\ell} = \frac{1}{2m_i} + \frac{1}{2m_j},$$
(19)

with

$$\tilde{C}_{ij,k\ell} = \left(\frac{x_{k\ell,i} - x_{k\ell,j}}{2}\right)^2.$$
(20)

Equation (19) can be written in the matrix form as

$$\widetilde{\mathbf{D}}\mathbf{A} = \boldsymbol{\alpha},\tag{21}$$

where  $\widetilde{\mathbf{D}}$  is an  $L_N \times L_N$  matrix, with  $\widetilde{\mathbf{D}}_{11} = \tilde{C}_{12,12}$ ,  $\widetilde{\mathbf{D}}_{12} = \tilde{C}_{12,13}, \dots, \widetilde{\mathbf{D}}_{21} = \tilde{C}_{13,12}, \dots, \widetilde{\mathbf{D}}_{N(N-1)/2N(N-1)/2} = \tilde{C}_{N(N-1),N(N-1)}$ , that is, using (20),

$$\widetilde{\mathbf{D}} := \frac{1}{4} \begin{pmatrix} (x_{12,1} - x_{12,2})^2 & (x_{13,1} - x_{13,2})^2 & \cdots & (x_{N-1N,1} - x_{N-1N,2})^2 \\ (x_{12,1} - x_{12,3})^2 & (x_{13,1} - x_{13,3})^2 & \cdots & (x_{N-1N,1} - x_{N-1N,3})^2 \\ \vdots & \vdots & \ddots & \vdots \\ (x_{12,N-1} - x_{12,N})^2 & (x_{13,N-1} - x_{13,N})^2 & \cdots & (x_{N-1N,N-1} - x_{N-1N,N})^2 \end{pmatrix}, \quad (22)$$

A and  $\alpha$  in (21) are two column matrices with  $L_N$  lines given by

$$\mathbf{A} := \begin{pmatrix} a_{12} \\ a_{13} \\ \vdots \\ a_{N-1N} \end{pmatrix}, \qquad \boldsymbol{\alpha} := \begin{pmatrix} \alpha_{12} \\ \alpha_{13} \\ \vdots \\ \alpha_{N-1N} \end{pmatrix}$$
(23)

with

$$\alpha_{ij} := \frac{1}{2m_i} + \frac{1}{2m_j}.$$
(24)

The matrix equation (21) can be inverted, thus giving  $L_N a_{ij}$  as functions of  $C_N x_{k\ell,m}$ ,

$$\mathbf{A} = \mathbf{\hat{D}}^{-1} \boldsymbol{\alpha}. \tag{25}$$

Needless to say that the analytical inversion of the matrix  $\tilde{\mathbf{D}}$  in the most general case, i.e., for the most general mass configuration, is far from being an easy task. Fortunately, we do not need the explicit expressions of  $a_{ij}$  in terms of the parameters  $x_{k\ell,m}$  to have access to the universal dynamical constraints as we will show in the following. Indeed taking the derivative of (21) with respect to  $x_{k\ell,m}$ ,  $(m \neq k, m \neq \ell)$ , one obtains, taking into account that  $\alpha_{ij}$  do not depend on  $x_{k\ell,m}$ , and after multiplying by  $\tilde{\mathbf{D}}^{-1}$ ,

$$\frac{\partial \mathbf{A}}{\partial x_{k\ell,m}} = -\widetilde{\mathbf{D}}^{-1} \frac{\partial \mathbf{D}}{\partial x_{k\ell,m}} \mathbf{A}.$$
(26)

Equation (26) shows that the matrix  $\tilde{\mathbf{B}}$  is minus the product of the inverse of the  $L_N \times L_N$  matrix  $\tilde{\mathbf{D}}$  by an  $L_N \times C_N$  matrix  $\tilde{\mathbf{M}}'$ 

$$\widetilde{\mathbf{B}} = -\widetilde{\mathbf{D}}^{-1}\widetilde{\mathbf{M}}'.$$
(27)

The matrix  $\tilde{\mathbf{M}}'$  is constructed in the following way: consider the sole column of the matrix  $\tilde{\mathbf{D}}$  which depends on a given  $x_{k\ell,m}$ ,  $k < \ell = 1, 2, ..., N$ ,  $m \neq k, m \neq \ell$ , m = 1, 2, ..., N, take its derivative with respect to  $x_{k\ell,m}$  and multiply the result by  $a_{k\ell}$ . The column obtained in this way is nothing but the column of the matrix  $\tilde{\mathbf{M}}'$  corresponding to the column index  $k\ell$ , m. Equation (27) shows that the rank condition on  $\tilde{\mathbf{B}}$  is equivalent to the same rank condition on a simpler matrix  $\tilde{\mathbf{M}}'$ . We can even replace this rank condition on  $\tilde{\mathbf{M}}'$  by the same rank condition on a simpler matrix. Indeed, we know from the properties of determinants [12] that when a column of a matrix is multiplied by a factor, the corresponding determinant is multiplied by the same factor. Therefore, the determinant of any  $L_N \times L_N$  matrix extracted from the matrix  $\tilde{\mathbf{M}}'$  shows in the form of a product of  $L_N$  factors  $a_{ij}$ , not necessarily all different, by the determinant of the same square matrix by putting formally all the factors  $a_{ij}$  equal to 1. We may then conclude that the rank condition on the matrix  $\tilde{\mathbf{M}}'$  by formally putting all  $a_{ij}$  equal to 1. At this point, we are in a position to give a three-step recipe in order to work out the universal dynamical constraints:

*First step: construction of the matrix*  $\mathbf{\tilde{M}}$ . Take the only column of the matrix  $\mathbf{\tilde{D}}$  which depends on a given  $x_{k\ell,m}$  and derive it with respect to  $x_{k\ell,m}$ . The result is nothing but the column of the matrix  $\mathbf{\tilde{M}}$  corresponding to the column index  $k\ell, m$ . Repeating the process for each  $k\ell, m$ ,  $k < \ell = 1, 2, ..., N, m \neq k, m \neq \ell, m = 1, 2, ..., N$  (for example, we may choose to vary *m* first, then  $\ell$ , and finally *k*), one constructs the matrix  $\mathbf{\tilde{M}}$ . It is worthwhile to emphasize that each column of the matrix  $\mathbf{\tilde{D}}$  gives rise to N - 2 columns of the matrix  $\mathbf{\tilde{M}}$ . Therefore, the columns of the matrix  $\mathbf{\tilde{M}}$  come in blocks labelled by  $k\ell$ , each consisting of N - 2 columns and involving the same number of parameters  $x_{k\ell,m}$ , namely N - 2 parameters, with given  $k\ell$ and varying *m*.

Second step: choice of the independent parameters. Since we know that the number of universal dynamical constraints is  $C_N - R_N$ , one can take advantage of these relations to eliminate the same number of parameters in favour of the remaining  $R_N$  parameters, which are considered as independent parameters. Many choices of such independent parameters are allowed. A choice which we found particularly interesting consists in taking all the parameters, except one of them, occurring in three blocks. We are then faced with two possible situations: either the number of parameters selected in this way equals the number of independent parameters, as in the N = 3 and N = 4 cases, and we have achieved our task, or the number of chosen parameters is smaller than the number of independent parameters and we must complete by further parameters taken out of the initially chosen three blocks. This last situation occurs for  $N \ge 5$ .

Third step: determination of the universal dynamical constraints. Choose  $L_N \times L_N$  matrices out of the matrix  $\widetilde{\mathbf{M}}$  by selecting  $L_N$  of its columns. For each chosen matrix calculate the corresponding determinant, write it in a factorized form, and equate it to zero. Then solve for the dependent parameters in terms of the independent ones. You may obtain more than one solution. Select the correct one by applying the following two criteria:

• The solution must correspond to the correct limits when the system exhibit symmetries for instance, all the parameters must be equal to zero in the equal mass case. • The parameters chosen as independent parameters in step 2 must be treated as independent parameters in the sense that an expression containing only independent parameters cannot be set to zero.

The minimal number of matrices to be considered in this step is the number of universal dynamical constraints, i.e.,  $C_N - R_N$ , but one may find itself in the necessity to consider additional matrices because the initially selected matrices may not exhaust the whole information implied by the rank condition. This point shows the great importance of the choice of the square matrices in this step. A clever choice of these matrices leads to a fast determination of the universal dynamical constraints. Let us say that it is merely a matter of skill.

Two comments on the universal dynamical constraints are in order:

First, as *N* increases by one unit, a further qualitative difficulty appears in the computation of the universal dynamical constraints. To state the things crudely: the three-body case is rather trivial compared to the four-body case, this latter in turn is a child's play when compared to the five-body case, and the cases  $N \ge 6$  seem to be intractable for the most general mass configuration.

Second, the universal dynamical constraints are not of kinematical nature, so we can ignore them, perform the maximization procedure, and verify *a posteriori* that they are numerically verified at the maximum. Nonetheless, the universal dynamical constraints are extremely important at least for practical reasons. Indeed with these relations at hand the optimization procedure can be performed over independent parameters rather than over the totality of the parameters, which makes it much more easier. This is particularly clear if we have in mind that we deal with nonlinear optimization problems.

Let us now give the explicit expressions of the universal dynamical constraints for the three-body case [1], the four-body case [2] and the five-body case [18]. We will illustrate our three-step recipe described above in the three-body case. But since we find this an almost trivial case, because of not exhibiting the typical difficulties inherent to the procedure, we will also show how our procedure works in the four-body case in appendix A.

#### 3.1. Three-body case

In this case, we have only one universal dynamical constraint, which may be expressed [1] as

$$e_1 = \frac{d_2 - c_3}{1 - c_3 d_2},\tag{28}$$

where we have made the following change of notation:

$$c_3 := x_{12,3}, \qquad d_2 := x_{13,2}, \qquad e_1 := x_{23,1}.$$
 (29)

Let us apply our three-step procedure described above to recover the result (28).

*First step.* Using (22) for N = 3 one obtains for the  $3 \times 3$  matrix  $\hat{\mathbf{D}}$  the following expression:

$$\widetilde{\mathbf{D}} = \frac{1}{4} \begin{pmatrix} 4 & (d_2 - 1)^2 & (e_1 - 1)^2 \\ (c_3 - 1)^2 & 4 & (e_1 + 1)^2 \\ (c_3 + 1)^2 & (d_2 + 1)^2 & 4 \end{pmatrix}.$$
(30)

Each column of  $\widetilde{\mathbf{D}}$  gives rise to one column of the matrix  $\widetilde{\mathbf{M}}$ , so  $\widetilde{\mathbf{M}}$  is also a 3 × 3 matrix

$$\widetilde{\mathbf{M}} = \frac{1}{2} \begin{pmatrix} 0 & d_2 - 1 & e_1 - 1 \\ c_3 - 1 & 0 & e_1 + 1 \\ c_3 + 1 & d_2 + 1 & 0 \end{pmatrix}.$$
(31)

Second step. Let us take here  $c_3$  and  $d_2$  as independent parameters.

Third step. Our rank condition translates here into a single relation

$$\det \tilde{\mathbf{M}} = 0, \tag{32}$$

which gives

$$c_3 d_2 e_1 - c_3 + d_2 - e_1 = 0. ag{33}$$

Solving the last equation for  $e_1$ , one gets (28).

## 3.2. Four-body case

With the following change of notation,

 $c_{3} := x_{12,3}, \quad c_{4} := x_{12,4}, \quad d_{2} := x_{13,2}, \quad d_{4} := x_{13,4}, \quad e_{2} := x_{14,2}, \quad e_{3} := x_{14,3},$   $f_{1} := x_{23,1}, \quad f_{4} := x_{23,4}, \quad g_{1} := x_{24,1}, \quad g_{3} := x_{24,3}, \quad h_{1} := x_{34,1}, \quad h_{2} := x_{34,2},$ the seven universal dynamical constraints can be expressed [2] as (34)

$$e_{3} = \frac{c_{3} - c_{4} - d_{2} + d_{4} + e_{2} + c_{4}d_{2} - c_{3}d_{4} - c_{3}e_{2} - d_{4}e_{2} + c_{3}d_{4}e_{2}}{1 - c_{4} - d_{2} + c_{4}d_{2}},$$

$$f_{1} = \frac{d_{2} - c_{3}}{1 - c_{3}d_{2}},$$

$$f_{4} = \frac{d_{4} - c_{4} + c_{4}d_{2} - c_{3}d_{4}}{1 - c_{3}d_{2}},$$

$$g_{1} = \frac{e_{2} - c_{4}}{1 - c_{4}e_{2}},$$

$$g_{3} = \frac{d_{4} + e_{2} - c_{4} - d_{2} + c_{3}d_{2} + c_{4}d_{2} - c_{3}d_{4} - d_{4}e_{2} - c_{3}d_{2}e_{2} + c_{3}d_{4}e_{2}}{1 - d_{2} - c_{4}e_{2} + c_{4}d_{2}e_{2}},$$

$$h_{1} = \frac{c_{3} - c_{4} - d_{2} + d_{4} + c_{4}d_{2} - c_{3}d_{4} - d_{4}e_{2} + c_{3}d_{4}e_{2}}{1 - c_{4} - d_{2} + d_{4} + c_{4}d_{2} - c_{3}d_{2}e_{2}},$$

$$h_{2} = \frac{e_{2} - d_{2} - c_{4}e_{2} + c_{3}d_{2} + c_{4}d_{2}e_{2} - c_{3}d_{2}e_{2}}{1 - c_{4} - d_{2} + d_{4} + c_{4}d_{2} - c_{3}d_{4} - d_{4}e_{2} + c_{3}d_{4}e_{2}}.$$
(35)

1

The reader interested in application of our three-step procedure to the four-body case may find full details in appendix A.

#### 3.3. Five-body case

If we make the following change of notation in the five-body case,

$$c_{3} = x_{12,3}, \quad c_{4} = x_{12,4}, \quad c_{5} = x_{12,5}, \quad d_{2} = x_{13,2}, \quad d_{4} = x_{13,4}, \quad d_{5} = x_{13,5}, \\ e_{2} = x_{14,2}, \quad e_{3} = x_{14,3}, \quad e_{5} = x_{14,5}, \quad f_{2} = x_{15,2}, \quad f_{3} = x_{15,3}, \quad f_{4} = x_{15,4}, \\ g_{1} = x_{23,1}, \quad g_{4} = x_{23,4}, \quad g_{5} = x_{23,5}, \quad h_{1} = x_{24,1}, \quad h_{3} = x_{24,3}, \quad h_{5} = x_{24,5}, \\ j_{1} = x_{25,1}, \quad j_{3} = x_{25,3}, \quad j_{4} = x_{25,4}, \quad k_{1} = x_{34,1}, \quad k_{2} = x_{34,2}, \quad k_{5} = x_{34,5}, \\ l_{1} = x_{35,1}, \quad l_{2} = x_{35,2}, \quad l_{4} = x_{35,4}, \quad n_{1} = x_{45,1}, \quad n_{2} = x_{45,2}, \quad n_{3} = x_{45,3}, \end{cases}$$

$$(36)$$

1

the 21 universal dynamical constraints [18] then read

$$e_{3} = \frac{c_{3}d_{4}e_{2} - c_{3}d_{4} - c_{3}e_{2} + c_{3} - d_{4}e_{2} + d_{4} + c_{4}d_{2} - d_{2} + e_{2} - c_{4}}{(1 - c_{4})(1 - d_{2})}$$

$$f_{2} = \frac{c_{5} + j_{1}}{1 + j_{1}c_{5}},$$

$$\begin{split} f_{3} &= \frac{j_{1}c_{5} - c_{5}d_{2}j_{1} - c_{3}d_{5} + j_{1}c_{3}d_{5} + c_{3} - d_{5}j_{1} - c_{3}j_{1} - d_{2} + d_{5} + j_{1}}{(1 - d_{2})(1 + j_{1}c_{5})}, \\ f_{4} &= \frac{j_{1}c_{4}e_{5} - c_{5}e_{2}j_{1} + c_{4} - e_{5}c_{4} - c_{4}j_{1} - e_{5}j_{1} + j_{1}c_{5} - e_{2} + e_{5} + j_{1}}{(1 - e_{2})(1 + j_{1}c_{5})}, \\ g_{1} &= \frac{c_{3} - d_{2}}{c_{3}d_{2} - 1}, \\ g_{4} &= \frac{c_{4}d_{2} - c_{3}d_{4} - c_{4} + d_{4}}{1 - c_{3}d_{2}}, \\ g_{5} &= \frac{d_{2}c_{5} - c_{3}d_{5} - c_{5} + d_{5}}{1 - c_{3}d_{2}}, \\ h_{1} &= \frac{e_{2} - c_{4}}{1 - c_{3}d_{2}}, \\ h_{3} &= \frac{c_{4}d_{2} - c_{4} + c_{3}d_{2} + e_{2} + d_{4} - c_{3}e_{2}d_{2} - c_{3}d_{4} + c_{3}d_{4}e_{2} - d_{4}e_{2} - d_{2}}{(1 - d_{2})(1 - c_{4}e_{2})}, \\ h_{5} &= \frac{c_{5}e_{2} - c_{4}e_{5} - c_{5} + e_{5}}{1 - c_{4}e_{2}}, \\ j_{3} &= \frac{c_{3}d_{5}j_{1} - c_{3}d_{2}j_{1} - c_{3}d_{5} + c_{3}d_{2} + j_{1} + c_{5}j_{1} - c_{5}d_{2}j_{1} - d_{5}j_{1} + d_{5} - d_{2}}{1 + c_{5} - d_{2} - d_{2}c_{5}}, \\ j_{4} &= \frac{j_{1} + j_{1}c_{5} - e_{5}j_{1} + c_{4}e_{5}j_{1} - c_{4}e_{2}j_{1} - c_{4}e_{5} + e_{5} - e_{2} + c_{4}e_{2}}{1 + c_{5} - d_{2} - c_{5}e_{2}}, \\ k_{1} &= \frac{c_{3} - c_{4} - d_{2} + d_{4} - c_{3}d_{4} + c_{4}d_{2} - d_{4}e_{2} + c_{3}d_{4}e_{2}}{1 - c_{4} - d_{2} + d_{4} - c_{3}d_{4} + c_{4}d_{2} - d_{4}e_{2} + c_{3}d_{4}e_{2}}, \\ k_{5} &= \frac{e_{1} - d_{2} + d_{4} - c_{3}d_{4} + c_{4}d_{2} - d_{4}e_{2} + c_{3}d_{4}e_{2}}{1 - c_{4} - d_{2} + d_{4} - c_{3}d_{4} + c_{4}d_{2} - d_{4}e_{2} + c_{3}d_{4}e_{2}}, \\ l_{1} &= \frac{c_{3} - d_{2} + j_{1} - c_{3}j_{1} + c_{5}j_{1} - c_{5}d_{2}j_{1}}{1 - c_{4} - d_{2} + d_{4} - c_{3}d_{4} + c_{4}d_{2} - d_{4}e_{2} + c_{3}d_{4}e_{2}}, \\ l_{2} &= \frac{c_{5} - d_{2} + j_{1} + c_{3}j_{1} + c_{3}j_{1} + c_{3}j_{1} + c_{3}j_{1}}{1 - c_{2}d_{2} + d_{5} - c_{3}d_{5} + c_{5}j_{1} - d_{5}d_{2}j_{1}}, \\ l_{2} &= \frac{c_{5} - d_{2} + j_{1} + c_{3}d_{2} - c_{5}d_{2} - c_{5}d_{2}}{1 - c_{4} - d_{2} + d_{5} - c_{3}d_{5} + c_{5}j_{1} - c_{3}d_{2}}}{1 - c_{4} - d_{2} + d_{5} - c_{3}d_{5} + c_{5}j_{1} - c_{5}d_{2}j_{1}}, \\ l_{2} &= \frac{c_{5} - d_$$

## 3.4. Particular configurations for the six-body case

As we have already noted, the calculations to obtain the universal dynamical constraints in the most general case become intractable from the six-body up. For  $N \ge 6$  the universal dynamical

constraints can be computed only for particular mass configurations. For the simplest such case, i.e., the six-body case, we can treat the configurations where up to three different masses are involved, i.e., the configurations  $(m_1, m_2, 4m_3)$ ,  $(m_1, 2m_2, 3m_3)$ ,  $(2m_1, 2m_2, 2m_3)$ , if we restrict ourselves to two-body interactions depending only on the constituent masses. The full details of the derivation of the corresponding universal dynamical constraints are included in appendix B, together with a discussion about how our general method can be adapted to work out the universal dynamical constraints when symmetries are present, i.e., for particular mass configurations. In the following, we will simply give the relations implied by the symmetries of the problem, together with the computed universal dynamical constraints.

3.4.1.  $(m_1, m_2, 4m_3)$ . Using symmetry arguments, it is easy to convince oneself that there are only three independent  $b_i$ ,

$$b_1, b_2, b_3 = b_4 = b_5 = b_6, \tag{38}$$

four independent  $a_{ij}$ ,

$$a_{12}, a_{13} = a_{14} = a_{15} = a_{16}, a_{23} = a_{24} = a_{25} = a_{26}, a_{34} = a_{35} = a_{36} = a_{45} = a_{46} = a_{56},$$
  
(39)

five independent parameters  $x_{ij,k}$ ,

$$x_{12,3} = x_{12,4} = x_{12,5} = x_{12,6} = c, \qquad x_{13,2} = x_{14,2} = x_{15,2} = x_{16,2} = d$$

$$x_{13,4} = x_{13,5} = x_{13,6} = x_{14,3} = x_{14,5} = x_{14,6} = x_{15,3} = x_{15,4}$$

$$= x_{15,6} = x_{16,3} = x_{16,4} = x_{16,5} = e$$

$$x_{23,1} = x_{24,1} = x_{25,1} = x_{26,1} = f$$

$$x_{23,4} = x_{23,5} = x_{23,6} = x_{24,3} = x_{24,5} = x_{24,6} = x_{25,3} = x_{25,4}$$
(40)

$$23,4 - x_{23},5 - x_{23},6 - x_{24},5 - x_{24},5 - x_{24},6 - x_{25},5$$

 $= x_{25,6} = x_{26,3} = x_{26,4} = x_{26,5} = g,$ 

and all the other parameters  $x_{ij,k}$  are equal to zero. In this case, we have two universal dynamical constraints which we can use to express f and g in terms of c, d and e:

$$f = \frac{c-d}{cd-1}, \qquad g = \frac{c-e-cd+ce}{cd-1}.$$
 (41)

3.4.2.  $(m_1, 2m_2, 3m_3)$ . Here, again by symmetry arguments, we have three independent  $b_i$ ,  $b_1, b_2 = b_3, b_4 = b_5 = b_6$ , (42)

five independent  $a_{ij}$ ,

 $a_{12} = a_{13}, a_{14} = a_{15} = a_{16}, a_{23}, a_{24} = a_{25} = a_{26} = a_{34} = a_{35} = a_{36}, a_{45} = a_{46} = a_{56},$  (43) seven independent parameters  $x_{ij,k}$ 

$$\begin{aligned} x_{12,3} &= x_{13,2} = c, \\ x_{12,4} &= x_{12,5} = x_{12,6} = x_{13,4} = x_{13,5} = x_{13,6} = d, \\ x_{14,2} &= x_{14,3} = x_{15,2} = x_{15,3} = x_{16,2} = x_{16,3} = e, \\ x_{14,5} &= x_{14,6} = x_{15,4} = x_{15,6} = x_{16,4} = x_{16,5} = f, \\ x_{24,1} &= x_{25,1} = x_{26,1} = x_{34,1} = x_{35,1} = x_{36,1} = g, \\ x_{24,3} &= x_{34,2} = x_{25,3} = x_{35,2} = x_{26,3} = x_{36,2} = h, \\ x_{24,5} &= x_{24,6} = x_{25,4} = x_{25,6} = x_{26,4} = x_{26,5} = x_{34,5} = x_{34,6} \\ &= x_{35,4} = x_{35,6} = x_{36,4} = x_{36,5} = i, \end{aligned}$$
(44)

and all the other  $x_{ij,k}$  are equal to zero. Here we have three universal dynamical constraints which allow us to express g, h and i in terms of c, d, e and f:

$$g = \frac{d-e}{de-1}, \qquad h = \frac{c+de-e-ce}{de-1}, \qquad i = \frac{d+df-f-de}{de-1}.$$
 (45)

3.4.3.  $(2m_1, 2m_2, 2m_3)$ . Using once again symmetry arguments, it is easy to conclude that there are three independent  $b_i$ ,

$$b_1 = b_2, b_3 = b_4, b_5 = b_6, \tag{46}$$

six independent  $a_{ij}$ ,

 $a_{12}, a_{13} = a_{14} = a_{23} = a_{24}, a_{15} = a_{16} = a_{25} = a_{26}, a_{34}, a_{35} = a_{36} = a_{45} = a_{46}, a_{56},$  (47) nine independent parameters  $x_{ij,k}$ ,

$$\begin{aligned} x_{13,2} &= x_{14,2} = x_{23,1} = x_{24,1} = c, \\ x_{13,4} &= x_{14,3} = x_{23,4} = x_{24,3} = d, \\ x_{13,5} &= x_{13,6} = x_{14,5} = x_{14,6} = x_{23,5} = x_{23,6} = x_{24,5} = x_{24,6} = e, \\ x_{15,2} &= x_{16,2} = x_{25,1} = x_{26,1} = f, \\ x_{15,3} &= x_{15,4} = x_{16,3} = x_{16,4} = x_{25,3} = x_{25,4} = x_{26,3} = x_{26,4} = g, \\ x_{15,6} &= x_{16,5} = x_{25,6} = x_{26,5} = h, \\ x_{35,1} &= x_{35,2} = x_{36,1} = x_{36,2} = x_{45,1} = x_{45,2} = x_{46,1} = x_{46,2} = i, \\ x_{35,4} &= x_{36,4} = x_{45,3} = x_{46,3} = j, \\ x_{35,6} &= x_{36,5} = x_{45,6} = x_{46,5} = k, \end{aligned}$$

and all the other  $x_{ij,k}$  are equal to zero. In this latter case, we have four universal dynamical constraints which we can use to express f, g, j and k in terms of c, d, e, h and i:

$$f = \frac{c+i+ei-ci}{1+ei}, \qquad g = \frac{e+i}{1+ei}, \qquad (49)$$
  
$$j = \frac{e+di+i-d}{1+e}, \qquad k = \frac{h-e+ei+ehi}{1+e}.$$

#### 4. Special configurations

Let us now consider in turn the three special configurations  $(N \times m)$ , i.e., an *N*-body system with the *N* particles having the same mass *m*,  $((N - 1) \times m, M)$ , i.e., an *N*-body system with N - 1 particles with the same mass *m* and a particle with mass  $M, m \neq M$ , and  $(n \times m, n' \times M)$ , i.e., an *N*-body system with *n* particles with the same mass *m* and *n'* particles with the same mass *M*, with  $m \neq M$ , n + n' = N, and both *n* and *n'* greater than 1. We will work in the hypothesis where the two-body potential depends only on the masses of the constituent particles. Here, the symmetry properties are sufficient to entirely determine the universal dynamical constraints for these three particular configurations. In addition to this fact, we have been able to prove [17] analytically the saturation of the optimized lower bound in the harmonic oscillator case for these same particular configurations. A separate detailed paper [17] is devoted to the analytical proof of saturability, including in particular the explicit computations of both the optimized lower bound and the ground state energy, in the harmonic oscillator case for the three special configurations mentioned above. So we will be very brief here.

## 4.1. $(N \times m)$ configurations

In this case

$$m_1 = m_2 = \dots = m_N = m, \tag{50}$$

and the system is invariant under any permutations of the N particles. This results in a single a and also in a single b,

$$a_{ij} = a, \qquad i < j = 1, \dots, N,$$
 (51)

$$b_i = b, \qquad i = 1, \dots, N, \tag{52}$$

and all the parameters  $x_{ij,k}$  must be equal to zero

$$x_{ij,k} = 0, \qquad i < j = 1, \dots, N, \quad k = 1, \dots, N, \qquad k \neq i, \quad k \neq j.$$
 (53)

Thus we have no parameter to adjust, one distinct value *a* for  $a_{ij}$  and one distinct value *b* for  $b_i$ . The N + N(N - 1)/2 relations obtained by identifying both sides of (5) reduce here to two relations, i.e.,

$$\frac{(N-1)}{4}a + b = \frac{1}{2m}, \qquad -\frac{1}{2}a + 2b = 0.$$
(54)

The linear system of equations (54) admits

$$a = \frac{2}{Nm}, \qquad b = \frac{1}{2Nm} \tag{55}$$

as a solution. Let us consider the case of a power law potential, i.e., a two-body potential of the form

$$v(\mathbf{r}_{ij}) = \lambda r_{ij}^{\nu},\tag{56}$$

with  $\lambda$  and  $\nu$  of the same sign. Then the optimized lower bound  $E_{olb}$  (14) simplifies in this particular case to

$$E_{\rm olb} = \frac{N(N-1)}{2} \left(\frac{2}{Nm}\right)^{\frac{\nu}{2+\nu}} |\lambda|^{\frac{2}{2+\nu}} E^{(2)}(1, \operatorname{sign}(\nu), \nu),$$
(57)

where  $E^{(2)}(\alpha, \lambda, \nu)$  denotes the ground state energy of the two-body Hamiltonian

$$H^{(2)} = \alpha p^2 + \lambda r^{\nu},\tag{58}$$

and sign(v) denotes the sign of v. To obtain (57), we make use of the scaling laws for power law potentials [13–16] which state, among other things, that the energy levels of a two-body Hamiltonian of the form (58) scale as

$$E^{(2)}(\alpha,\lambda,\nu) = \alpha^{\frac{\nu}{2+\nu}} |\lambda|^{\frac{2}{2+\nu}} E^{(2)}(1,\operatorname{sign}(\nu),\nu).$$
(59)

In the harmonic oscillator case, i.e. for v = 2,

$$E^{(2)}(1,1,2) = 3,$$
 (60)

and (57) simplifies to

$$E_{\rm olb} = 3N\left(N-1\right)\sqrt{\frac{\lambda}{2Nm}}.$$
(61)

On the other hand, one can show [17] that the ground state energy of the *N*-body harmonic oscillator is also given by (61). This means that the optimized lower bound is saturated, i.e., equal to the exact result, in the harmonic case for the particular mass configuration  $(N \times m)$ .

#### 4.2. $((N-1) \times m, M)$ configurations

One can always, without loss of generality, number the N - 1 particles with the same mass *m* from 1 to N - 1 and the single particle with mass *M* by *N*, that is,

$$m_1 = m_2 = \dots = m_{N-1} = m, \qquad m_N = M.$$
 (62)

Under the conditions specified above, the system is invariant under any permutations of the N - 1 particles with the same mass *m*. This results in the following relations,

$$a_{ij} = a_{mm}$$
  $i < j = 1, 2, ..., N - 1,$   $a_{iN} = a_{mM}$   $i < N,$  (63)

$$b_1 = b_2 = \dots = b_{N-1} = b, \tag{64}$$

and

$$x_{ij,k} = 0 \qquad i < j < N, \quad k \neq i, \quad k \neq j,$$
  

$$x_{iN,k} = \ell \qquad i < N, \qquad k \neq i, \quad k \neq N.$$
(65)

We have thus only one variational parameter  $\ell$  to adjust and two distinct values  $a_{mm}$  and  $a_{mM}$  for  $a_{ij}$ .

The N + N(N - 1)/2 relations obtained by identifying both sides of (5) reduce here to four relations, namely,

$$b + \frac{N-2}{4}a_{mm} + \frac{1}{4}a_{mM} + \frac{N-2}{4}\ell^2 a_{mM} = \frac{1}{2m},$$
  

$$b_N + \frac{N-1}{4}a_{mM} = \frac{1}{2M},$$
  

$$2b - \frac{1}{2}a_{mm} + \ell a_{mM} + \frac{N-3}{2}\ell^2 a_{mM} = 0,$$
  

$$b + b_N - \frac{1}{2}a_{mM} - \frac{N-2}{2}\ell a_{mM} = 0.$$
  
(66)

Equations (66) may be considered as a system of linear equations with four unknowns  $a_{mm}, a_{mM}, b, b_N$  and one parameter  $\ell$ . The resolution of this system is trivial and gives for  $a_{mm}$  and  $a_{mM}$  the following expressions in terms of the parameter  $\ell$ :

$$a_{mm}(\ell) = 2 \frac{(\ell+1)(\ell N - 3\ell + 1 + N)M - (\ell - 1)^2 m}{(\ell N + N - 2\ell)^2 m M},$$
  

$$a_{mM}(\ell) = 2 \frac{(N-1)m + M}{(\ell N + N - 2\ell)^2 m M}.$$
(67)

Let us consider as an example the case of a two-body interaction described by a power law potential

$$\begin{aligned}
\nu_{mm}(r_{ij}) &= \lambda_{mm} r_{ij}^{\nu_{mm}}, & i < j = 1, 2, \dots, N-1, \\
\nu_{mM}(r_{iN}) &= \lambda_{mM} r_{iN}^{\nu_{mM}}, & i = 1, 2, \dots, N-1,
\end{aligned} \tag{68}$$

where the real  $\lambda_{mm}$  and  $\lambda_{mM}$  have the same signs as  $\nu_{mm}$  and  $\nu_{mM}$  respectively. The optimized lower bound  $E_{olb}$  reads in this case

$$E_{\text{olb}} = \max_{\ell} E(\ell), \tag{69}$$

where

$$E(\ell) := \frac{(N-1)(N-2)}{2} |\lambda_{mm}|^{\frac{2}{2+\nu_{mm}}} (a_{mm}(\ell))^{\frac{\nu_{mm}}{\nu_{mm+2}}} E^{(2)}(1, \operatorname{sign}(\nu_{mm}), \nu_{mm}) + (N-1) |\lambda_{mM}|^{\frac{2}{2+\nu_{mM}}} (a_{mM}(\ell))^{\frac{\nu_{mM}}{\nu_{mM+2}}} E^{(2)}(1, \operatorname{sign}(\nu_{mM}), \nu_{mM}).$$
(70)

To obtain (70), we have made use of the scaling laws (59) for power law potentials. In the harmonic oscillator case, i.e.,

$$V_{ij}(\mathbf{r}_{ij}) = V_{mm}(\mathbf{r}_{ij}) = \lambda_{mm}r_{ij}^2 \qquad i < j < N,$$
  

$$V_{iN}(\mathbf{r}_{iN}) = V_{mM}(\mathbf{r}_{iN}) = \lambda_{mM}r_{iN}^2 \qquad i < N,$$
(71)

it is more convenient to work with a new parameter h related to the parameter  $\ell$  by

$$h := \frac{(N-2)(1-\ell)}{(2-N)(1-\ell)+2(N-1)}.$$
(72)

In terms of the new parameter h (72),  $a_{mm}$  and  $a_{mM}$  read

$$a_{mm}(h) = \frac{2}{(N-1)m} - \frac{2((N-1)m+M)}{(N-2)^2(N-1)mM}h^2,$$
(73)

$$a_{mM}(h) = \frac{((N-1)m+M)}{2mM(N-1)^2}(1+h)^2,$$
(74)

and the optimized lower bound  $E_{olb}$  (69) takes the form

$$E_{\text{olb}} = \max_{h} E(h), \tag{75}$$

where, taking into account of the result (60),

$$E(h) = 3(N-1) \left( \frac{(N-2)}{2} \sqrt{\lambda_{mm}} \sqrt{\frac{2}{(N-1)m} - \frac{2((N-1)m+M)}{(N-2)^2(N-1)mM}} h^2 + \sqrt{\lambda_{mM}} \sqrt{\frac{(N-1)m+M}{2mM(N-1)^2}} \sqrt{(1+h)^2} \right).$$
(76)

Here the maximization implied by (75) can be worked out analytically, and one can show [17] that the value  $h_0$  of h corresponding to the optimized lower bound, which is obtained by equating the derivative of E(h) (76) with respect to h to zero, is given by

$$h_0 = (N-1)\sqrt{\frac{M}{(N-1)m+M}}\sqrt{\frac{\lambda_{mM}}{(N-1)\lambda_{mm}+\lambda_{mM}}}.$$
(77)

Substituting  $h_0$  (77) in E(h) (76) one gets for the optimized lower bound  $E_{olb}$  (75) the following expression,

$$E_{\rm obb} = E(h_0) = \frac{3}{\sqrt{2}} \left\{ (N-2)\sqrt{\frac{(N-1)\lambda_{mm} + \lambda_{mM}}{m}} + \sqrt{\frac{\lambda_{mM}}{m}}\sqrt{\frac{(N-1)m + M}{M}} \right\},$$
(78)

which is identical to the *N*-body harmonic oscillator ground state energy [17]. Thus the optimized lower bound  $E_{olb}$  (78) is saturated for harmonic forces. The interested reader may consult [17] for details.

## 4.3. $(n \times m, n' \times M)$ configurations

Here both *n* and *n'* are greater than 1, which means that the system is at least a four-body system. We can always number the *n* particles with the same mass *m* as 1, 2, ..., n and the remaining *n'* particles with the same mass *M* as n + 1, n + 2, ..., N. Of course n + n' = N:

$$m_1 = m_2 = \dots = m_n = m, \qquad m_{n+1} = m_{n+2} = \dots = m_N = M.$$
 (79)

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Since the system is invariant under any permutations of particles with the same mass,

$$\begin{aligned} a_{ij} &= a_{mm}, & i < j \le n, \\ a_{ij} &= a_{mM}, & i = 1, \dots, n, \quad j = n+1, \dots, N, \\ a_{ij} &= a_{MM}, & n < i < j \le N, \end{aligned}$$
 (80)

$$b_1 = b_2 = \dots = b_n = b_m, \qquad b_{n+1} = b_{n+2} = \dots = b_N = b_M,$$
 (81)

and

$$\begin{aligned} x_{ij,q} &= 0, & i < j \le n & \text{or} & n < i < j \le N, \\ x_{ij,q} &= \ell, & i = 1, \dots, n, & j = n+1, \dots, N, & 1 \le q \le n, q \neq i, \\ x_{ij,q} &= p, & i = 1, \dots, n, & j = n+1, \dots, N, & n < q \le N, & q \neq j. \end{aligned}$$
(82)

Thus, here we have two different values,  $b_m$ ,  $b_M$ , for  $b_i$ , three different values,  $a_{mm}$ ,  $a_{mM}$ ,  $a_{MM}$ , for  $a_{ij}$ , and two parameters,  $\ell$  and p, to adjust. The N + N(N - 1)/2 relations obtained by identifying both sides of (5) reduce in this case to the following five relations:

$$b_{m} + \frac{1}{4}(n-1)a_{mm} + \frac{n'}{4}(\ell^{2}(n-1)+1)a_{mM} = \frac{1}{2m},$$
  

$$b_{M} + \frac{n}{4}(p^{2}(n'-1)+1)a_{mM} + \frac{1}{4}(n'-1)a_{MM} = \frac{1}{2M},$$
  

$$2b_{m} - \frac{1}{2}a_{mm} + \left(\ell + \frac{\ell^{2}}{2}(n-2)\right)n'a_{mM} = 0,$$
  

$$2b_{M} - \frac{1}{2}a_{MM} + \left(p + \frac{p^{2}}{2}(n'-2)\right)na_{mM} = 0,$$
  

$$b_{m} + b_{M} + \frac{1}{2}((n'-1)p - 1 - \ell(n-1) + p\ell(n-1)(n'-1))a_{mM} = 0.$$
  
(83)

Equations (83) can be considered as a system of five linear equations with five unknowns,  $a_{mm}$ ,  $a_{mM}$ ,  $a_{MM}$ ,  $b_m$ ,  $b_M$ . Solving this system, one gets for  $a_{mm}$ ,  $a_{mM}$  and  $a_{MM}$  the following expressions in terms of  $\ell$  and p:

$$a_{mm}(\ell, p) = 2 \frac{(n - npn' + pn + 2n' - 2\ell n' + n\ell n')(1 - pn' + p + \ell n')M - (\ell - 1)^2 n'm}{(n' + n - \ell n' + n\ell n' - npn' + pn)^2 mM},$$
(84)

$$a_{mM}(\ell, p) = 2 \frac{n'M + nm}{(n' + n - \ell n' + n\ell n' - npn' + pn)^2 mM},$$
(85)

$$a_{MM}(\ell, p) = 2 \frac{(1 - \ell + n\ell - pn)(n\ell n' - \ell n' + 2pn - npn' + 2n + n')m - n(p+1)^2 M}{(n' + n - \ell n' + n\ell n' - npn' + pn)^2 m M}.$$
(86)

Let us consider again the case of a two-body interaction described by a power law potential, that is,

$$\begin{aligned}
\nu_{mm}(r_{ij}) &= \lambda_{mm} r_{ij}^{\nu_{mm}}, & i < j = 1, 2, \dots, n, \\
\nu_{mM}(r_{ij}) &= \lambda_{mM} r_{ij}^{\nu_{mM}}, & i = 1, 2, \dots, n, \quad j = n+1, \quad n+2, \dots, N, \\
\nu_{MM}(r_{ij}) &= \lambda_{MM} r_{ij}^{\nu_{MM}}, & i < j = n+1, \quad n+2, \dots, N,
\end{aligned} \tag{87}$$

where  $\lambda_{mm}$ ,  $\lambda_{mM}$  and  $\lambda_{MM}$  have the same signs as  $\nu_{mm}$ ,  $\nu_{mM}$  and  $\nu_{MM}$  respectively. Then the optimized lower bound  $E_{olb}$  reads

$$E_{\text{olb}} = \max_{\ell, p} E(\ell, p), \tag{88}$$

where

$$E(\ell, p) := \frac{1}{2}n(n-1)|\lambda_{mm}|^{\frac{2}{2+\nu_{mm}}} (a_{mm}(\ell, p))^{\frac{\nu_{mm}}{\nu_{mm}+2}} E^{(2)}(1, \operatorname{sign}(\nu_{mm}), \nu_{mm}) + nn'|\lambda_{mM}|^{\frac{2}{2+\nu_{mM}}} (a_{mM}(\ell, p))^{\frac{\nu_{mM}}{\nu_{mM}+2}} E^{(2)}(1, \operatorname{sign}(\nu_{mM}), \nu_{mM}) + \frac{1}{2}n'(n'-1)|\lambda_{MM}|^{\frac{2}{2+\nu_{MM}}} (a_{MM}(\ell, p))^{\frac{\nu_{MM}}{\nu_{MM}+2}} E^{(2)}(1, \operatorname{sign}(\nu_{MM}), \nu_{MM}),$$
(89)

and we again make use of the scaling laws (59) for power law potentials. In the harmonic oscillator case, i.e., for

$$V_{ij}(r_{ij}) = V_{mm}(r_{ij}) = \lambda_{mm}r_{ij}^2 \qquad i < j = 1, 2, ..., n,$$
  

$$V_{ij}(r_{ij}) = V_{MM}(r_{ij}) = \lambda_{MM}r_{ij}^2 \qquad i < j = n + 1, \quad n + 2, ..., N,$$
  

$$V_{ij}(r_{ij}) = V_{mM}(r_{iN}) = \lambda_{mM}r_{ij}^2 \qquad i = 1, 2, ..., n, \quad j = n + 1, \quad n + 2, ..., N,$$
(90)

it is more convenient to work with new parameters h and c defined in terms of the original ones  $\ell$  and p by the following relations:

$$h = \frac{(n-1)(N-n)(1-\ell)}{(N-n)(1-\ell) + n(N-n)(\ell-p) + n(1+p)},$$
(91)

$$c = \frac{n(N-n-1)(1+p)}{(N-n)(1-\ell) + n(N-n)(\ell-p) + n(1+p)}.$$
(92)

In terms of the new parameters h(91) and c(92),  $a_{mm}$ ,  $a_{mM}$  and  $a_{MM}$  can be re-expressed as

$$a_{mm}(h,c) = \frac{2}{nm} - \frac{2(nm + (N-n)M)}{n(N-n)(n-1)^2 mM} h^2,$$
(93)

$$a_{mM}(h,c) = \frac{nm + (N-n)M}{2n^2(N-n)^2mM}(1+h+c)^2,$$
(94)

$$a_{MM}(h,c) = \frac{2}{(N-n)M} - \frac{2(nm + (N-n)M)}{n(N-n)(N-n-1)^2mM}c^2.$$
(95)

It is easy to see that, when expressed in terms of h and c,  $E(\ell, p)$  (89) takes the following form,

$$E(h,c) = \frac{3}{2} \left( n(n-1)\sqrt{\lambda_{mm}} \sqrt{\frac{2}{nm}} \sqrt{1 - \frac{nm + (N-n)M}{(N-n)(n-1)^2 M}} h^2 + \sqrt{\lambda_{mM}} \sqrt{\frac{2(nm + (N-n)M)}{mM}} \sqrt{(1+h+c)^2} + (N-n)(N-n-1)\sqrt{\lambda_{MM}} \sqrt{\frac{2}{(N-n)M}} \sqrt{1 - \frac{nm + (N-n)M}{n(N-n-1)^2 m}} c^2 \right), \quad (96)$$

where we have made use of the result (60). The optimized lower bound  $E_{\rm olb}$  (88) then reads

$$E_{\text{olb}} = \max_{h,c} E(h,c) \,. \tag{97}$$

Here again the maximization procedure implied by (97) can be worked out analytically [17] to the end. One can show [17] that the values  $h_0$ , of h, and  $c_0$ , of c, corresponding to the

optimized lower bound, obtained by equating to zero the partial derivatives of E(h, c) (96) with respect to h and c, are given by

$$h_0 = (N-n)(n-1)\sqrt{\frac{M}{nm+(N-n)M}}\sqrt{\frac{\lambda_{mM}}{n\lambda_{mm}+(N-n)\lambda_{mM}}}$$
(98)

$$c_0 = n\left(N - n - 1\right)\sqrt{\frac{m}{nm + (N - n)M}}\sqrt{\frac{\lambda_{mM}}{(N - n)\lambda_{MM} + n\lambda_{mM}}}.$$
(99)

The optimized lower bound  $E_{olb}$  (97) is then given by

$$E_{\rm olb} = E(h_0, c_0). \tag{100}$$

Replacing  $h_0$  and  $c_0$  by their respective expressions (98) and (99), one finally gets for the optimized lower bound the following expression,

$$E_{\text{olb}} = E(h_0, c_0) = \frac{3}{\sqrt{2}} \left( (n-1)\sqrt{\frac{n\lambda_{mm} + (N-n)\lambda_{mM}}{m}} + \sqrt{\lambda_{mM}} \sqrt{\frac{nm + (N-n)M}{mM}} + (N-n-1)\sqrt{\frac{n\lambda_{mM} + (N-n)\lambda_{MM}}{M}} \right),$$
(101)

which is nothing but the ground state energy of the *N*-body harmonic oscillator obtained in [17] for the mass configuration  $(n \times m, (N - n) \times M)$ . This means that the optimized lower bound is saturated, i.e., the optimized lower bound is equal to the ground state energy, for the *N*-body harmonic oscillator in the case of mass configurations of the type  $(n \times m, (N - n) \times M)$ . Still the interested reader is referred to [17] for more details.

#### 5. Conclusion

We have presented in this paper a general methodology for obtaining lower bounds for the ground state energy of an N-body Hamiltonian obeying non-relativistic kinematics and with a potential energy consisting of a sum of two-body contributions. Under these two conditions, one is able to derive such lower bounds for arbitrary N.

The starting point is a particular decomposition of the kinetic energy term (5) involving N + N(N-1)/2 + N(N-1)(N-2)/2 parameters constrained by N + N(N-1)/2 conditions, which can be used to express N + N(N-1)/2 parameters in terms of the remaining  $N(N-1)(N-2)/2 = C_N$  ones. This means that we are faced with a decomposition involving  $C_N$  arbitrary parameters. Then making use of the well-known invariance of the ground state under translations and of the variational principle, one ends with a lower bound which has the original property to depend on  $C_N$  arbitrary parameters. For each set of values of these  $C_N$  parameters, one obtains a lower bound for the Hamiltonian ground state energy. The best of these lower bounds, one which is nearest to the ground state energy, named optimized lower bound, is obviously the maximum of these lower bounds. We are thus involved with a maximization problem over  $C_N$  variables. We have shown that the values of the  $C_N$  parameters corresponding to the optimized lower bound satisfy  $C_N - R_N$  relations, which have the nice property to be independent of the particular form of the potential. We named these relations universal dynamical constraints. The calculations leading to the universal dynamical constraints are tractable in the general case up to N = 5, that is, for N = 3, N = 4, N = 5,

where we obtain respectively 1, 7, 21 constraints. For N > 5, i.e. for N = 6, 7, ..., the calculations are intractable in the most general case, but can be worked out when the system exhibits a sufficient degree of symmetry. In these cases symmetry arguments allow one to determine a number of these constraints and the remaining relations are then worked out. As a general rule, the number of universal dynamical constraints obtained, other than those determined by symmetry considerations, is the number of independent parameters minus the number of independent  $a_{ij}$  plus 1. There are cases where the symmetry conditions alone allow one to determine completely the constraints. These are the three configurations  $(N \times m)$ ,  $((N - 1) \times m, M)$  and  $(n \times m, n' \times M)$ , with both n and n' greater than 1. The universal dynamical constraints are very useful since they may be implemented from the beginning before working out the optimization procedure, simplifying it considerably. This remark takes its whole significance if we have in mind that we deal with a nonlinear optimization problem.

Our preliminary investigations show, on the one hand, that the optimized lower bound is always better than other lower bounds derived earlier [19–27]. (We will discuss this point in detail in a forthcoming paper [28].) On the other hand, the optimized lower bound proves to be identical to the ground state energy, i.e., the optimized lower bound is saturated, in the case of the *N*-body harmonic oscillator for all the mass configurations we have considered and we are convinced that this is a general property. But, although the property of saturability has never been taken by default, this is only a numerical evidence for saturability and does not constitute, strictly speaking, a mathematical proof of saturability. Moreover, to our knowledge, there is no analytical proof of saturability of the optimized lower bound in the harmonic case. Recently we succeeded to fill partially this gap. Indeed, we have given an analytical proof of saturability of the optimized lower bound in the *N*-body harmonic oscillator case for the particular mass configurations  $(N \times m)$ ,  $((N - 1) \times m, M)$  and  $(n \times m, n' \times M)$ , with both *n* and *n'* greater than 1, but for arbitrary *N*.

#### Acknowledgment

This work is supported by Le Ministère de L'Enseignement Supérieur et de la Recherche Scientifique of Algeria under grant no D2501/11/2003.

#### Appendix A

Let us adopt here the same notation as in subsection 3.2, i.e.,

$$c_3 := x_{12,3}, \quad c_4 := x_{12,4}, \quad d_2 := x_{13,2}, \quad d_4 := x_{13,4}, \quad e_2 := x_{14,2}, \quad e_3 := x_{14,3}, \\ f_1 := x_{23,1}, \quad f_4 := x_{23,4}, \quad g_1 := x_{24,1}, \quad g_3 := x_{24,3}, \quad h_1 := x_{34,1}, \quad h_2 := x_{34,2}, \end{cases}$$
(A.1)

and apply step by step the procedure described in section 3 in order to retrieve the universal dynamical constraints in the four-body case (35).

*First step.* The 6  $\times$  6 matrix  $\tilde{\mathbf{D}}$  is given by

$$\widetilde{\mathbf{D}} = \frac{1}{4} \begin{pmatrix} 4 & (d_2 - 1)^2 & (e_2 - 1)^2 & (f_1 - 1)^2 & (g_1 - 1)^2 & (h_1 - h_2)^2 \\ (c_3 - 1)^2 & 4 & (e_3 - 1)^2 & (f_1 + 1)^2 & (g_1 - g_3)^2 & (h_1 - 1)^2 \\ (c_4 - 1)^2 & (d_4 - 1)^2 & 4 & (f_1 - f_4)^2 & (g_1 + 1)^2 & (h_1 + 1)^2 \\ (c_3 + 1)^2 & (d_2 + 1)^2 & (e_2 - e_3)^2 & 4 & (g_3 - 1)^2 & (h_2 - 1)^2 \\ (c_4 + 1)^2 & (d_2 - d_4)^2 & (e_2 + 1)^2 & (f_4 - 1)^2 & 4 & (h_2 + 1)^2 \\ (c_3 - c_4)^2 & (d_4 + 1)^2 & (e_3 + 1)^2 & (f_4 + 1)^2 & (g_3 + 1)^2 & 4 \end{pmatrix}.$$
(A.2)

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Each column of the  $6 \times 6$  matrix  $\tilde{\mathbf{D}}$  gives rise to two columns of the matrix  $\tilde{\mathbf{M}}$ . For instance, the derivative of the first column of the matrix  $\tilde{\mathbf{D}}$  with respect to  $c_3$  gives rise to the first column of the matrix  $\tilde{\mathbf{M}}$ , the derivative of the first column of the matrix  $\tilde{\mathbf{D}}$  with respect to  $c_4$  gives rise to the second column of the matrix  $\tilde{\mathbf{M}}$ , the derivative of the second column of the matrix  $\tilde{\mathbf{D}}$  with respect to  $c_4$  gives rise to the second column of the matrix  $\tilde{\mathbf{M}}$ , the derivative of the second column of the matrix  $\tilde{\mathbf{D}}$  with respect to  $d_2$  gives rise to the third column of the matrix  $\tilde{\mathbf{M}}$ , and so on. The  $6 \times 12$  matrix  $\tilde{\mathbf{M}}$  obtained in this way is then given by

$$\widetilde{\mathbf{M}} = \frac{1}{2} \\ \times \begin{pmatrix} 0 & 0 & d_2 - 1 & 0 & e_2 - 1 & 0 & f_1 - 1 & 0 & g_1 - 1 & 0 & h_1 - h_2 & h_2 - h_1 \\ c_3 - 1 & 0 & 0 & 0 & 0 & e_3 - 1 & f_1 + 1 & 0 & g_1 - g_3 & g_3 - g_1 & h_1 - 1 & 0 \\ 0 & c_4 - 1 & 0 & d_4 - 1 & 0 & 0 & f_1 - f_4 & f_4 - f_1 & g_1 + 1 & 0 & h_1 + 1 & 0 \\ c_3 + 1 & 0 & d_2 + 1 & 0 & e_2 - e_3 & e_3 - e_2 & 0 & 0 & 0 & g_3 - 1 & 0 & h_2 - 1 \\ 0 & c_4 + 1 & d_2 - d_4 & d_4 - d_2 & e_2 + 1 & 0 & 0 & f_4 - 1 & 0 & 0 & 0 & h_2 + 1 \\ c_3 - c_4 & c_4 - c_3 & 0 & d_4 + 1 & 0 & e_3 + 1 & 0 & f_4 + 1 & 0 & g_3 + 1 & 0 & 0 \end{pmatrix}.$$
(A.3)

Second step. Before going further, let us note that since two matrices differing by an overall multiplicative factor have the same rank, we find it more convenient to work with the matrix  $2\widetilde{\mathbf{M}}$  than with the matrix  $\widetilde{\mathbf{M}}$  itself. We find it also convenient to refer to the two columns of the matrix  $2\widetilde{\mathbf{M}}$  containing  $c_3$  and  $c_4$  as block C, to the two columns containing  $d_2$  and  $d_4$  as block D and so on. Consider the first three blocks of the matrix  $2\widetilde{\mathbf{M}}$ , namely the blocks C, D and E. Six parameters are involved. Choose five among them, for instance  $c_3$ ,  $c_4$ ,  $d_2$ ,  $d_4$  and  $e_2$ , as independent parameters.

*Third step.* Now take the *C*, *D* and *E* blocks. You obtain in this way the following  $6 \times 6$  matrix:

$$\begin{pmatrix} 0 & 0 & d_2 - 1 & 0 & e_2 - 1 & 0 \\ c_3 - 1 & 0 & 0 & 0 & 0 & e_3 - 1 \\ 0 & c_4 - 1 & 0 & d_4 - 1 & 0 & 0 \\ c_3 + 1 & 0 & d_2 + 1 & 0 & e_2 - e_3 & e_3 - e_2 \\ 0 & c_4 + 1 & d_2 - d_4 & d_4 - d_2 & e_2 + 1 & 0 \\ c_3 - c_4 & c_4 - c_3 & 0 & d_4 + 1 & 0 & e_3 + 1 \end{pmatrix}.$$
 (A.4)

Calculate the determinant of this matrix, which we will refer to as CDE and put it in a factorized form. The result is

$$CDE = -(c_4d_2e_3 - d_2e_3 - c_4d_2 + 2c_3d_2 - d_2 - 4 - c_3 - d_4 - c_3d_4 - e_3 + 2d_4e_3 - e_2 - c_3e_2 + c_3d_4e_2 - d_4e_2 - c_4 - c_4e_3 + 2c_4e_2)(d_2 - d_2e_3 - c_4d_2 + c_4d_2e_3 - c_3 - d_4 + c_3d_4 + e_3 - e_2 + c_3e_2 + d_4e_2 - c_3d_4e_2 - c_4e_3 + c_4).$$
(A.5)

Equate CDE to zero. This results in either

$$c_4d_2e_3 - d_2e_3 - c_4d_2 + 2c_3d_2 - d_2 - 4 - c_3 - d_4 - c_3d_4 - e_3 + 2d_4e_3 - e_2 - c_3e_2 + c_3d_4e_2 - d_4e_2 - c_4 - c_4e_3 + 2c_4e_2 = 0,$$
(A.6)

or

$$d_2 - d_2e_3 - c_4d_2 + c_4d_2e_3 - c_3 - d_4 + c_3d_4 + e_3 - e_2 + c_3e_2 + d_4e_2 - c_3d_4e_2 - c_4e_3 + c_4 = 0.$$
(A.7)

On the one hand, the first solution (A.6) clearly does not conform with the equal mass case since, due to the presence of 4, it is not homogeneous in the parameters and must be rejected. On the other hand, one can solve (A.7) for  $e_3$  and gets the first universal dynamical constraint

$$e_3 = \frac{c_4d_2 - c_4 - d_2 - d_4e_2 + d_4 - c_3d_4 + e_2 + c_3 + c_3d_4e_2 - c_3e_2}{(1 - c_4)(1 - d_2)}.$$
 (A.8)

To determine the second and third constraints, construct two  $6 \times 6$  matrices by taking the blocks *C*, *E*, *F* for one of them and the blocks *D*, *E*, *F* for the other. Calculate their respective determinants *CEF* and *DEF*. In both cases the determinant factorizes as the product of two terms, one of which cannot be put to zero since it does not conform with the equal mass case. This is a general feature which reproduces itself in the following. Thus *CEF* = 0 and *DEF* = 0 give, respectively,

$$e_{3}f_{1} - e_{3} + c_{4}e_{3} - c_{4}e_{3}f_{1} - f_{1} - c_{3}f_{1} + e_{2} - e_{2}c_{4} + c_{4}e_{2}f_{1} + c_{3}e_{2}f_{1} + f_{4} + c_{3}f_{4} - c_{3}e_{2}f_{4} - e_{2}f_{4} = 0.$$

$$(A.9)$$

$$-e_{2}f_{1} - e_{2} + d_{4}e_{2}f_{1} + d_{4}e_{2} - f_{4} + f_{1} - d_{2}f_{4} + d_{2}f_{1} + e_{3} + e_{3}f_{4} + d_{2}e_{3}f_{4}$$

$$-d_2e_3f_1 - d_4e_3f_1 - d_4e_3 = 0. (A.10)$$

Taking into account the expression of  $e_3$ , (A.8), (A.9) and (A.10) can be put, respectively, in the form

$$\{ ((e_2 - 1)(-c_3 + c_3d_4 + f_1c_4d_2 - c_4d_2 + c_4 - f_1c_3d_4 - d_4 - f_1 + f_4 - c_4f_1 + c_3f_4 - c_3f_4d_2 + c_3f_1d_2 - d_2f_4 + d_4f_1 + d_2))/(d_2 - 1) \} = 0.$$

$$\{ ((d_4 - 1)(e_2 - 1)(d_4 - c_3d_4 - f_1c_3d_4 + d_4f_1 + c_3 - c_4 - d_2) \} = 0.$$

$$(A.11)$$

$$-c_4 f_1 + c_4 d_2 + c_3 f_4 d_2 + f_1 c_4 d_2 - c_3 f_1 d_2 - f_4 -d_2 f_4 + c_3 f_4 + f_1)/((d_2 - 1)(c_4 - 1))) = 0.$$
(A.12)

In (A.11)  $e_2 - 1$  cannot be put to zero since  $e_2$  has been taken as an independent parameter. It follows that the second factor in the numerator on the left-hand side of (A.11) is necessarily zero, i.e.,

$$-c_{3} + c_{3}d_{4} + f_{1}c_{4}d_{2} - c_{4}d_{2} + c_{4} - f_{1}c_{3}d_{4} - d_{4} - f_{1} + f_{4} - c_{4}f_{1} + c_{3}f_{4} - c_{3}f_{4}d_{2} + c_{3}f_{1}d_{2} - d_{2}f_{4} + d_{4}f_{1} + d_{2} = 0.$$
(A.13)

In the same manner neither  $d_4 - 1$  nor  $e_2 - 1$  in (A.12) can be put to zero since  $d_4$  and  $e_2$  have been taken as independent parameters. So the third factor in the numerator on the left-hand side of (A.12) necessarily vanishes, i.e.,

$$d_4 - c_3 d_4 - f_1 c_3 d_4 + d_4 f_1 + c_3 - c_4 - d_2 - c_4 f_1 + c_4 d_2 + c_3 f_4 d_2 + f_1 c_4 d_2 - c_3 f_1 d_2 - f_4 - d_2 f_4 + c_3 f_4 + f_1 = 0.$$
(A.14)

One can solve (A.13) for  $f_4$  and gets

$$f_4 = \frac{c_3d_4 - c_3 + f_1c_4d_2 - c_4d_2 + c_4 - f_1c_3d_4 - d_4 - f_1 - c_4f_1 + c_3f_1d_2 + d_4f_1 + d_2}{-1 - c_3 + c_3d_2 + d_2}.$$
(A.15)

Substituting for  $f_4$  in (A.14) its expression (A.15), one gets

$$2\frac{(-f_1 + c_3 f_1 d_2 - c_3 + d_2) (-c_3 d_4 + c_3 - d_2 + c_4 d_2 + d_4 - c_4)}{(d_2 - 1) (c_3 + 1)} = 0.$$
(A.16)

In (A.16) the factor  $-c_3d_4 + c_3 - d_2 + c_4d_2 + d_4 - c_4$  cannot be put to zero since it involves only independent parameters. Hence the first factor in the numerator on the left-hand side of (A.16) necessarily vanishes, i.e.,

$$-f_1 + c_3 f_1 d_2 - c_3 + d_2 = 0. (A.17)$$

Solving (A.17) for  $f_1$ , one gets a second universal dynamical constraint

$$f_1 = \frac{c_3 - d_2}{-1 + c_3 d_2}.\tag{A.18}$$

Substituting (A.18) for  $f_1$  in (A.15), one obtains a third universal dynamical constraint, namely,

$$f_4 = \frac{c_3 d_4 - c_4 d_2 + c_4 - d_4}{-1 + c_3 d_2}.$$
(A.19)

To get the fourth and fifth constraints, we need two more  $6 \times 6$  matrices. Construct one of them by taking the blocks *C*, *D*, *G* and the other by taking the blocks *D*, *E*, *G*. Putting CDG = 0 and DEG = 0, and rejecting in each case the solution which does not satisfy the correct limits, one obtains respectively

$$c_4d_2g_3 - c_4g_3 + d_2g_3 - g_3 - d_2 + c_3d_2 + d_4 - c_3d_4 - c_3d_2g_1 - c_4d_2g_1 + c_4g_1 + g_1 + c_3d_4g_1 - d_4g_1 = 0,$$
(A.20)

and

$$d_4e_2g_3 + d_4g_3 - e_2g_3 - g_3 - d_2 + g_1 - d_2g_1 + d_4 + d_2e_3 + d_2e_3g_1 - d_4e_3 - d_4e_3g_1 + e_2g_1 - d_4e_2g_1 = 0.$$
(A.21)

Equation (A.20) can be solved for  $g_3$ ,

$$g_3 = \frac{d_4g_1 - c_3d_2 - d_4 + c_3d_4 + d_2 + c_4d_2g_1 - c_4g_1 - g_1 + c_3d_2g_1 - c_3d_4g_1}{-c_4 + d_2 - 1 + c_4d_2}.$$
 (A.22)

Replacing  $e_3$  and  $g_3$  by their expressions, (A.8) and (A.22) respectively, (A.21) can be put in the form

$$2\frac{(d_4-1)(d_4-d_2)(c_3-1)(-g_1-c_4+e_2+c_4e_2g_1)}{(d_2-1)(c_4-1)(1+c_4)} = 0.$$
 (A.23)

Because we have taken  $c_3$ ,  $d_2$  and  $d_4$  as independent parameters, none of the three factors  $d_4 - 1$ ,  $d_4 - d_2$ ,  $c_3 - 1$  can be put equal to zero. It follows that in order to satisfy (A.23), one must have

$$-g_1 - c_4 + e_2 + c_4 e_2 g_1 = 0. (A.24)$$

Solving (A.24) for  $g_1$ , one gets a fourth constraint

$$g_1 = \frac{-e_2 + c_4}{-1 + c_4 e_2}.\tag{A.25}$$

Now substituting (A.25) for  $g_1$  in (A.22), one gets a fifth constraint

$$g_3 = \frac{c_4d_2 - c_4 - d_4e_2 - e_2c_3d_2 + c_3d_2 + c_3d_4e_2 + d_4 - c_3d_4 - d_2 + e_2}{(d_2 - 1)(-1 + c_4e_2)}.$$
 (A.26)

It remains to obtain the two last constraints, namely the sixth and seventh constraints. To this end consider two other matrices. Construct one of them by taking the C, D and H blocks and the other by taking C, G and H blocks. Putting their determinants equal to zero and retaining in both cases the solution which gives the correct limit, one obtains, respectively,

$$c_{3}d_{4}h_{2} + c_{3}h_{2} - h_{2} - d_{4}h_{2} + h_{1} + c_{4} - c_{4}h_{1} + d_{4}h_{1} - c_{3}$$
  
$$-c_{3}d_{4}h_{1} + c_{4}d_{2}h_{1} - c_{4}d_{2} + c_{3}d_{2} - c_{3}d_{2}h_{1} = 0$$
(A.27)

and

$$-g_{3}h_{1} - h_{1} - c_{4}g_{3}h_{1} - c_{4}h_{1} + h_{2} - c_{4} + c_{4}g_{1} + c_{4}g_{1}h_{2} + c_{3}h_{2} + c_{3} - g_{1}c_{3}h_{2} - g_{1}c_{3} + g_{3}h_{2} + g_{3}c_{4}h_{2} = 0.$$
(A.28)

Solving (A.27) for  $h_1$ , one gets

$$h_1 = \frac{c_3 d_4 h_2 + c_3 h_2 - h_2 - d_4 h_2 - c_3 + c_4 - c_4 d_2 + c_3 d_2}{c_4 + c_3 d_4 - c_4 d_2 - d_4 - 1 + c_3 d_2}.$$
 (A.29)

Making use of the expressions for  $g_1$  (A.25)  $g_3$  (A.26) and  $h_1$  (A.29), (A.28) can be put in the form

$$2\{((1+c_4)(c_4-c_3)(c_4d_2h_2+c_4e_2-d_2c_4e_2-c_4h_2-c_3d_2+e_2c_3d_2-c_3d_4h_2+d_2+h_2c_3d_4e_2+d_4h_2-h_2d_4e_2-d_2h_2-e_2+h_2))/((-c_4-c_3d_4+c_4d_2+d_4+1-c_3d_2)(-1+c_4e_2))\} = 0.$$
(A.30)

None of the two factors  $1 + c_4$  and  $c_4 - c_3$  involved in the numerator on the left-hand side of (A.30) can be put to zero, since both  $c_3$  and  $c_4$  have been chosen to be independent parameters. This means that in order to satisfy (A.30), one must have

$$c_4d_2h_2 + c_4e_2 - d_2c_4e_2 - c_4h_2 - c_3d_2 + e_2c_3d_2 - c_3d_4h_2 + d_2 + h_2c_3d_4e_2 + d_4h_2 - h_2d_4e_2 - d_2h_2 - e_2 + h_2 = 0.$$
(A.31)

One can solve (A.31) for  $h_2$  to obtain the sixth constraint

$$h_2 = \frac{c_3d_2 - c_4e_2 + d_2c_4e_2 - d_2 + e_2 - e_2c_3d_2}{-c_3d_4 - c_4 + c_4d_2 + d_4 - d_4e_2 - d_2 + c_3d_4e_2 + 1}.$$
 (A.32)

Substituting (A.32) for  $h_2$  in (A.29), one gets the seventh and last universal dynamical constraint

$$h_1 = \frac{c_4 d_2 - c_4 - d_2 - c_3 e_2 + c_3 + e_2}{-c_3 d_4 - c_4 + c_4 d_2 + d_4 - d_4 e_2 - d_2 + c_3 d_4 e_2 + 1}.$$
(A.33)

## **Appendix B**

For  $N \ge 6$  the universal dynamical constraints can be computed only for special mass configurations. Let us illustrate in the six-body case how our method can be adapted to work out the universal dynamical constraints for particular mass configurations. We can treat the cases where up to three different masses are involved, i.e., the configurations  $(m_1, m_2, 4m_3), (m_1, 2m_2, 3m_3), (2m_1, 2m_2, 2m_3)$ , if we restrict ourselves to two-body interactions depending only on the constituent masses. Let us consider in turn these three mass configurations and derive the corresponding universal dynamical constraints.

#### *B.1.* $(m_1, m_2, 4m_3)$

In this case the kinetic energy decomposition (2) reduces to

$$\frac{1}{2m_1}p_1^2 + \frac{1}{2m_2}p_2^2 + \frac{1}{2m_3}p_3^2 + \frac{1}{2m_3}p_4^2 + \frac{1}{2m_3}p_5^2 + \frac{1}{2m_3}p_6^2$$

$$= (b_1p_1 + b_2p_2 + b_3p_3 + b_3p_4 + b_3p_5 + b_3p_6)(p_1 + p_2 + p_3 + p_4 + p_5 + p_6)$$

$$+ \frac{a_{12}}{4}(p_1 - p_2 + cp_3 + cp_4 + cp_5 + cp_6)^2$$

$$+ \frac{a_{13}}{4}(p_1 - p_3 + dp_2 + ep_4 + ep_5 + ep_6)^2$$

$$+ \frac{a_{13}}{4}(p_1 - p_5 + dp_2 + ep_3 + ep_4 + ep_6)^2$$

$$+ \frac{a_{13}}{4}(p_1 - p_6 + dp_2 + ep_3 + ep_4 + ep_5)^2$$

$$+ \frac{a_{23}}{4}(p_2 - p_3 + fp_1 + gp_4 + gp_5 + gp_6)^2$$

$$+\frac{a_{23}}{4}(p_2 - p_4 + fp_1 + gp_3 + gp_5 + gp_6)^2 +\frac{a_{23}}{4}(p_2 - p_5 + fp_1 + gp_3 + gp_4 + gp_6)^2 +\frac{a_{23}}{4}(p_2 - p_6 + fp_1 + gp_3 + gp_4 + gp_5)^2 +\frac{a_{34}}{4}(p_3 - p_4)^2 + \frac{a_{34}}{4}(p_3 - p_5)^2 + \frac{a_{34}}{4}(p_3 - p_6)^2 +\frac{a_{34}}{4}(p_4 - p_5)^2 + \frac{a_{34}}{4}(p_4 - p_6)^2 + \frac{a_{34}}{4}(p_5 - p_6)^2.$$
(B.1)

Identifying both sides of (B.1), and eliminating  $b_1$ ,  $b_2$  and  $b_3$ , one obtains the following set of equations for  $a_{12}$ ,  $a_{13}$ ,  $a_{23}$  and  $a_{34}$  with c, d, e, f, h and g as parameters,

$$\begin{pmatrix} 4 & 4(d-1)^2 & 4(f-1)^2 & 0\\ (c-1)^2 & 3e^2 - 6e + 7 & 2f - 6fg + 4f^2 + 3g^2 + 1 & 3\\ (c+1)^2 & 2d - 6de + 4d^2 + 3e^2 + 1 & 3g^2 - 6g + 7 & 3\\ 0 & (e+1)^2 & (g+1)^2 & 4 \end{pmatrix}$$
$$\times \begin{pmatrix} a_{12}\\ a_{13}\\ a_{23}\\ a_{34} \end{pmatrix} = \begin{pmatrix} \frac{2}{m_1} + \frac{2}{m_2}\\ \frac{2}{m_1} + \frac{2}{m_3}\\ \frac{2}{m_3}\\ \frac{2}{m_3} \end{pmatrix}.$$
(B.2)

It is easy to see that the values of the parameters c, d, e, f, g corresponding to the optimized lower bound are such that the matrix

$$\begin{pmatrix} 0 & 8(d-1) & 0 & 8(f-1) & 0\\ 2(c-1) & 0 & 6(e-1) & 2(1+4f-3g) & 6(g-f)\\ 2(c+1) & 2(1+4d-3e) & 6(e-d) & 0 & 6(g-1)\\ 0 & 0 & 2(e+1) & 0 & 2(g+1) \end{pmatrix},$$
(B.3)

must be of rank 3 at most, i.e., any  $4 \times 4$  matrix extracted from the  $4 \times 5$  matrix (B.3) must be of determinant zero. This results in two relations

$$f = \frac{c-d}{cd-1}, \qquad g = \frac{c-e-cd+ce}{cd-1}.$$
 (B.4)

## B.2. $(m_1, 2m_2, 3m_3)$

In this particular case, the kinetic energy decomposition (2) simplifies to

$$\begin{aligned} \frac{1}{2m_1}p_1^2 + \frac{1}{2m_2}p_2^2 + \frac{1}{2m_2}p_3^2 + \frac{1}{2m_3}p_4^2 + \frac{1}{2m_3}p_5^2 + \frac{1}{2m_3}p_6^2 \\ &= (b_1p_1 + b_2p_2 + b_2p_3 + b_4p_4 + b_4p_5 + b_4p_6)(p_1 + p_2 + p_3 + p_4 + p_5 + p_6) \\ &+ \frac{a_{12}}{4}(p_1 - p_2 + cp_3 + dp_4 + dp_5 + dp_6)^2 \\ &+ \frac{a_{12}}{4}(p_1 - p_3 + cp_2 + dp_4 + dp_5 + dp_6)^2 \\ &+ \frac{a_{14}}{4}(p_1 - p_4 + ep_2 + ep_3 + fp_5 + fp_6)^2 \\ &+ \frac{a_{14}}{4}(p_1 - p_5 + ep_2 + ep_3 + fp_4 + fp_6)^2 \\ &+ \frac{a_{14}}{4}(p_1 - p_6 + ep_2 + ep_3 + fp_4 + fp_5)^2 \end{aligned}$$

$$+\frac{a_{23}}{4}(p_2 - p_3)^2 +\frac{a_{24}}{4}(p_2 - p_4 + gp_1 + hp_3 + ip_5 + ip_6)^2 +\frac{a_{24}}{4}(p_2 - p_5 + gp_1 + hp_3 + ip_4 + ip_6)^2 +\frac{a_{24}}{4}(p_2 - p_6 + gp_1 + hp_3 + ip_4 + ip_5)^2 +\frac{a_{24}}{4}(p_3 - p_4 + gp_1 + hp_2 + ip_5 + ip_6)^2 +\frac{a_{24}}{4}(p_3 - p_5 + gp_1 + hp_2 + ip_4 + ip_6)^2 +\frac{a_{24}}{4}(p_3 - p_6 + gp_1 + hp_2 + ip_4 + ip_5)^2 +\frac{a_{45}}{4}(p_4 - p_5)^2 + \frac{a_{45}}{4}(p_4 - p_6)^2 + \frac{a_{45}}{4}(p_5 - p_6)^2.$$
(B.5)

Identifying both sides of (B.5), and eliminating  $b_1$ ,  $b_2$  and  $b_4$ , one gets the following set of five linear equations for  $a_{12}$ ,  $a_{14}$ ,  $a_{23}$ ,  $a_{24}$  and  $a_{45}$  with c, d, e, f, g, h and i as parameters

$$\begin{pmatrix} \frac{c^2 - 2c + 5}{2} & \frac{3(e - 1)^2}{2} & \frac{1}{2} & \frac{3(2g^2 - 2gh - 2g + h^2 + 1)}{2} & 0\\ (d - 1)^2 & (f^2 - 2f + 3) & 0 & (2g - 4gi + 3g^2 + 2i^2 + 1) & 1\\ \frac{(2d - 2cd + c^2 + 2d^2 + 1)}{2} & \frac{2e - 4ef + 3e^2 + 2f^2 + 1}{2} & \frac{1}{2} & \frac{(2h - 4i - 4hi + 3h^2 + 4i^2 + 7)}{2} & 1\\ \frac{c + 1}{2} & 0 & 1 & \frac{3(h - 1)^2}{2} & 0\\ 0 & \frac{(f + 1)^2}{2} & 0 & (i + 1)^2 & \frac{3}{2} \end{pmatrix}$$

$$\times \begin{pmatrix} a_{12} \\ a_{14} \\ a_{23} \\ a_{24} \\ a_{45} \end{pmatrix} = \begin{pmatrix} \frac{2}{m_1} + \frac{2}{m_2} \\ \frac{2}{m_3} \\ \frac{2}{m_3} \\ \frac{2}{m_3} \end{pmatrix}.$$
(B.6)

Here, it is easy to see that the values of the parameters c, d, e, f, g, h and i corresponding to the optimized lower bound are such that the  $5 \times 7$  matrix

$$\begin{pmatrix} (c-1) & 0 & 3(e-1) & 0 & 3(2g-h-1) & 3(h-g) & 0 \\ 0 & 2(d-1) & 0 & 2(f-1) & 2(3g-2i+1) & 0 & 4(i-g) \\ (c-d) & (2d-c+1) & (1-2f+3e) & 2(f-e) & 0 & (1-2i+3h) & 2(2i-h-1) \\ (c+1) & 0 & 0 & 0 & 0 & 3(h-1) & 0 \\ 0 & 0 & 0 & (f+1) & 0 & 0 & 2(i+1) \end{pmatrix},$$
(B.7)

is of rank 4 at most. This means that every  $5 \times 5$  matrix extracted from the previous matrix by selecting five of its columns must be of determinant zero. This results in three relations between the values of the parameters c, d, e, f, g, h and i corresponding to the optimized lower bound, namely,

$$g = \frac{d-e}{de-1}, \qquad h = \frac{c+de-e-ce}{de-1}, \qquad i = \frac{d+df-f-de}{de-1}.$$
 (B.8)

## $B.3. (2m_1, 2m_2, 2m_3)$

Here, the kinetic energy decomposition (2) reduces to

$$\begin{aligned} \frac{1}{2m_1}p_1^2 + \frac{1}{2m_1}p_2^2 + \frac{1}{2m_2}p_3^2 + \frac{1}{2m_2}p_4^2 + \frac{1}{2m_3}p_5^2 + \frac{1}{2m_3}p_6^2 \\ &= (b_1p_1 + b_1p_2 + b_3p_3 + b_3p_4 + b_5p_5 + b_5p_6)(p_1 + p_2 + p_3 + p_4 + p_5 + p_6) \\ &+ \frac{a_{12}}{4}(p_1 - p_2)^2 \\ &+ \frac{a_{13}}{4}(p_1 - p_3 + cp_2 + dp_4 + ep_5 + ep_6)^2 \\ &+ \frac{a_{13}}{4}(p_1 - p_4 + cp_2 + dp_3 + ep_5 + ep_6)^2 \\ &+ \frac{a_{15}}{4}(p_1 - p_5 + fp_2 + gp_3 + gp_4 + hp_6)^2 \\ &+ \frac{a_{13}}{4}(p_2 - p_3 + cp_1 + dp_4 + ep_5 + ep_6)^2 \\ &+ \frac{a_{13}}{4}(p_2 - p_3 + cp_1 + dp_4 + ep_5 + ep_6)^2 \\ &+ \frac{a_{13}}{4}(p_2 - p_5 + fp_1 + gp_3 + gp_4 + hp_5)^2 \\ &+ \frac{a_{13}}{4}(p_2 - p_5 + fp_1 + gp_3 + gp_4 + hp_6)^2 \\ &+ \frac{a_{15}}{4}(p_2 - p_5 + fp_1 + gp_3 + gp_4 + hp_6)^2 \\ &+ \frac{a_{15}}{4}(p_3 - p_4)^2 \\ &+ \frac{a_{34}}{4}(p_3 - p_4)^2 \\ &+ \frac{a_{35}}{4}(p_3 - p_5 + ip_1 + ip_2 + jp_4 + kp_5)^2 \\ &+ \frac{a_{35}}{4}(p_4 - p_5 + ip_1 + ip_2 + jp_3 + kp_5)^2 \\ &+ \frac{a_{35}}{4}(p_4 - p_5 + ip_1 + ip_2 + jp_3 + kp_5)^2 \\ &+ \frac{a_{35}}{4}(p_4 - p_5 + ip_1 + ip_2 + jp_3 + kp_5)^2 \\ &+ \frac{a_{35}}{4}(p_5 - p_6)^2. \end{aligned}$$
(B.9)

The identification of the left-hand side of (B.9) with its right-hand side leads us after elimination of  $b_1$ ,  $b_3$  and  $b_5$  to a linear system of six equations for the six a, namely  $a_{12}$ ,  $a_{13}$ ,  $a_{15}$ ,  $a_{34}$ ,  $a_{35}$  and  $a_{56}$ , with c, d, e, f, g, h, i, j and k as parameters

$$2 \begin{pmatrix} 1 & (c-1)^2 & (f-1)^2 & 0 & 0 & 0 \\ \frac{1}{2} & 3+c^2+c-cd-d+d^2 & 1+2g^2-2g-2fg+f^2 & \frac{1}{2} & 1+2i^2-2ij+j^2-2i & 0 \\ \frac{1}{2} & 1+c^2-2ce-2e+2e^2 & 3+f^2-h+f-fh+h^2 & 0 & 1+2i^2+k^2+2i-2ik & \frac{1}{2} \\ 0 & (d+1)^2 & 0 & 1 & (j-1)^2 & 0 \\ 0 & 1+d^2+2e^2+2e-2de & 2g-2gh+2g^2+1+h^2 & \frac{1}{2} & 3+j^2+k^2+j-k-jk & \frac{1}{2} \\ 0 & 0 & (h+1)^2 & 0 & (k+1)^2 & 1 \end{pmatrix}$$

$$\times \begin{pmatrix} a_{12} \\ a_{13} \\ a_{15} \\ a_{34} \\ a_{35} \\ a_{56} \end{pmatrix} = \begin{pmatrix} \frac{\overline{m_1}}{\overline{m_1}} \\ \frac{2}{m_1} + \frac{2}{m_2} \\ \frac{2}{m_1} + \frac{2}{m_3} \\ \frac{2}{m_2} \\ \frac{2}{m_2} + \frac{2}{m_3} \\ \frac{2}{m_3} \end{pmatrix}.$$
 (B.10)

It is easy to show that the values of the parameters c, d, e, f, g, h, i, j and k, corresponding to the optimized lower bound are such that the  $6 \times 9$  matrix

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is of rank 5 at most, i.e., any  $6 \times 6$  matrix extracted from the previous matrix by selecting six of its columns must be of determinant zero. This results in four relations among the values of the nine parameters c, d, e, f, g, h, i, j and k, when the optimized lower bound is reached, namely,

$$f = \frac{c+i+ei-ci}{1+ei}, \qquad g = \frac{e+i}{1+ei}, \qquad j = \frac{e+di+i-d}{1+e}, \qquad k = \frac{h-e+ei+ehi}{1+e}.$$
(B.12)

The same pattern occurs for N-body systems with  $N \ge 7$ . The calculations leading to the universal dynamical constraints are intractable in the most general case, but can be worked out when the system exhibits a sufficient degree of symmetry, reducing thereby the number of independent parameters  $x_{ij,k}$  and the number of independent  $a_{ij}$ . It is easy to see that the number of universal dynamical constraints is the number of independent parameters  $x_{ii,k}$ minus the number of independent  $a_{ij}$  plus 1. Indeed,  $a_{ij}$  are determined by a matrix equation similar to (21), where the matrix playing the role of  $\tilde{\mathbf{D}}$  is a square matrix, whose number of lines is the number of independent  $a_{ij}$ . Each of the parameters  $x_{ij,k}$  appears in one and only one column of the square matrix. Now, consider one of the independent parameters  $x_{ii,k}$ , select the single column which contains it, and take the derivative of this column with respect to this same parameter. This results in a new non-vanishing column. Repeating the process for each of the independent parameters results in a number of columns which is the same as the number of independent  $x_{ii,k}$ . Putting together these columns, one can construct a  $p \times q$  matrix, where p, the number of lines, is the number of independent  $a_{ij}$ , and q, the number of columns, is the number of independent  $x_{ij,k}$ . The universal dynamical constraints are then obtained by requiring the matrix obtained in this way to be of rank p-1 at most, i.e., any  $p \times p$  matrix extracted from the  $p \times q$  matrix by selecting p of its columns must be of determinant zero.

This results in q - p + 1 conditions among the parameters, i.e., q - p + 1 universal dynamical constraints. This general rule is verified in particular for the three particular configurations of the six-body system considered above. Obviously, the above rule supposes the number of independent parameters  $x_{ij,k}$  greater than or equal to the number of independent  $a_{ij}$ . Now, what happens when the number of independent parameters  $x_{ij,k}$  is lower than the number of independent  $a_{ij}$ ? Here, there are no further universal dynamical constraints at all, other than those deduced from symmetry arguments. For *N*-body systems, with arbitrary *N*, this situation occurs only for three particular mass configurations, considered in detail in section 4.

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