An analytical proof of saturability of an optimized lower bound for *N*-body Hamiltonians for some mass configurations, with arbitrary *N*

2006 J. Phys. A: Math. Gen. 39 5857

(http://iopscience.iop.org/0305-4470/39/20/015)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 5857–5872 doi:10.1088/0305-4470/39/20/015

An analytical proof of saturability of an optimized lower bound for N-body Hamiltonians for some mass configurations, with arbitrary N

KheirEddine Boudjemaa[1] **and Sami R Zouzou**

Laboratoire de Physique Théorique, Département de Physique, Faculté des Sciences, Université Mentouri-Constantine, Algeria

E-mail: szouzou2000@yahoo.fr

Received 7 January 2006, in final form 8 January 2006
Published 3 May 2006
Online at stacks.iop.org/JPhysA/39/5857

Abstract

We begin by deriving explicit formulae for the energy levels of a system of N harmonic oscillators for two special mass configurations but for arbitrary N. Under the same conditions, we can perform analytically all the calculational procedure leading to an optimized lower bound for the ground state energy of an N-body system. The lower bound obtained in this way proves to be identical to the exact result. It is the first time, to our knowledge, that an explicit analytical proof of saturability has been worked out.

PACS number: 03.65.−w

1. Introduction

N-body problems constitute a challenge. Even the most simple of them, that is the one-body 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 N-body problem increases quickly with N. One alternative to overcome the non-analytic solvability is to have recourse to numerical investigations. Again these numerical computations complicate rapidly with N requiring thereby considerable calculational facilities. A second alternative is to focus on exact results. Among these, exact lower bounds for N-body Hamiltonians occupy a particular place. Recently we have derived an optimized lower bound for the ground state energies of N-body systems, with arbitrary N. Before going further, it is worthwhile emphasizing that the whole procedure applies only to systems of N particles interacting via translationally invariant two-body forces in the context of nonrelativistic kinematics. In particular three-body forces cannot be included in our present scheme. The lower bound we have obtained seems to be very promising. Indeed

[1] Also at Centre Universitaire de Khenchela, Algérie.

our investigations [1] show the superiority of this lower bound over earlier derived naive [2–7] and improved [8–10] lower bounds, and the saturability in the harmonic oscillator case [11, 12], which means that the optimized lower bound becomes equal to the exact result in the case of a system of N harmonic oscillators. But there is a small problem from the point of view of mathematical rigour. Although the saturability has been checked out numerically in all configurations considered, this does not constitute a rigorous proof of saturability. Our goal in this paper is to fill, partially, this lack. We will analytically prove in the following that the optimized lower bound we have obtained is saturated in the case of a system of N harmonic oscillators for two particular mass configurations, but with arbitrary N. We will begin by recalling quickly the derivation of this optimized lower bound. Then we will return to our primary concern in this paper. We will consider in turn two special configurations, where in each case we will establish the expressions of the exact energy levels of the system of N harmonic oscillators, together with the explicit exact expression of the optimized lower bound. Comparing the two expressions leads to the announced result, i.e., the saturability of the optimized lower bound for two special mass configurations, but for arbitrary N.

2. Optimized lower bound

We will be very brief here since the details of the derivation of the optimized lower bound can be found elsewhere. Let us consider N-body systems with nonrelativistic kinematics and translationally invariant two-body forces, i.e., systems described by Hamiltonians of the form

$$H = \sum_{i=1}^{N} \frac{1}{2m_i}\boldsymbol{p}_i^2 + \sum_{i<j=1}^{N} V^{(ij)}(\boldsymbol{r}_{ij}), \tag{1}$$

where $m_i, \boldsymbol{r}_i, \boldsymbol{p}_i$ stand respectively for the mass, the position and the momentum of the ith particle. $\boldsymbol{r}_{ij} := \boldsymbol{r}_i - \boldsymbol{r}_j, i \neq j = 1, 2, \ldots, N$. It will be noted that the two-body force is given by the pair potential $V^{(ij)}$. Our procedure [12] extends to N-body systems, with arbitrary N, optimized lower bounds obtained in the past for the three-body [13] and the four-body [14–17] cases, and very recently for the five-body case [11]. Our starting point has been the decomposition

$$\sum_{i=1}^{N} \frac{1}{2m_i}\boldsymbol{p}_i^2 = \left(\sum_{j=1}^{N} b_j \boldsymbol{p}_j\right)\left(\sum_{i=1}^{N} \boldsymbol{p}_i\right) + \sum_{i<j=1}^{N} a_{ij}\boldsymbol{p}_{ij}^2 \tag{2}$$

of the kinetic part of the Hamiltonian involving the parameters b_j, $j = 1, \ldots, N$, and the necessary positive parameters $a_{ij}, i < j = 1, 2, \ldots, N$. $\boldsymbol{p}_{ij}$ is a linear combination of the various momenta $\boldsymbol{p}_k$,

$$\boldsymbol{p}_{ij} = \sum_{k=1}^{N} \frac{x_{ij,k}}{2}\boldsymbol{p}_k. \tag{3}$$

Here the factor one-half is introduced for convenience. The coefficients $x_{ij,k}$ entering the linear combination are chosen such that $\boldsymbol{r}_{ij}$ and $\boldsymbol{p}_{ij}$ are conjugate variables of one another, that is satisfying canonical commutation relations

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

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

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

It will be remarked that the parameters b_j, a_{ij} and $x_{ij,k}$ are constrained by relations obtained by identifying the two 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_j 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 $x_{ij,i}$ to be equal to 1 by a redefinition of a_{ij} and of $x_{ij,k}$ for $k \neq i = 1, 2, \ldots, N$. Then imposing the canonical commutation relations, (4), one ends with $x_{ij,j} = -1$. Thus, we are left with $N(N-1)(N-2)/2$ parameters $x_{ij,k}$. The decomposition of the Hamiltonian, (1), corresponding to the decomposition of the kinetic energy term, (5), is

$$H = \left(\sum_{j=1}^{N} b_j \boldsymbol{p}_j\right)\left(\sum_{i=1}^{N} \boldsymbol{p}_i\right) + \sum_{i<j=1}^{N}\left(\frac{a_{ij}}{4}\left(\sum_{k=1}^{N} x_{ij,k}\boldsymbol{p}_k\right)^2 + V^{(ij)}(\boldsymbol{r}_{ij})\right). \tag{6}$$

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

$$\begin{aligned} E &= \langle\Psi|H|\Psi\rangle \\ &= \langle\Psi|\left(\sum_{j=1}^{N} b_j \boldsymbol{p}_j\right)\left(\sum_{i=1}^{N} \boldsymbol{p}_i\right)|\Psi\rangle + \sum_{i<j=1}^{N}\langle\Psi|\left(\frac{a_{ij}}{4}\left(\sum_{k=1}^{N} x_{ij,k}\boldsymbol{p}_k\right)^2 + V^{(ij)}(\boldsymbol{r}_{ij})\right)|\Psi\rangle. \end{aligned} \tag{7}$$

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

$$\left(\sum_{i=1}^{N} \boldsymbol{p}_i\right)|\Psi\rangle = \mathbf{o}, \tag{8}$$

and thus the contribution of the first term on the right-hand side of (7) vanishes. It results that

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

But by virtue of the variational principle

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

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

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

It follows that

$$E \geqslant \sum_{i<j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})]. \tag{12}$$

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

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

for each set of values of the parameters $x_{k\ell,m}$. The best of these bounds, denoted by E_{olb}, corresponds obviously to those values of $x_{k\ell,m}$ which maximize $\sum_{i<j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})]$. Thus

$$E_{\mathrm{olb}} = \max_{x_{k\ell,m}} \sum_{i<j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})]. \tag{13}$$

E_{olb} is called optimized lower bound.

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

$$\sum_{i<j=1}^{N} \frac{\partial E_{ij}^{(2)}}{\partial a_{ij}} \frac{\partial a_{ij}}{\partial x_{k\ell,m}} = 0, \qquad m \neq k, \qquad m \neq \ell, \quad k < l = 1, 2, \ldots, N. \tag{14}$$

Since $\partial E_{ij}^{(2)} \big/ \partial a_{ij}$ are not all zero, the rectangular matrix $\widetilde{B}$ with $N(N-1)/2$ lines and $N(N-1)(N-2)/2$ columns with matrix elements $\partial E_{ij}^{(2)} \big/ \partial a_{k\ell,m}$, where ij and $k\ell, m$ correspond respectively to the line and column indices, must be at most of rank $N(N-1)/2-1$. This means that every $N(N-1)/2 \times N(N-1)/2$ square matrix extracted from the matrix $\widetilde{B}$, by selecting $N(N-1)/2$ of its columns, must be of determinant zero. This results in $N(N-1)(N-2)/2 - N(N-1)/2 + 1$ relations among the values of $x_{k\ell,m}$ at the maximum. The general methodology for obtaining these relations can be found in [12] and their explicit forms for the three-body, four-body and five-body cases are given respectively in [13], [14] and [11]. Let us now consider in turn the two special configurations $((N-1) \times m, M)$, 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 $m \neq M$ and $n + n' = N$. We will work in the hypothesis where the two-body potential depends only on the masses of the particles constituting the pair.

3. Configurations $((N-1) \times m, M)$

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

$$m_1 = m_2 = \cdots = m_{N-1} = m, \qquad m_N = M.$$

3.1. Energy levels of the system of N harmonic oscillators

To solve the system of N harmonic oscillators, we have to first introduce a set of Jacobi coordinates and the corresponding conjugate momenta, together with the centre of mass coordinate and its conjugate momentum, i.e., the total momentum. We then express the Hamiltonian, (1), in terms of these new coordinates and their conjugate momenta. Subtracting the centre of mass kinetic energy, i.e., separating the centre of mass motion, one ends with the relative Hamiltonian.

A natural choice of the Jacobi coordinates is the following:

$$\begin{aligned}
\boldsymbol{\rho}_1 &= -\boldsymbol{r}_2 + \boldsymbol{r}_1, \\
\boldsymbol{\rho}_2 &= -\boldsymbol{r}_3 + \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2), \\
&\vdots
\end{aligned}$$

$$
\begin{aligned}
\boldsymbol{\rho}_i &= -\boldsymbol{r}_{i+1} + \frac{1}{i}(\boldsymbol{r}_1 + \boldsymbol{r}_2 + \cdots + \boldsymbol{r}_i),\\
&\vdots\\
\boldsymbol{\rho}_{N-2} &= -\boldsymbol{r}_{N-1} + \frac{1}{N-2}(\boldsymbol{r}_1 + \cdots + \boldsymbol{r}_{N-1}),\\
\boldsymbol{\rho}_{N-1} &= -\boldsymbol{r}_N + \frac{1}{N-1}(\boldsymbol{r}_1 + \cdots + \boldsymbol{r}_N).
\end{aligned}
\tag{15}
$$

One can express the individual coordinates of the particles in terms of the Jacobi coordinates, (15), and the centre of mass coordinate $\boldsymbol{R}$ defined as

$$
\boldsymbol{R} = \frac{m(\boldsymbol{r}_1 + \cdots + \boldsymbol{r}_{N-1}) + M\boldsymbol{r}_N}{(N-1)m + M}. \tag{16}
$$

The result is

$$
\begin{aligned}
\boldsymbol{r}_1 &= \frac{1}{2}\boldsymbol{\rho}_1 + \frac{1}{3}\boldsymbol{\rho}_2 + \frac{1}{4}\boldsymbol{\rho}_3 + \cdots + \frac{1}{N-1}\boldsymbol{\rho}_{N-2} + \frac{M}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R},\\
\boldsymbol{r}_2 &= -\frac{1}{2}\boldsymbol{\rho}_1 + \frac{1}{3}\boldsymbol{\rho}_2 + \frac{1}{4}\boldsymbol{\rho}_3 + \cdots + \frac{1}{N-1}\boldsymbol{\rho}_{N-2} + \frac{M}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R},\\
\boldsymbol{r}_3 &= -\frac{2}{3}\boldsymbol{\rho}_2 + \frac{1}{4}\boldsymbol{\rho}_3 + \cdots + \frac{1}{N-1}\boldsymbol{\rho}_{N-2} + \frac{M}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R},\\
&\vdots\\
\boldsymbol{r}_i &= -\frac{i-1}{i}\boldsymbol{\rho}_{i-1} + \frac{1}{i+1}\boldsymbol{\rho}_i + \cdots + \frac{1}{N-1}\boldsymbol{\rho}_{N-2} + \frac{M}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R},\\
&\vdots\\
\boldsymbol{r}_{N-2} &= -\frac{N-3}{N-2}\boldsymbol{\rho}_{N-3} + \frac{1}{N-1}\boldsymbol{\rho}_{N-2} + \frac{1}{N-1}\boldsymbol{\rho}_{N-2} + \frac{M}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R},\\
\boldsymbol{r}_{N-1} &= -\frac{N-2}{N-1}\boldsymbol{\rho}_{N-2} + \frac{M}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R},\\
\boldsymbol{r}_N &= -\frac{(N-1)m}{(N-1)m+M}\boldsymbol{\rho}_{N-1} + \boldsymbol{R}.
\end{aligned}
\tag{17}
$$

The potential energy V,

$$
V = \lambda_{mm}\sum_{i<j=1}^{N-1}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 + \lambda_{mM}\sum_{i=1}^{N-1}(\boldsymbol{r}_i - \boldsymbol{r}_N)^2, \tag{18}
$$

can be put in the form

$$
V = ((N-2)\lambda_{mm} + \lambda_{mM})\sum_{i=1}^{N-1}\boldsymbol{r}_i^2 + \lambda_{mM}(N-1)\boldsymbol{r}_N^2 - 2\lambda_{mm}\sum_{i<j=1}^{N-1}\boldsymbol{r}_i\cdot\boldsymbol{r}_j - 2\lambda_{mM}\sum_{i=1}^{N-1}\boldsymbol{r}_i\cdot\boldsymbol{r}_N. \tag{19}
$$

Replacing $\boldsymbol{r}_i$ by their expressions, one gets

$$
\sum_{i=1}^{N-1}\boldsymbol{r}_i^2 = \sum_{i=1}^{N-2}\frac{i}{i+1}\boldsymbol{\rho}_i^2 + \frac{(N-1)M^2}{((N-1)m+M)^2}\boldsymbol{\rho}_{N-1}^2 + (N-1)\boldsymbol{R}^2 + 2\frac{(N-1)M}{(N-1)m+M}\boldsymbol{\rho}_{N-1}\cdot\boldsymbol{R}, \tag{20}
$$

$$\boldsymbol{r}_N^2 = \frac{(N-1)m^2}{((N-1)m+M)^2}\boldsymbol{\rho}_{N-1}^2 + \boldsymbol{R}^2 - 2\frac{(N-1)m}{(N-1)m+M}\boldsymbol{\rho}_{N-1}\cdot\boldsymbol{R}, \tag{21}$$

$$\sum_{i<j=1}^{N-1}\boldsymbol{r}_i\cdot\boldsymbol{r}_j = -\frac{1}{2}\sum_{i=1}^{N-2}\frac{i}{i+1}\boldsymbol{\rho}_i^2 + \frac{1}{2}\frac{(N-1)(N-2)M^2}{((N-1)m+M)^2}\boldsymbol{\rho}_{N-1}^2 + \frac{1}{2}(N-1)(N-2)\boldsymbol{R}^2 + \frac{(N-1)(N-2)M}{(N-1)m+M}\boldsymbol{\rho}_{N-1}\cdot\boldsymbol{R}, \tag{22}$$

$$\sum_{i=1}^{N-1}\boldsymbol{r}_i\cdot\boldsymbol{r}_N = -\frac{(N-1)^2Mm}{((N-1)m+M)^2}\boldsymbol{\rho}_{N-1}^2 + (N-1)\boldsymbol{R}^2 + \frac{(N-1)M-(N-1)^2m}{(N-1)m+M}\boldsymbol{\rho}_{N-1}\cdot\boldsymbol{R}. \tag{23}$$

Putting all together, one obtains

$$V = ((N-1)\lambda_{mm} + \lambda_{mM})\sum_{i=1}^{N-2}\frac{i}{i+1}\boldsymbol{\rho}_i^2 + \lambda_{mM}(N-1)\boldsymbol{\rho}_{N-1}^2. \tag{24}$$

The momenta conjugate to Jacobi coordinates, (15), are

$$\begin{aligned}
\boldsymbol{p}_{\rho_1} &= \frac{1}{2}(-\boldsymbol{p}_2 + \boldsymbol{p}_1),\\
\boldsymbol{p}_{\rho_2} &= \frac{2}{3}\left(-\boldsymbol{p}_3 + \frac{1}{2}(\boldsymbol{p}_1 + \boldsymbol{p}_2)\right),\\
&\vdots\\
\boldsymbol{p}_{\rho_i} &= \frac{i}{i+1}\left(-\boldsymbol{p}_{i+1} + \frac{1}{i}(\boldsymbol{p}_1 + \cdots + \boldsymbol{p}_i)\right), \qquad (25)\\
&\vdots\\
\boldsymbol{p}_{\rho_{N-2}} &= \frac{N-2}{N-1}\left(-\boldsymbol{p}_{N-1} + \frac{1}{N-2}(\boldsymbol{p}_1 + \boldsymbol{p}_2 + \cdots + \boldsymbol{p}_{N-2})\right),\\
\boldsymbol{p}_{\rho_{N-1}} &= -\frac{(N-1)m}{(N-1)m+M}\boldsymbol{p}_N + \frac{M}{(N-1)m+M}(\boldsymbol{p}_1 + \boldsymbol{p}_2 + \cdots + \boldsymbol{p}_{N-1}).
\end{aligned}$$

Equation (25), together with the expression of the centre of mass momentum, i.e., that of the total momentum $\boldsymbol{P}$,

$$\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2 + \cdots + \boldsymbol{p}_{N-1} + \boldsymbol{p}_N, \tag{26}$$

may be inverted to get the expressions of the individual momenta in terms of the Jacobi momenta, (25), and the centre of mass momentum, (26), which when inserted in the kinetic part of the Hamiltonian gives

$$T := \sum_{i=1}^{N}\frac{1}{2m_i}\boldsymbol{p}_i^2 = \frac{\boldsymbol{P}^2}{2((N-1)m+M)} + \sum_{i=1}^{N-2}\frac{\boldsymbol{p}_{\rho_i}^2}{\frac{2im}{i+1}} + \frac{\boldsymbol{p}_{\rho_{N-1}}^2}{\frac{2(N-1)mM}{(N-1)m+M}}. \tag{27}$$

Thus the Hamiltonian, (1), may be written in terms of the Jacobi coordinates, (15), their conjugate momenta, (25), and the centre of mass momentum, (26), as

$$H = \frac{1}{2((N-1)m+M)}\boldsymbol{P}_R^2 + \sum_{i=1}^{N-2}\left(\frac{1}{\frac{2im}{i+1}}\boldsymbol{p}_{\rho_i}^2 + ((N-1)\lambda_{mm} + \lambda_{mM})\frac{i}{i+1}\boldsymbol{\rho}_i^2\right) + \frac{1}{\frac{2(N-1)mM}{(N-1)m+M}}\boldsymbol{p}_{\rho_{N-1}}^2 + \lambda_{mM}(N-1)\boldsymbol{\rho}_{N-1}^2. \tag{28}$$

From (28), one deduces the Hamiltonian of relative motion H_R by subtracting the centre of mass kinetic energy. This results in

$$H_R = \sum_{i=1}^{N-2}\left(\frac{1}{\frac{2im}{i+1}}p_{\rho_i}^2 + ((N-1)\lambda_{mm} + \lambda_{mM})\frac{i}{i+1}\rho_i^2\right) + \frac{1}{\frac{2(N-1)mM}{(N-1)m+M}}p_{\rho_{N-1}}^2 + \lambda_{mM}(N-1)\rho_{N-1}^2. \tag{29}$$

H_R thus shows as a sum of $N-1$ independent harmonic oscillators. Then the energy levels are sums of the energy levels of the $N-1$ harmonic oscillators.

$$E_{j_1,j_2,\ldots,j_{N-1}} = \sum_{i=1}^{N-2}(2j_i+3)\sqrt{\frac{(N-1)\lambda_{mm}+\lambda_{mM}}{2m}} + (2j_{N-1}+3)\sqrt{\frac{\lambda_{mM}((N-1)m+M)}{2mM}}, \tag{30}$$

where $j_1, j_2, \ldots, j_{N-1}$ are natural integers. The ground state energy E corresponds to $j_1 = 0, j_2 = 0, \ldots, j_{N-1} = 0$

$$E = 3(N-2)\sqrt{\frac{(N-1)\lambda_{mm}+\lambda_{mM}}{2m}} + 3\sqrt{\frac{((N-1)m+M)\lambda_{mM}}{2mM}}. \tag{31}$$

3.2. Optimized lower bounds

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

$$\begin{aligned} &a_{ij} = a_{mm} \qquad i < j = 1, 2, \ldots, N-1, \\ &a_{iN} = a_{mM} \qquad i < N, \end{aligned} \tag{32}$$

$$b_1 = b_2 = \cdots = b_{N-1} = b, \tag{33}$$

and

$$\begin{aligned} &x_{ij,k} = 0 \qquad i < j < N, \quad k \neq i, \quad k \neq j, \\ &x_{iN,k} = \ell \qquad i < N, \quad k \neq i, \quad k \neq N. \end{aligned} \tag{34}$$

We thus have only one variational parameter ℓ 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

$$\begin{aligned} &b + \frac{N-2}{4}a_{mm} + \frac{1}{4}a_{mM} + \frac{N-2}{4}\ell^2 a_{mM} = \frac{1}{2m}, \\ &b_N + \frac{N-1}{4}a_{mM} = \frac{1}{2M}, \\ &2b - \frac{1}{2}a_{mm} + \ell a_{mM} + \frac{N-3}{2}\ell^2 a_{mM} = 0, \\ &b + b_N - \frac{1}{2}a_{mM} - \frac{N-2}{2}\ell a_{mM} = 0. \end{aligned} \tag{35}$$

Equation (35) may be considered as a system of linear equations with four unknowns a_{mm}, a_{mM}, b, b_N and one parameter ℓ. The resolution of this system is trivial and gives for a_{mm} and a_{mM} the following expressions in terms of the parameter ℓ:

$$\begin{aligned} &a_{mm}(\ell) = 2\frac{(\ell+1)(\ell N - 3\ell + 1 + N)M - (\ell-1)^2 m}{(\ell N + N - 2\ell)^2 mM}, \\ &a_{mM}(\ell) = 2\frac{(N-1)m + M}{(\ell N + N - 2\ell)^2 mM}. \end{aligned} \tag{36}$$

For a harmonic oscillator problem

$$\begin{aligned} V_{ij}(\boldsymbol{r}_{ij}) &= V_{mm}(\boldsymbol{r}_{ij}) = \lambda_{mm} r_{ij}^2 \qquad && i < j < N, \\ V_{iN}(\boldsymbol{r}_{iN}) &= V_{mM}(\boldsymbol{r}_{iN}) = \lambda_{mM} r_{iN}^2 \qquad && i < N. \end{aligned} \tag{37}$$

Then, if we define $E(\ell)$ as

$$E(\ell) := \frac{(N-1)(N-2)}{2} E^{(2)}[a_{mm}(\ell), \lambda_{mm}, 2] + (N-1) E^{(2)}[a_{mM}(\ell), \lambda_{mM}, 2], \tag{38}$$

where $E^{(2)}[a, \lambda, 2]$, with λ positive, denotes the ground state energy of the two-body harmonic oscillator Hamiltonian $H_{\text{ho}}^{(2)}$ defined by

$$H_{\text{ho}}^{(2)} := a\boldsymbol{p}^2 + \lambda r^2, \tag{39}$$

the optimized lower bound E_{olb}, (13), reads

$$E_{\text{olb}} = \max_{\ell} E(\ell). \tag{40}$$

Making use of the result, [18], which simply follows from the observation that the well-known expression $3\omega/2$ (in units where $\hbar = 1$ of course) for the ground state energy of the three-dimensional isotropic harmonic oscillator written in its familiar form $\boldsymbol{p}^2/2m + m\omega^2 r^2/2$ is nothing but three times the square root of the product of the two factors in front of $\boldsymbol{p}^2$ and r^2, $1/2m$ and $m\omega^2/2$ respectively,

$$E^{(2)}[a, \lambda, 2] = 3\sqrt{a\lambda}, \tag{41}$$

(38) simplifies to

$$E(\ell) = 3\frac{(N-1)(N-2)}{2}\sqrt{\lambda_{mm}}\sqrt{a_{mm}(\ell)} + 3(N-1)\sqrt{\lambda_{mM}}\sqrt{a_{mM}(\ell)}. \tag{42}$$

Before going further, it is more convenient to put $a_{mm}(\ell)$ and $a_{mM}(\ell)$, (36), in a slightly different form

$$\begin{aligned} a_{mm}(\ell) &= \frac{2}{(N-1)m} + \frac{2(\ell-1)^2((N-1)m+M)}{(N-\ell+(N-1)\ell)^2(N-1)mM}, \\ a_{mM}(\ell) &= \frac{4}{(N-\ell+(N-1)\ell)^2}\frac{(N-1)m+M}{2mM}. \end{aligned} \tag{43}$$

It is also convenient to make the following change of variable:

$$h := \frac{(N-2)(1-\ell)}{(2-N)(1-\ell)+2(N-1)}. \tag{44}$$

In terms of the new parameter h, (44), a_{mm} and a_{mM} read

$$a_{mm}(h) = \frac{2}{(N-1)m} - \frac{2((N-1)m+M)}{(N-2)^2(N-1)mM}h^2, \tag{45}$$

$$a_{mM}(h) = \frac{((N-1)m+M)}{2mM(N-1)^2}(1+h)^2, \tag{46}$$

and the optimized lower bound E_{olb} reads

$$E_{\text{olb}} = \max_{h} E(h), \tag{47}$$

where

$$\begin{aligned} E(h) = 3(N-1)\Bigg(&\frac{(N-2)}{2}\sqrt{\lambda_{mm}}\sqrt{\frac{2}{(N-1)m} - \frac{2((N-1)m+M)}{(N-2)^2(N-1)mM}h^2} \\ &+ \sqrt{\lambda_{mM}}\sqrt{\frac{(N-1)m+M}{2mM(N-1)^2}}\sqrt{(1+h)^2}\Bigg). \end{aligned} \tag{48}$$

Let us conjecture that $1 + h$ is positive, when $E(h)$ reaches its maximum. Then, in the neighbourhood of the maximum,

$$\frac{\partial E(h)}{\partial h} = 3(N-1)\left\{-\sqrt{\lambda_{mm}}\frac{(N-1)m+M}{(N-2)(N-1)mM}\frac{h}{\sqrt{\frac{2}{(N-1)m} - \frac{2((N-1)m+M)h^2}{(N-2)^2(N-1)mM}}}\right.$$
$$\left. + \sqrt{\lambda_{mM}}\sqrt{\frac{(N-1)m+M}{2mM(N-1)^2}}\right\}. \tag{49}$$

Putting $\partial E(h)/\partial h$, (49), to zero, one gets the value h_0 of h corresponding to the optimized lower bound,

$$h_0 = (N-1)\sqrt{\frac{M}{(N-1)m+M}}\sqrt{\frac{\lambda_{mM}}{(N-1)\lambda_{mm}+\lambda_{mM}}}. \tag{50}$$

Substituting h_0, (50), in $E(h)$, (48), one gets for the optimized lower bound, E_{olb}, the following expression:

$$E_{\text{olb}} = E(h_0) = \frac{3}{\sqrt{2}}\left\{(N-2)\sqrt{\frac{(N-1)\lambda_{mm}+\lambda_{mM}}{m}} + \sqrt{\frac{\lambda_{mM}}{m}}\sqrt{\frac{(N-1)m+M}{M}}\right\}, \tag{51}$$

which is identical to the ground state energy of the system of N harmonic oscillators, (31). Thus the optimized lower bound, E_{olb}, (51), is saturated for harmonic forces.

4. Configuration $(n \times m, n' \times M)$

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 $1, \ldots, n$ and the remaining n' particles with the same mass M as $n+1, \ldots, N$. Of course $n + n' = N$.

$$\begin{aligned} &m_1 = m_2 = \cdots = m_n = m; \\ &m_{n+1} = m_{n+2} = \cdots = m_N = M. \end{aligned} \tag{52}$$

As in the previous section, we begin by deriving the explicit expression of the exact energy levels of the system of N harmonic oscillators and then that of the optimized lower bound.

4.1. Energy levels of the system of N harmonic oscillators

As in section 3.1, we begin by introducing a set of $N - 1$ Jacobi coordinates. Here, a natural choice of the Jacobi coordinates is to consider relative coordinates inside the cluster of the n particles with the same mass m, relative coordinates inside the cluster of the n' particles with the same mass M, and the relative coordinate between the two clusters. To be more explicit, a natural choice of the Jacobi coordinates in the case of the special configuration $(n \times m, n' \times M)$ is the following:

$$\begin{aligned} &\boldsymbol{\rho}_i = -\boldsymbol{r}_{i+1} + \frac{1}{i}\sum_{k=1}^{i}\boldsymbol{r}_k \qquad 1 \leqslant i < n, \\ &\boldsymbol{\rho}_n = \frac{1}{n}\sum_{k=1}^{n}\boldsymbol{r}_k - \frac{1}{n'}\sum_{k=n+1}^{N}\boldsymbol{r}_k, \\ &\boldsymbol{\rho}_i = -\boldsymbol{r}_{i+1} + \frac{1}{i-n}\sum_{k=n+1}^{i}\boldsymbol{r}_k \qquad n < i < N. \end{aligned} \tag{53}$$

The centre of mass coordinate of the system is given by

$$\boldsymbol{R} = \frac{1}{nm + n'M}\left(m\sum_{k=1}^{n}\boldsymbol{r}_k + M\sum_{k=n+1}^{N}\boldsymbol{r}_k\right). \tag{54}$$

Inverting (53) and (54), one gets the expressions of the individual particle coordinates in terms of the Jacobi coordinates together with the centre of mass coordinate. The result is

$$\begin{aligned}
\boldsymbol{r}_1 &= \frac{1}{2}\boldsymbol{\rho}_1 + \sum_{k=2}^{n-1}\frac{1}{k+1}\boldsymbol{\rho}_k + \frac{n'M}{nm+n'M}\boldsymbol{\rho}_n + \boldsymbol{R},\\
&\vdots\\
\boldsymbol{r}_i &= -\frac{(i-1)}{i}\boldsymbol{\rho}_{i-1} + \sum_{k=i}^{n-1}\frac{1}{k+1}\boldsymbol{\rho}_k + \frac{n'M}{nm+n'M}\boldsymbol{\rho}_n + \boldsymbol{R} \qquad 1 < i < n,\\
&\vdots\\
\boldsymbol{r}_n &= -\frac{n-1}{n}\boldsymbol{\rho}_{n-1} + \frac{n'M}{nm+n'M}\boldsymbol{\rho}_n + \boldsymbol{R},\\
\boldsymbol{r}_{n+1} &= \frac{1}{2}\boldsymbol{\rho}_{n+1} + \sum_{k=n+2}^{N-1}\frac{1}{k-n+1}\boldsymbol{\rho}_k - \frac{nm}{nm+n'M}\boldsymbol{\rho}_n + \boldsymbol{R},\\
&\vdots\\
\boldsymbol{r}_i &= -\frac{i-n-1}{i-n}\boldsymbol{\rho}_{i-1} + \sum_{k=i}^{N-1}\frac{1}{k-n+1}\boldsymbol{\rho}_k - \frac{nm}{nm+n'M}\boldsymbol{\rho}_n + \boldsymbol{R} \qquad n < i < N,\\
&\vdots\\
\boldsymbol{r}_N &= -\frac{N-n-1}{N-n}\boldsymbol{\rho}_{N-1} - \frac{nm}{nm+n'M}\boldsymbol{\rho}_n + \boldsymbol{R}.
\end{aligned} \tag{55}$$

The potential energy V,

$$V = \lambda_{mm}\sum_{i<j=1}^{n}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 + \lambda_{MM}\sum_{i<j=n+1}^{N}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 + \lambda_{mM}\sum_{i=1}^{n}\sum_{j=n+1}^{N}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2, \tag{56}$$

can be rewritten as

$$\begin{aligned}
V &= ((n-1)\lambda_{mm} + n'\lambda_{mM})\sum_{i=1}^{n}\boldsymbol{r}_i^2 + ((n'-1)\lambda_{MM} + n\lambda_{mM})\sum_{i=n+1}^{N}\boldsymbol{r}_i^2\\
&\quad - 2\left(\lambda_{mm}\sum_{i=1}^{n}\sum_{j=i+1}^{n}\boldsymbol{r}_i\cdot\boldsymbol{r}_j + \lambda_{MM}\sum_{i=n+1}^{N}\sum_{j=i+1}^{N}\boldsymbol{r}_i\cdot\boldsymbol{r}_j + \lambda_{mM}\sum_{i=1}^{n}\sum_{j=n+1}^{N}\boldsymbol{r}_i\cdot\boldsymbol{r}_j\right).
\end{aligned} \tag{57}$$

Substituting the expressions of the $\boldsymbol{r}_i, i = 1, \ldots, N$, (55), one obtains for the various contributions to V involved in (57) the following expressions:

$$\sum_{i=1}^{n}\boldsymbol{r}_i^2 = n\boldsymbol{R}^2 + \frac{2nn'M}{nm+n'M}\boldsymbol{\rho}_n\cdot\boldsymbol{R} + n\frac{n'^2M^2}{(nm+n'M)^2}\boldsymbol{\rho}_n^2 + \sum_{k=1}^{n-1}\frac{k}{k+1}\boldsymbol{\rho}_k^2. \tag{58}$$

$$\sum_{i=n+1}^{N} \boldsymbol{r}_i^2 = n'\boldsymbol{R}^2 - \frac{2nn'm}{nm+n'M}\boldsymbol{\rho}_n \cdot \boldsymbol{R} + n'\frac{n^2m^2}{(nm+n'M)^2}\boldsymbol{\rho}_n^2 + \sum_{k=n+1}^{N-1} \frac{k-n}{k-n+1}\boldsymbol{\rho}_k^2. \tag{59}$$

$$\sum_{i=1}^{n}\sum_{j=i+1}^{n} \boldsymbol{r}_i \cdot \boldsymbol{r}_j = \frac{1}{2}n(n-1)\boldsymbol{R}^2 + n(n-1)\frac{n'M}{nm+n'M}\boldsymbol{\rho}_n \cdot \boldsymbol{R} + \frac{1}{2}n(n-1)\frac{n'^2M^2}{(nm+n'M)^2}\boldsymbol{\rho}_n^2 - \frac{1}{2}\sum_{k=1}^{n-1}\frac{k}{k+1}\boldsymbol{\rho}_k^2. \tag{60}$$

$$\sum_{i=n+1}^{N}\sum_{j=i+1}^{N} \boldsymbol{r}_i \cdot \boldsymbol{r}_j = \frac{1}{2}n'(n'-1)\boldsymbol{R}^2 - n'(n'-1)\frac{nm}{nm+n'M}\boldsymbol{\rho}_n \cdot \boldsymbol{R} + \frac{1}{2}n'(n'-1)\frac{n^2m^2}{(nm+n'M)^2}\boldsymbol{\rho}_n^2 - \frac{1}{2}\sum_{k=n+1}^{N-1}\frac{k-n}{k-n+1}\boldsymbol{\rho}_k^2. \tag{61}$$

$$\sum_{i=1}^{n}\sum_{j=n+1}^{N} \boldsymbol{r}_i \cdot \boldsymbol{r}_j = nn'\boldsymbol{R}^2 + nn'\frac{-nm+n'M}{nm+n'M}\boldsymbol{\rho}_n \cdot \boldsymbol{R} - nn'\frac{nmn'M}{(nm+n'M)^2}\boldsymbol{\rho}_n^2. \tag{62}$$

Putting all together, (58), (59), (60), (61), and (62), in (57), one obtains

$$V = (n\lambda_{mm} + n'\lambda_{mM})\sum_{i=1}^{n-1}\frac{i}{i+1}\boldsymbol{\rho}_i^2 + nn'\lambda_{mM}\boldsymbol{\rho}_n^2 + (\lambda_{MM}n' + \lambda_{mM}n)\sum_{i=n+1}^{N-1}\frac{i-n}{i-n+1}\boldsymbol{\rho}_i^2. \tag{63}$$

The conjugate momenta corresponding to the Jacobi coordinates, (53), are

$$\begin{aligned}
\boldsymbol{p}_{\rho_i} &= \frac{i}{i+1}\left(-\boldsymbol{p}_{i+1} + \frac{1}{i}\sum_{j=1}^{i}\boldsymbol{p}_j\right) \qquad 1 \leqslant i < n,\\
\boldsymbol{p}_{\rho_n} &= \frac{n'M}{nm+n'M}\sum_{j=1}^{n}\boldsymbol{p}_j - \frac{nm}{nm+n'M}\sum_{j=n+1}^{N}\boldsymbol{p}_j,\\
\boldsymbol{p}_{\rho_i} &= \frac{i-n}{i-n+1}\left(-\boldsymbol{p}_{i+1} + \frac{1}{i-n}\sum_{j=n+1}^{i}\boldsymbol{p}_j\right) \qquad n < i < N,
\end{aligned} \tag{64}$$

where $\boldsymbol{p}_i, i = 1, \ldots, N$, are the momenta corresponding to the individual particle coordinates $\boldsymbol{r}_i, i = 1, \ldots, N$. The total momentum $\boldsymbol{P}$ is the sum of the individual momenta

$$\boldsymbol{P} = \boldsymbol{p}_1 + \cdots + \boldsymbol{p}_n + \boldsymbol{p}_{n+1} + \cdots + \boldsymbol{p}_N. \tag{65}$$

Inverting (64) and (65), one obtains the individual momenta in terms of the conjugate momenta of the Jacobi coordinates together with the total momentum. Then substituting the expressions obtained in this way in the kinetic part of the Hamiltonian, (1), one gets

$$T := \sum_{i=1}^{N}\frac{1}{2m_i}\boldsymbol{p}_i^2 = \frac{1}{2(nm+n'M)}\boldsymbol{P}^2 + \sum_{i=1}^{n-1}\frac{1}{\frac{2i}{i+1}}\boldsymbol{p}_{\rho_i}^2 + \frac{1}{2\frac{nmn'M}{nm+n'M}}\boldsymbol{p}_n^2 + \sum_{i=n+1}^{N-1}\frac{1}{\frac{2(i-n)}{i-n+1}M}\boldsymbol{p}_{\rho_i}^2. \tag{66}$$

Putting together the kinetic and potential parts of the Hamiltonian, (66) and (63) respectively, one obtains the Hamiltonian expressed in terms of the Jacobi coordinates, (53), their conjugate momenta, (64), together with the total momentum, (65),

$$H = \frac{1}{2(nm+n'M)}\boldsymbol{P}^2 + \sum_{i=1}^{n-1}\left(\frac{1}{\frac{2i}{i+1}}\boldsymbol{p}_{\rho_i}^2 + (n\lambda_{mm} + n'\lambda_{mM})\frac{i}{i+1}\boldsymbol{\rho}_i^2\right) + \left(\frac{1}{2\frac{nmn'M}{nm+n'M}}\boldsymbol{p}_n^2 + nn'\lambda_{mM}\boldsymbol{\rho}_n^2\right) + \sum_{i=n+1}^{N-1}\left(\frac{1}{\frac{2(i-n)}{i-n+1}M}\boldsymbol{p}_{\rho_i}^2 + (\lambda_{MM}n' + \lambda_{mM}n)\frac{i-n}{i-n+1}\boldsymbol{\rho}_i^2\right). \tag{67}$$

Subtracting the centre of mass kinetic energy, one obtains the relative Hamiltonian H_R

$$H_R = \sum_{i=1}^{n-1}\left(\frac{1}{\frac{2i}{i+1}}\boldsymbol{p}_{\rho_i}^2 + (n\lambda_{mm} + n'\lambda_{mM})\frac{i}{i+1}\boldsymbol{\rho}_i^2\right) + \left(\frac{1}{2\frac{nmn'M}{nm+n'M}}\boldsymbol{p}_n^2 + nn'\lambda_{mM}\boldsymbol{\rho}_n^2\right) + \sum_{i=n+1}^{N-1}\left(\frac{1}{\frac{2(i-n)}{i-n+1}M}\boldsymbol{p}_{\rho_i}^2 + (\lambda_{MM}n' + \lambda_{mM}n)\frac{i-n}{i-n+1}\boldsymbol{\rho}_i^2\right). \tag{68}$$

Thus H_R shows a sum of $N-1$ independent harmonic oscillators. The energy levels are therefore sums of the energy levels of the $N-1$ independent harmonic oscillators. It follows that the energy levels are given by

$$E_{j_1,j_2,\ldots,j_{n-1},j_n,j_{n+1},\ldots,j_{n+n'-1}} = \sum_{i=1}^{n-1}(2j_i+3)\sqrt{\frac{\lambda_{mm}n + \lambda_{mM}n'}{2m}} + (2j_n+3)\sqrt{\frac{\lambda_{mM}(nm+n'M)}{2mM}} + \sum_{i=1}^{n'-1}(2j_{n+i}+3)\sqrt{\frac{\lambda_{MM}n' + \lambda_{mM}n}{2M}}, \tag{69}$$

with j_i, $i = 1, \ldots, n+n'-1$, natural integers, $j_i \geqslant 0$. The ground state energy E corresponds to all j_i equal to zero. Thus

$$E = 3(n-1)\sqrt{\frac{\lambda_{mm}n + \lambda_{mM}n'}{2m}} + 3(n'-1)\sqrt{\frac{\lambda_{MM}n' + \lambda_{mM}n}{2M}} + 3\sqrt{\frac{\lambda_{mM}(nm+n'M)}{2mM}}. \tag{70}$$

4.2. Optimized lower bounds

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

$$\begin{aligned} a_{ij} &= a_{mm} && i < j \leqslant n, \\ a_{ij} &= a_{mM} && i = 1, \ldots, n, \quad j = n+1, \ldots, N, \\ a_{ij} &= a_{MM} && n < i < j \leqslant N, \end{aligned} \tag{71}$$

$$\begin{aligned} &b_1 = b_2 = \cdots = b_n = b_m, \\ &b_{n+1} = b_{n+2} = \cdots = b_N = b_M, \end{aligned} \tag{72}$$

and

$$\begin{aligned} x_{ij,q} &= 0 && i < j \leqslant n \quad \text{or} \quad n < i < j \leqslant N, \\ x_{ij,q} &= \ell && i = 1, \ldots, n \quad j = n+1, \ldots, N \quad 1 \leqslant q \leqslant n \quad q \neq i, \\ x_{ij,q} &= p && i = 1, \ldots, n \quad j = n+1, \ldots, N \quad n < q \leqslant N \quad q \neq j. \end{aligned} \tag{73}$$

Thus, here we have three different values, a_{mm}, a_{mM}, a_{MM}, for a_{ij}, and two parameters, ℓ 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:

$$\begin{aligned}
&b_m + \frac{1}{4}(n-1)a_{mm} + \frac{n'}{4}(\ell^2(n-1)+1)a_{mM} = \frac{1}{2m},\\
&b_M + \frac{n}{4}(p^2(n'-1)+1)a_{mM} + \frac{1}{4}(n'-1)a_{MM} = \frac{1}{2M},\\
&2b_m - \frac{1}{2}a_{mm} + \left(\ell + \frac{\ell^2}{2}(n-2)\right)n'a_{mM} = 0,\\
&2b_M - \frac{1}{2}a_{MM} + \left(p + \frac{p^2}{2}(n'-2)\right)na_{mM} = 0,\\
&b_m + b_M + \frac{1}{2}((n'-1)p - 1 - \ell(n-1) + p\ell(n-1)(n'-1))a_{mM} = 0.
\end{aligned} \tag{74}$$

Equation (74) 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 ℓ and p:

$$a_{mm}(\ell,p) = 2\frac{(n - npn' + pn + 2n' - 2\ell n' + n\ell n')(1 - pn' + p + \ell n')M - (\ell-1)^2 n'm}{(n' + n - \ell n' + n\ell n' - npn' + pn)^2 mM}, \tag{75}$$

$$a_{mM}(\ell,p) = 2\frac{n'M + nm}{(n' + n - \ell n' + n\ell n' - npn' + pn)^2 mM}, \tag{76}$$

$$a_{MM}(\ell,p) = 2\frac{(1 - \ell + n\ell - pn)(n\ell n' - \ell n' + 2pn - npn' + 2n + n')m - n(p+1)^2 M}{(n' + n - \ell n' + n\ell n' - npn' + pn)^2 mM}. \tag{77}$$

Taking into account the expression of the ground state energy, (41), of the three-dimensional isotropic harmonic oscillator, (39), the optimized lower bound E_{olb} can be put in the form

$$E_{\mathrm{olb}} = \max_{\ell,p} E(\ell,p), \tag{78}$$

where $E(\ell,p)$ is defined by

$$\begin{aligned}
E(\ell,p) := 3\Bigg(&\frac{n(n-1)}{2}\sqrt{\lambda_{mm}a_{mm}(\ell,p)} + n(N-n)\sqrt{\lambda_{mM}a_{mM}(\ell,p)}\\
&+ \frac{(N-n)(N-n-1)}{2}\sqrt{\lambda_{MM}a_{MM}(\ell,p)}\Bigg).
\end{aligned} \tag{79}$$

$a_{mm}(\ell,p)$, $a_{mM}(\ell,p)$ and $a_{MM}(\ell,p)$ are given by (75), (76) and (77), respectively. Before going further, let us put $a_{mm}(\ell,p)$, $a_{mM}(\ell,p)$, and $a_{MM}(\ell,p)$ in a slightly different form

$$a_{mm}(\ell,p) = \frac{2}{nm} - \frac{2(N-n)((N-n))M + nm)(\ell-1)^2}{nmM(N - (N-n)\ell + n(N-n)\ell - n(N-n)p + np)^2}, \tag{80}$$

$$a_{mM}(\ell,p) = 2\frac{nm + (N-n)M}{mM(N - (N-n)\ell + n(N-n)\ell - n(N-n)p + np)^2}, \tag{81}$$

$$a_{MM}(\ell,p) = \frac{2}{(N-n)M} - \frac{2n(nm + (N-n)M)(p+1)^2}{(N-n)mM(N - (N-n)\ell + n(N-n)\ell - n(N-n)p + np)^2}. \tag{82}$$

Let us now make the following change of variables:

$$h = \frac{(n-1)(N-n)(1-\ell)}{(N-n)(1-\ell) + n(N-n)(\ell - p) + n(1+p)}, \tag{83}$$

$$c = \frac{n(N-n-1)(1+p)}{(N-n)(1-\ell) + n(N-n)(\ell - p) + n(1+p)}. \tag{84}$$

In terms of the new parameters h, (83), and c, (84), a_{mm}, a_{mM} and a_{MM} can be re-expressed as

$$a_{mm}(h,c) = \frac{2}{nm} - \frac{2(nm + (N-n)M)}{n(N-n)(n-1)^2 mM} h^2, \tag{85}$$

$$a_{mM}(h,c) = \frac{nm + (N-n)M}{2n^2(N-n)^2 mM}(1+h+c)^2, \tag{86}$$

$$a_{MM}(h,c) = \frac{2}{(N-n)M} - \frac{2(nm + (N-n)M)}{n(N-n)(N-n-1)^2 mM} c^2. \tag{87}$$

It is easy to see that, when expressed in terms of h and c, $E(\ell, p)$, (79), takes the following form:

$$\begin{aligned} E(h,c) = \frac{3}{2}\Bigg(& n(n-1)\sqrt{\lambda_{mm}}\sqrt{\frac{2}{nm}}\sqrt{1 - \frac{nm + (N-n)M}{(N-n)(n-1)^2 M} h^2} \\ & + \sqrt{\lambda_{mM}}\sqrt{\frac{2(nm + (N-n)M)}{mM}}\sqrt{(1+h+c)^2} \\ & + (N-n)(N-n-1)\sqrt{\lambda_{MM}}\sqrt{\frac{2}{(N-n)M}}\sqrt{1 - \frac{nm + (N-n)M}{n(N-n-1)^2 m} c^2}\Bigg), \end{aligned} \tag{88}$$

and the optimized lower bound $E_{\rm olb}$ reads

$$E_{\rm olb} = \max_{h,c} E(h,c). \tag{89}$$

Let us compute the partial derivatives of $E(h,c)$ with respect to h and c. We got

$$\begin{aligned} \frac{\partial E(h,c)}{\partial h} = \frac{3}{\sqrt{2}}\Bigg(& \sqrt{\lambda_{mM}}\sqrt{\frac{nm + (N-n)M}{mM}} \\ & - n(n-1)\sqrt{\frac{\lambda_{mm}}{nm}} \frac{1}{\sqrt{1 - \frac{nm + (N-n)M}{(n-1)^2 (N-n)M} h^2}} \frac{nm + (N-n)M}{(n-1)^2 (N-n)M} h\Bigg), \end{aligned} \tag{90}$$

and

$$\begin{aligned} \frac{\partial E(h,c)}{\partial c} = \frac{3}{\sqrt{2}}\Bigg(& \sqrt{\lambda_{mM}}\sqrt{\frac{nm + (N-n)M}{mM}} - (N-n)(N-n-1) \\ & \times \sqrt{\frac{\lambda_{MM}}{(N-n)M}} \frac{1}{\sqrt{1 - \frac{nm + (N-n)M}{(N-n-1)^2 nm} c^2}} \frac{nm + (N-n)M}{(N-n-1)^2 nm} c\Bigg), \end{aligned} \tag{91}$$

where we have conjectured that $1 + h + c > 0$ in a neighbourhood of the maximum of $E(h,c)$, (88). Equating $\partial E(h,c)/\partial h$ and $\partial E(h,c)/\partial c$ to zero, one gets the values of h, h_0, and of c, c_0, corresponding to the maximum of $E(h,c)$, that is to the optimized lower bound. The result is

$$h_0 = (N-n)(n-1)\sqrt{\frac{M}{nm+(N-n)M}}\sqrt{\frac{\lambda_{mM}}{n\lambda_{mm}+(N-n)\lambda_{mM}}}, \tag{92}$$

$$c_0 = n(N-n-1)\sqrt{\frac{m}{nm+(N-n)M}}\sqrt{\frac{\lambda_{mM}}{(N-n)\lambda_{MM}+n\lambda_{mM}}}. \tag{93}$$

One finally gets after replacing h_0 and c_0 by their explicit expressions, (92) and (93) respectively, the following expression for the optimized lower bound E_{olb},

$$E_{\text{olb}} = E(h_0, c_0) = \frac{3}{\sqrt{2}}\left((n-1)\sqrt{\frac{n\lambda_{mm}+(N-n)\lambda_{mM}}{m}} + \sqrt{\lambda_{mM}}\sqrt{\frac{nm+(N-n)M}{mM}} + (N-n-1)\sqrt{\frac{n\lambda_{mM}+(N-n)\lambda_{MM}}{M}}\right), \tag{94}$$

which is nothing but the ground state energy of the system of N harmonic oscillators for the $(n \times m, (N-n) \times M)$ mass configuration, (70). This again means that the optimized lower bound is saturated for the system of N harmonic oscillators in the case of mass configurations of the type $(n \times m, (N-n) \times M)$.

5. Conclusion

In [12], we derived an optimized lower bound for the ground state energy of an N-body Hamiltonian, with non-relativistic kinematics and translationally invariant two-body forces, by extending for arbitrary N a procedure used previously for the three-body case [13], the four-body case [14] and very recently for the five-body case [11] . This lower bound proves to be superior to previously derived naive [2–7] and improved [8–10] lower bounds. Furthermore, the optimized lower bound we obtain in this way coincides with the ground state energy in the particular case of harmonic interactions for all the mass configurations we have considered. But this is a numerical evidence and a numerical result remains a numerical result and cannot be considered, strictly speaking, as a proof of saturability, although we have the 'intime conviction' that the optimized lower bound we have obtained is always saturated in the case of harmonic forces, independently of the particular mass configuration under study.

This paper fills partially this lack in that we have succeeded to analytically prove the saturability of the optimized lower bound we obtained in [12] in the case of harmonic forces for particular mass configurations but for arbitrary N.

For the most general configuration, we think that analytical proof of saturability is out of reach for $N > 5$, since for $N > 5$, we know from the beginning that analytical expressions of the energy levels of the system of N harmonic oscillators should not be available since the problem is equivalent to solving an algebraic equation of degree $N-1$ [11].

Acknowledgments

This work was supported by Le Ministère de L'Enseignement Supérieur et la Recherche Scientifique of Algeria under grant D2501/11/2003.

References

[1] Boudjemaa Kh and Zouzou S R Comparison of lower bounds on N-body Hamiltonians (in preparation)

[2] Fisher M E and Ruelle D 1966 *J. Math. Phys.* **7** 260

[3] Dyson F J and Lenard A 1967 *J. Math. Phys.* **8** 423

[4] Lévy-Leblond J-M 1969 *J. Math. Phys.* **10** 806

[5] Ader J-P, Richard J-M and Taxil P 1982 *Phys. Rev.* D **25** 2370

[6] Nussinov S 1983 *Phys. Rev. Lett.* **51** 2081

[7] Richard J-M 1984 *Phys. Lett.* B **139** 408

[8] Hall R L and Post H R 1967 *Proc. Phys. Soc.* **90** 381

[9] Basdevant J-L, Martin A and Richard J-M 1990 *Nucl. Phys.* B **343** 60

[10] Basdevant J-L, Martin A and Richard J-M 1990 *Nucl. Phys.* B **343** 69

[11] Boudjemaa Kh and Zouzou S R 2005 Optimized lower bound for five-body Hamiltonians *J. Math. Phys.* (submitted)

[12] Boudjemaa Kh and Zouzou S R 2005 Optimized lower bound for *N*-body Hamiltonians *J. Phys. A: Math. Gen.* (submitted)

[13] Basdevant J-L, Martin A, Richard J-M and Wu T T 1993 *Nucl. Phys.* B **393** 111

[14] Benslama A, Metatla A, Bachkhaznadji A, Zouzou S R, Krikeb A, Basdevant J-L, Richard J-M and Wu T T 1998 *Few-Body Syst.* **24** 39

[15] Metatla A 1997 *Thèse de magister* Université de Constantine

[16] Krikeb A 1999 *Thèse de Doctorat* Université Claude Bernard, Lyon

[17] Bouaouina B 1999 *Thèse de magister* Université de Constantine

[18] Richard J-M 1992 *Phys. Rep.* **56** 1 (see p 22)