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COMPARISON OF VARIOUS LOWER BOUNDS FOR THE GROUND STATE ENERGY OF AN N-BODY SYSTEM

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This paper is devoted to a comparison of various lower bounds, the so-called optimized, naïve and improved lower bounds on the ground state energies of N-body systems with non-relativistic kinematics and translationally invariant two-body interactions. The optimized lower bound proves, in all cases, to be better than the improved and the naïve bounds.

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1. Introduction

As is generally admitted, the N-body problem is extremely difficult to deal with. Even the most simple cases of a one-body problem in a central potential or the two-body problem with translationally and rotationally invariant interaction can be solved only for particular forms of the interaction potential. This leads to the development of approximate methods of resolution of the Schrödinger equation. However, the things complicate quickly with N, requiring considerable calculational facilities. An alternative to numerical calculations are exact results. Among them, the lower bounds for the ground state energy occupy a particular place. Recently, we have generalized a lower bound initially derived for three- [1] and four-body [2] systems to N-body systems [3–5], with arbitrary N, under the two assumptions of non-relativistic kinematics and translationally invariant two-body interactions, that is to N-body systems governed by Hamiltonians of the form

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$$H=\sum_{i=1}^{N}\frac{1}{2m_i}\vec{p}_i^{\,2}+\sum_{i<j=1}^{N}V^{(ij)}(\vec{r}_{ij})\,, \tag{1.1}$$

where m_i, $\vec{r}_i$, $\vec{p}_i$ stand, respectively, for the mass, the position and the linear momentum of the ith particle. $\vec{r}_{ij}:=\vec{r}_i-\vec{r}_j$, $i\neq j=1,\ldots,N$. This bound, named optimized lower bound, proves to be very interesting. Among other things, it proves to be saturated in the case of harmonic interactions, for all mass configurations and all values of the coupling constants. This property of saturability is something like a label of quality of the optimized lower bound. Other lower bounds on the market, the so-called naïve and improved lower bounds, do not satisfy this property of saturability. The objective of this paper is to compare the optimized, the naïve and the improved lower bounds for different forms of the two-body interaction potentials. This paper is organized as follows. In Section 2 and 3 the naïve and the improved lower bounds are presented in turn, and then compared to each other in Section 4. The optimized lower bound is presented in Section 5. Section 6 is devoted to numerical results and Section 7 to a general conclusion and perspectives.

2. Naïve lower bound

Historically, the naïve lower bound [6–11] was the first to be established. Its starting point is the following decomposition of the kinetic energy term

$$\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2m_i}=\frac{1}{N-1}\sum_{i<j=1}^{N}\left(\frac{\vec{p}_i^{\,2}}{2m_i}+\frac{\vec{p}_j^{\,2}}{2m_j}\right)\,. \tag{2.1}$$

The Hamiltonian H may then be rewritten as a sum of two-body Hamiltonians $H_{ij}^{\prime(2)}$

$$H=\sum_{i=1}^{N}H_{ij}^{\prime(2)} \tag{2.2}$$

with

$$H_{ij}^{\prime(2)}=\frac{1}{N-1}\left(\frac{\vec{p}_i^{\,2}}{2m_i}+\frac{\vec{p}_j^{\,2}}{2m_j}\right)+V^{(ij)}\left(\vec{r}_{ij}\right)\,. \tag{2.3}$$

$H_{ij}^{\prime(2)}$ may be rewritten as

$$H_{ij}^{\prime(2)}=\frac{\vec{P}_{ij}^{\,2}}{2(N-1)(m_i+m_j)}+\frac{\vec{p}_{ij}^{\,2}}{2\mu_{ij}}+V^{(ij)}\left(\vec{r}_{ij}\right)\,, \tag{2.4}$$

where $\vec{P}_{ij}$ denotes the sum of the momenta $\vec{p}_i$ and $\vec{p}_j$

$$\vec{P}_{ij} := \vec{p}_i + \vec{p}_j \,, \tag{2.5}$$

$\vec{p}_{ij}$ is a conjugate momentum of $\vec{r}_{ij} := \vec{r}_i - \vec{r}_j$

$$\vec{p}_{ij} := \frac{m_i m_j}{m_i + m_j}\left(\frac{\vec{p}_i}{m_i} - \frac{\vec{p}_j}{m_j}\right) = \frac{m_j \vec{p}_i - m_i \vec{p}_j}{m_i + m_j}\,, \tag{2.6}$$

and μ_{ij} is the reduced mass of two particles of masses $(N-1)m_i$ and $(N-1)m_j$

$$\mu_{ij} = (N-1)\frac{m_i m_j}{m_i + m_j}\,. \tag{2.7}$$

Thus

$$H = \sum_{i<j=1}^{N} \frac{\vec{P}_{ij}^2}{2(N-1)m_i m_j} + \sum_{i<j=1}^{N} H_{ij}^{(2)}\,, \tag{2.8}$$

with

$$H_{ij}^{(2)} = \frac{\vec{p}_{ij}^{\,2}}{2\mu_{ij}} + V^{(ij)}\left(\vec{r}_{ij}\right)\,. \tag{2.9}$$

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

$$E = \langle\Psi|H|\Psi\rangle = \langle\Psi|\sum_{i<j=1}^{N} \frac{\vec{P}_{ij}^2}{2(N-1)(m_i + m_j)}|\Psi\rangle + \langle\Psi|\sum_{i<j=1}^{N} H_{ij}^{(2)}|\Psi\rangle\,. \tag{2.10}$$

Since $\vec{P}_{ij}^2/\left(2(N-1)m_i m_j\right)$ is a positive definite operator, then

$$\langle\Psi|\frac{\vec{P}_{ij}^2}{2(N-1)m_i m_j}|\Psi\rangle \geq 0\,. \tag{2.11}$$

This is on one hand. On the other hand, by virtue of the variational principle

$$\langle\Psi|H_{ij}^{(2)}|\Psi\rangle \geq E_{ij}^{(2)}(\mu_{ij})\,, \tag{2.12}$$

where $E_{ij}^{(2)}\left(\mu_{ij}\right)$ denotes the ground state energy of the two-body Hamiltonian $H_{ij}^{(2)}$. Hence

$$E \geq \sum_{i<j=1}^{N} E_{ij}^{(2)}\left(\mu_{ij}\right)\,. \tag{2.13}$$

The right-hand side of the inequality (2.13) is called the naïve lower bound and is denoted $E_{\text{naïve}}$, namely

$$E_{\text{naïve}} = \sum_{i<j=1}^{N} E_{ij}^{(2)}\left(\mu_{ij}\right) . \tag{2.14}$$

One easily sees that one default of the naïve lower bound is to replace the expectation value of each one of the positive definite operators $\vec{P}_{ij}^2/\left(2(N-1)m_i m_j\right)$ by zero, which is a rather crude approximation. This has lead to the development of another lower bound, known in the literature as the improved lower bound. We will present this bound in the next section, but before that let us consider the important particular case of a two-body power law potential

$$V^{(ij)}\left(\vec{r}_{ij}\right) = \lambda_{ij} r_{ij}^{\nu_{ij}} , \tag{2.15}$$

where λ_{ij}, the coupling constant, and ν_{ij} the exponent of the power law potential are of the same sign. By virtue of the scaling laws [12, 13]

$$E^{(2)}\left(a, |\lambda|, \nu\right) = a^{\frac{\nu}{2+\nu}} |\lambda|^{\frac{2}{2+\nu}} E^{(2)}\left(1, 1, \nu\right) , \tag{2.16}$$

where $E^{(2)}\left(a, |\lambda|, \nu\right)$ and $E^{(2)}\left(1, 1, \nu\right)$ stand respectively for the ground state energies of the two Hamiltonians

$$H^{(2)}(a, |\lambda|, \nu) := a\vec{p}^2 + \text{sign}(\nu)|\lambda| r^{\nu} \tag{2.17}$$

and

$$H^{(2)}(\nu) := \vec{p}^2 + \text{sign}(\nu) r^{\nu} . \tag{2.18}$$

The naïve lower bound may then be put in the form

$$E_{\text{naïve}} = \sum_{i<j=1}^{N} \left(2\mu_{ij}\right)^{\frac{-\nu_{ij}}{2+\nu_{ij}}} |\lambda_{ij}|^{\frac{2}{2+\nu_{ij}}} E^{(2)}\left(1, 1, \nu_{ij}\right) . \tag{2.19}$$

Let us consider now in turn, mass configurations up to three distinct masses. Throughout this paper, we will restrict ourselves to the case where λ_{ij} and ν_{ij} depend only on the masses m_i and m_j of the two involved particles.

2.1. Configuration $(N \times m)$

This is the case of a system with all masses equal. Thus

$$\mu_{ij} = (N-1)\frac{m}{2} , \qquad i < j = 1, \ldots, N , \tag{2.20}$$

is independent of the pair under consideration. Moreover, we have one coupling constant $\lambda_{ij} = \lambda$ and one power $\nu_{ij} = \nu$. Therefore, the naïve lower bound simplifies to

$$E_{\text{naïve}} = \frac{N\,(N-1)}{2}\,((N-1)m)^{\frac{-\nu}{2+\nu}}\,|\lambda|^{\frac{2}{2+\nu}}\,E^{(2)}(1,1,\nu)\,. \tag{2.21}$$

2.2. Configuration $(n_1 \times m_1,\, n_2 \times m_2)$

This is the case of systems constituted of n_1 ($n_1 < N$) particles of mass m_1 and n_2 ($n_2 = N - n_1$) particles of mass m_2. We have then three different reduced masses

$$\begin{aligned}
\mu_{ij} &= \mu_{m_1m_1} = (N-1)\,\frac{m_1}{2}\,, && i<j=1,\ldots,n_1\,,\\
\mu_{ij} &= \mu_{m_2m_2} = (N-1)\,\frac{m_2}{2}\,, && i<j=n_1+1,\ldots,N\,,\\
\mu_{ij} &= \mu_{m_1m_2} = (N-1)\,\frac{m_1m_2}{m_1+m_2}\,, && i=1,\ldots,n_1\,,\quad j=n_1+1,\ldots,N\,,
\end{aligned} \tag{2.22}$$

three coupling constants

$$\begin{aligned}
\lambda_{ij} &= \lambda_{m_1m_1}\,, && i<j=1,\ldots,n_1\,,\\
\lambda_{ij} &= \lambda_{m_2m_2}\,, && i<j=n_1+1,\ldots,N\,,\\
\lambda_{ij} &= \lambda_{m_1m_2}\,, && i=1,\ldots,n_1\,,\quad j=n_1+1,\ldots,N\,,
\end{aligned} \tag{2.23}$$

and three exponents

$$\begin{aligned}
\nu_{ij} &= \nu_{m_1m_1}\,, && i<j=1,\ldots,n_1\,,\\
\nu_{ij} &= \nu_{m_2m_2}\,, && i<j=n_1+1,\ldots,N\,,\\
\nu_{ij} &= \nu_{m_1m_2}\,, && i=1,\ldots,n_1\,,\quad j=n_1+1,\ldots,N\,.
\end{aligned} \tag{2.24}$$

The general expression of the naïve lower bound simplifies to

$$\begin{aligned}
E_{\text{naïve}} = {} & \frac{n_1\,(n_1-1)}{2}\,(2\mu_{m_1m_1})^{\frac{-\nu_{m_1m_1}}{2+\nu_{m_1m_1}}}\,|\lambda_{m_1m_1}|^{\frac{2}{2+\nu_{m_1m_1}}}\,E^{(2)}(1,1,\nu_{m_1m_1})\\
&+\frac{n_2\,(n_2-1)}{2}\,(2\mu_{m_2m_2})^{\frac{-\nu_{m_2m_2}}{2+\nu_{m_2m_2}}}\,|\lambda_{m_2m_2}|^{\frac{2}{2+\nu_{m_2m_2}}}\,E^{(2)}(1,1,\nu_{m_2m_2})\\
&+n_1n_2\,(2\mu_{m_1m_2})^{\frac{-\nu_{m_1m_2}}{2+\nu_{m_1m_2}}}\,|\lambda_{m_1m_2}|^{\frac{2}{2+\nu_{m_1m_2}}}\,E^{(2)}(1,1,\nu_{m_1m_2})\,,
\end{aligned} \tag{2.25}$$

where $\mu_{m_1m_1}$, $\mu_{m_2m_2}$ and $\mu_{m_1m_2}$ are given by (2.22).

2.3. *Configuration* $(n_1 \times m_1,\ n_2 \times m_2,\ n_3 \times m_3)$

Here we consider systems where three distinct masses m_1, m_2 and m_3 are involved. The particles with masses m_1, m_2 and m_3 are in numbers of n_1, n_2 and n_3 respectively with $n_1 + n_2 + n_3 = N$. For this configuration, we have 6 reduced masses, 6 exponents and 6 coupling constants

$$\begin{aligned}
\mu_{ij} &= \mu_{m_1m_1} = (n_1-1)\,\frac{m_1}{2}\,, && i<j=1,\ldots,n_1\,,\\
\mu_{ij} &= \mu_{m_2m_2} = (n_2-1)\,\frac{m_2}{2}\,, && i<j=n_1+1,\ldots,n_1+n_2\,,\\
\mu_{ij} &= \mu_{m_3m_3} = (n_3-1)\,\frac{m_3}{2}\,, && i<j=n_1+n_2+1,\ldots,N\,,\\
\mu_{ij} &= \mu_{m_1m_2} = (N-1)\,\frac{m_1m_2}{m_1+m_2}\,, && i=1,\ldots,n_1\,,\\
& && j=n_1+1,\ldots,n_1+n_2\,,\\
\mu_{ij} &= \mu_{m_1m_3} = (N-1)\,\frac{m_1m_3}{m_1+m_3}\,, && i=1,\ldots,n_1\,,\\
& && j=n_1+n_2+1,\ldots,N\,,\\
\mu_{ij} &= \mu_{m_2m_3} = (N-1)\,\frac{m_2m_3}{m_2+m_3}\,, && i=n_1+1,\ldots,n_1+n_2\,,\\
& && j=n_1+n_2+1,\ldots,N\,,
\end{aligned} \tag{2.26}$$

$$\begin{aligned}
\nu_{ij} &= \nu_{m_1m_1}\,, && i<j=1,\ldots,n_1\,,\\
\nu_{ij} &= \nu_{m_2m_2}\,, && i<j=n_1+1,\ldots,n_1+n_2\,,\\
\nu_{ij} &= \nu_{m_3m_3}\,, && i<j=n_1+n_2+1,\ldots,N\,,\\
\nu_{ij} &= \nu_{m_1m_2}\,, && i=1,\ldots,n_1\,, \quad j=n_1+1,\ldots,n_1+n_2\,,\\
\nu_{ij} &= \nu_{m_1m_3}\,, && i=1,\ldots,n_1\,, \quad j=n_1+n_2+1,\ldots,N\,,\\
\nu_{ij} &= \nu_{m_2m_3}\,, && i=n_1+1,\ldots,n_1+n_2\,,\\
& && j=n_1+n_2+1,\ldots,N\,,
\end{aligned} \tag{2.27}$$

and

$$\begin{aligned}
\lambda_{ij} &= \lambda_{m_1m_1}\,, && i<j=1,\ldots,n_1\,,\\
\lambda_{ij} &= \lambda_{m_2m_2}\,, && i<j=n_1+1,\ldots,n_1+n_2\,,\\
\lambda_{ij} &= \lambda_{m_3m_3}\,, && i<j=n_1+n_2+1,\ldots,N\,,\\
\lambda_{ij} &= \lambda_{m_1m_2}\,, && i=1,\ldots,n_1\,, \quad j=n_1+1,\ldots,n_1+n_2\,,\\
\lambda_{ij} &= \lambda_{m_1m_3}\,, && i=1,\ldots,n_1\,, \quad j=n_1+n_2+1,\ldots,N\,,\\
\lambda_{ij} &= \lambda_{m_2m_3}\,, && i=n_1+1,\ldots,n_1+n_2\,,\\
& && j=n_1+n_2+1,\ldots,N\,.
\end{aligned} \tag{2.28}$$

The naïve lower bound then reduces to

$$\begin{aligned} E_{\text{naïve}} &= \frac{n_1\,(n_1-1)}{2}\,(2\mu_{m_1m_1})^{\frac{-\nu_{m_1m_1}}{2+\nu_{m_1m_1}}}\,|\lambda_{m_1m_1}|^{\frac{2}{2+\nu_{m_1m_1}}}\,E^{(2)}(1,1,\nu_{m_1m_1}) \\ &+ \frac{n_2\,(n_2-1)}{2}\,(2\mu_{m_2m_2})^{\frac{-\nu_{m_2m_2}}{2+\nu_{m_2m_2}}}\,|\lambda_{m_2m_2}|^{\frac{2}{2+\nu_{m_2m_2}}}\,E^{(2)}(1,1,\nu_{m_2m_2}) \\ &+ \frac{n_3\,(n_3-1)}{2}\,(2\mu_{m_3m_3})^{\frac{-\nu_{m_3m_3}}{2+\nu_{m_3m_3}}}\,|\lambda_{m_3m_3}|^{\frac{2}{2+\nu_{m_3m_3}}}\,E^{(2)}(1,1,\nu_{m_3m_3}) \\ &+ n_1n_2\,(2\mu_{m_1m_2})^{\frac{-\nu_{m_1m_2}}{2+\nu_{m_1m_2}}}\,|\lambda_{m_1m_2}|^{\frac{2}{2+\nu_{m_1m_2}}}\,E^{(2)}(1,1,\nu_{m_1m_2}) \\ &+ n_1n_3\,(2\mu_{m_1m_3})^{\frac{-\nu_{m_1m_3}}{2+\nu_{m_1m_3}}}\,|\lambda_{m_1m_3}|^{\frac{2}{2+\nu_{m_1m_3}}}\,E^{(2)}(1,1,\nu_{m_1m_3}) \\ &+ n_2n_3\,(2\mu_{m_2m_3})^{\frac{-\nu_{m_2m_3}}{2+\nu_{m_2m_3}}}\,|\lambda_{m_2m_3}|^{\frac{2}{2+\nu_{m_2m_3}}}\,E^{(2)}(1,1,\nu_{m_2m_3})\,. \end{aligned} \tag{2.29}$$

3. Improved lower bound

A default of the naïve lower bound is that the centre of mass energy is not separated from the Hamiltonian and this leads, as we have already noticed, to the replacement of the expectation values of positive definite operators by zero, a rather crude approximation. This fact motivated the development of another lower bound, the so-called improved lower bound [14–16] which we will present in what follows. Here the starting point is the following identity

$$\sum_{i=1}^{N}\frac{\vec{p}_i^{\,2}}{2m_i} = \frac{\boldsymbol{P}^2}{2M} + \sum_{i<j=1}^{N}\frac{(m_j\vec{p}_i - m_i\vec{p}_j)^2}{2m_im_jM}\,, \tag{3.1}$$

where $\boldsymbol{P}^2/(2M)$ stands for the centre of mass kinetic energy ($M=\sum_{i=1}^{N} m_i$). The Hamiltonian of the system may then be rewritten as

$$H = \frac{\boldsymbol{P}^2}{2M} + \sum_{i<j=1}^{N}\widetilde{H}_{ij}^{(2)}\,, \tag{3.2}$$

where $\widetilde{H}_{ij}^{(2)}$ is a two-body Hamiltonian

$$\widetilde{H}_{ij}^{(2)} = \frac{(m_j\vec{p}_i - m_i\vec{p}_j)^2}{2m_im_jM} + V^{(ij)}\left(\vec{r}_{ij}\right)\,. \tag{3.3}$$

It is clear that

$$\vec{p}_{ij} := \frac{m_j\vec{p}_i - m_i\vec{p}_j}{m_i+m_j}\,, \qquad i<j=1,\dots,N \tag{3.4}$$

is a conjugate momentum of $\vec{r}_{ij}$ and it is more judicious to rewrite $\widetilde{H}_{ij}^{(2)}$ by explicitly showing $\vec{p}_{ij}$

$$\widetilde{H}_{ij}^{(2)} = \frac{\vec{p}_{ij}^{\,2}}{2\widetilde{\mu}_{ij}} + V^{(ij)}\left(\vec{r}_{ij}\right) \tag{3.5}$$

with

$$\widetilde{\mu}_{ij} = \frac{m_i m_j M}{\left(m_i + m_j\right)^2}\,, \qquad i < j = 1, \ldots, N\,. \tag{3.6}$$

Denoting again by $|\Psi\rangle$ the normalized ground state of the system and E the corresponding energy we have

$$E = \langle\Psi|H|\Psi\rangle = \langle\Psi|\frac{\boldsymbol{P}^2}{2M}|\Psi\rangle + \sum_{i<j=1}^{N} \langle\Psi|\widetilde{H}_{ij}^{(2)}|\Psi\rangle\,. \tag{3.7}$$

Since $|\Psi\rangle$ is invariant under translations, it follows that $\boldsymbol{P}\,|\Psi\rangle = \mathbf{0}$ and

$$\langle\Psi|\,\frac{\boldsymbol{P}^2}{2M}\,|\Psi\rangle = 0\,. \tag{3.8}$$

Applying the variational principle

$$\langle\Psi|\,\widetilde{H}_{ij}^{(2)}\,|\Psi\rangle \geq E_{ij}^{(2)}\left(\widetilde{\mu}_{ij}\right)\,, \tag{3.9}$$

where $E_{ij}^{(2)}\left(\widetilde{\mu}_{ij}\right)$ stands for the ground state energy of the two-body Hamiltonian $\widetilde{H}_{ij}^{(2)}$. Thus

$$E \geq \sum_{i<j=1}^{N} E_{ij}^{(2)}\left(\widetilde{\mu}_{ij}\right)\,. \tag{3.10}$$

We obtain in this way a lower bound, the right hand side of the previous inequality, called improved lower bound and denoted E_{improved}, *i.e.*,

$$E_{\text{improved}} = \sum_{i<j=1}^{N} E_{ij}^{(2)}\left(\widetilde{\mu}_{ij}\right)\,. \tag{3.11}$$

As in the case of the naïve lower bound, let us consider the interesting case of a two-body power law potential, (2.15). Making use of scaling laws, (2.16), we have in this case

$$E_{\text{improved}} = \sum_{i<j=1}^{N} \left(\frac{2m_i m_j M}{\left(m_i + m_j\right)^2}\right)^{\frac{-\nu_{ij}}{2+\nu_{ij}}} \left|\lambda_{ij}\right|^{\frac{2}{2+\nu_{ij}}} E^{(2)}(1, 1, \nu_{ij})\,, \tag{3.12}$$

where $E^{(2)}(1,1,\nu_{ij})$ stands for the ground state energy of the Hamiltonian $H^{(2)}(\nu_{ij})$, (2.18). As in the case of the naïve lower bound, let us consider in turn the mass configurations $(N\times m)$, $(n_1\times m_1, n_2\times m_2)$ and $(n_1\times m_1, n_2\times m_2, n_3\times m_3)$ with always the same assumptions on the exponents ν_{ij} and the coupling constants λ_{ij}, that is ν_{ij} and λ_{ij} depending uniquely on the masses of the two involved particles.

3.1. *Configuration* $(N\times m)$

We have one reduced mass

$$\widetilde{\mu}_{ij}=\widetilde{\mu}=\frac{Nm}{4}\,, \tag{3.13}$$

one exponent $\nu_{ij}=\nu$ and one coupling constant $\lambda_{ij}=\lambda$, in which case the improved lower bound, (3.12), reduces to

$$E_{\text{improved}}=\frac{N\,(N-1)}{2}\left(\frac{Nm}{2}\right)^{\frac{-\nu}{2+\nu}}|\lambda|^{\frac{2}{2+\nu}}\,E^{(2)}(1,1,\nu)\,. \tag{3.14}$$

3.2. *Configuration* $(n_1\times m_1,\ n_2\times m_2)$

We have three values of the exponents, (2.24), three coupling constants, (2.23), and three reduced masses

$$\begin{aligned}
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_1m_1}=\frac{n_1m_1+(N-n_1)\,m_2}{4}\,, \qquad i<j=1,\ldots,n_1\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_2m_2}=\frac{n_1m_1+(N-n_1)\,m_2}{4}\,, \qquad i<j=n_1+1,\ldots,N\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_1m_2}=\frac{m_1m_2(n_1m_1+(N-n_1)\,m_2)}{(m_1+m_2)^2}\,,\\
&\quad i=1,\ldots,n_1\,, \qquad j=n_1+1,\ldots,N\,.
\end{aligned} \tag{3.15}$$

The improved lower bound then reduces to

$$\begin{aligned}
E_{\text{improved}} = {}& \tfrac{n_1(n_1-1)}{2}\,(2\widetilde{\mu}_{m_1m_1})^{\frac{-\nu_{m_1m_1}}{2+\nu_{m_1m_1}}}|\lambda_{m_1m_1}|^{\frac{2}{2+\nu_{m_1m_1}}}\,E^{(2)}(1,1,\nu_{m_1m_1})\\
&+\tfrac{n_2(n_2-1)}{2}\,(2\widetilde{\mu}_{m_2m_2})^{\frac{-\nu_{m_2m_2}}{2+\nu_{m_2m_2}}}|\lambda_{m_2m_2}|^{\frac{2}{2+\nu_{m_2m_2}}}\,E^{(2)}(1,1,\nu_{m_2m_2})\\
&+n_1n_2(2\widetilde{\mu}_{m_1m_2})^{\frac{-\nu_{m_1m_2}}{2+\nu_{m_1m_2}}}|\lambda_{m_1m_2}|^{\frac{2}{2+\nu_{m_1m_2}}}\,E^{(2)}(1,1,\nu_{m_1m_2})\,.
\end{aligned} \tag{3.16}$$

3.3. Configuration $(n_1 \times m_1,\ n_2 \times m_2,\ n_3 \times m_3)$

We have six reduced masses

$$\begin{aligned}
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_1m_1} = \frac{n_1m_1+n_2m_2+n_3m_3}{4}\,, \qquad i<j=1,\dots,n_1\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_2m_2} = \frac{n_1m_1+n_2m_2+n_3m_3}{4}\,, \qquad i<j=n_1+1,\dots,n_1+n_2\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_3m_3} = \frac{n_1m_1+n_2m_2+n_3m_3}{4}\,, \qquad i<j=n_1+n_2+1,\dots,N\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_1m_2} = m_1m_2\frac{(n_1m_1+n_2m_2+n_3m_3)}{(m_1+m_2)^2}\,,\\
&\quad i=1,\dots,n_1\,, \qquad j=n_1+1,\dots,n_1+n_2\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_1m_3} = m_1m_3\frac{(n_1m_1+n_2m_2+n_3m_3)}{(m_1+m_3)^2}\,,\\
&\quad i=1,\dots,n_1\,, \qquad j=n_1+n_2+1,\dots,N\,,\\
\widetilde{\mu}_{ij} &= \widetilde{\mu}_{m_2m_3} = m_2m_3\frac{(n_1m_1+n_2m_2+n_3m_3)}{(m_2+m_3)^2}\,,\\
&\quad i=n_1+1,\dots,n_1+n_2\,, \qquad j=n_1+n_2+1,\dots,N\,, \qquad (3.17)
\end{aligned}$$

six values of the exponent ν_{ij}, (2.27), and six coupling constants λ_{ij}, (2.28). The improved lower bound then reduces to

$$\begin{aligned}
E_{\text{improved}} &= \frac{n_1(n_1-1)}{2}\left(2\widetilde{\mu}_{m_1m_1}\right)^{\frac{-\nu_{m_1m_1}}{2+\nu_{m_1m_1}}}\left|\lambda_{m_1m_1}\right|^{\frac{2}{2+\nu_{m_1m_1}}} E^{(2)}(1,1,\nu_{m_1m_1})\\
&+ \frac{n_2(n_2-1)}{2}\left(2\widetilde{\mu}_{m_2m_2}\right)^{\frac{-\nu_{m_2m_2}}{2+\nu_{m_2m_2}}}\left|\lambda_{m_2m_2}\right|^{\frac{2}{2+\nu_{m_2m_2}}} E^{(2)}(1,1,\nu_{m_2m_2})\\
&+ \frac{n_3(n_3-1)}{2}\left(2\widetilde{\mu}_{m_3m_3}\right)^{\frac{-\nu_{m_3m_3}}{2+\nu_{m_3m_3}}}\left|\lambda_{m_3m_3}\right|^{\frac{2}{2+\nu_{m_3m_3}}} E^{(2)}(1,1,\nu_{m_3m_3})\\
&+ n_1n_2\left(2\widetilde{\mu}_{m_1m_1}\right)^{\frac{-\nu_{m_1m_2}}{2+\nu_{m_1m_2}}}\left|\lambda_{m_1m_2}\right|^{\frac{2}{2+\nu_{m_1m_2}}} E^{(2)}(1,1,\nu_{m_1m_2})\\
&+ n_1n_3\left(2\widetilde{\mu}_{m_1m_3}\right)^{\frac{-\nu_{m_1m_3}}{2+\nu_{m_1m_3}}}\left|\lambda_{m_1m_3}\right|^{\frac{2}{2+\nu_{m_1m_3}}} E^{(2)}(1,1,\nu_{m_1m_3})\\
&+ n_2n_3\left(2\widetilde{\mu}_{m_2m_3}\right)^{\frac{-\nu_{m_2m_3}}{2+\nu_{m_2m_3}}}\left|\lambda_{m_2m_3}\right|^{\frac{2}{2+\nu_{m_2m_3}}} E^{(2)}(1,1,\nu_{m_2m_3})\,. \qquad (3.18)
\end{aligned}$$

4. Comparison of the naïve and improved lower bounds

In reality, the goal at the origin of the introduction of the improved lower bound is only partially reached. Let us content ourselves with two examples. One example where the improved lower bound is better than the naïve lower bound and a counter-example where it is the naïve lower bound that is better than the improved one.

First example

Let us consider the case of masses all equal $m_1 = \ldots = m_N = m$. The naïve and improved lower bounds then reduce respectively to

$$E_{\text{naïve}} = \frac{N(N-1)}{2} E^{(2)}\left(\frac{(N-1)m}{2}\right), \tag{4.1}$$

$$E_{\text{improved}} = \frac{N(N-1)}{2} E^{(2)}\left(\frac{Nm}{4}\right). \tag{4.2}$$

It is clear that the reduced mass, $Nm/4$, involved in E_{improved} is lower than the reduced mass, $(N-1)m/2$, involved in $E_{\text{naïve}}$. Making use of the Feynman–Hellmann theorem [17] which states that for a Hamiltonian H depending on a parameter

$$H = H(\alpha), \tag{4.3}$$

the corresponding energy levels depend on α according to

$$\frac{\partial E(\alpha)}{\partial \alpha} = \langle \Psi(\alpha)| \frac{\partial H(\alpha)}{\partial \alpha} |\Psi(\alpha)\rangle, \tag{4.4}$$

with

$$H(\alpha)|\Psi(\alpha)\rangle = E(\alpha)|\Psi(\alpha)\rangle, \tag{4.5}$$

to the case of the Hamiltonian $H^{(2)} = \vec{p}^2/(2\mu) + V(\vec{r})$, with the reduced mass μ as a parameter, one obtains

$$\frac{\partial E(\mu)}{\partial \mu} = -\langle \Psi(\mu)| \frac{\vec{p}^2}{2\mu^2} |\Psi(\mu)\rangle. \tag{4.6}$$

Since $\vec{p}^2/(2\mu)$ is a positive definite operator

$$\frac{\partial E(\mu)}{\partial \mu} \leq 0, \tag{4.7}$$

then $E(\mu)$ decreases with μ. This is nothing else but the translation of the intuitively well understood property that the inertia favors binding. Hence

$$E^{(2)}\left(\frac{Nm}{4}\right) > E^{(2)}\left(\frac{(N-1)m}{2}\right) \tag{4.8}$$

and

$$E_{\text{improved}} > E_{\text{naïve}}. \tag{4.9}$$

Second example

Let us consider the mass configuration $((N-1)\times m_1, 1\times m_2)$, where the naïve and the improved lower bounds reduce respectively to

$$E_{\text{naïve}} = \tfrac{(N-1)(N-2)}{2} E^{(2)}\left(\tfrac{(N-1)m_1}{2}\right) + (N-1)\, E^{(2)}\left(\tfrac{(N-1)m_1 m_2}{m_1+m_2}\right)$$

and

$$\begin{aligned} E_{\text{improved}} &= \tfrac{(N-1)(N-2)}{2} E^{(2)}\left(\tfrac{(N-1)m_1+m_2}{4}\right) \\ &\quad + (N-1)\, E^{(2)}\left(m_1 m_2 \tfrac{(N-1)m_1+m_2}{(m_1+m_2)^2}\right) . \end{aligned}$$

In the case of a power law potential with the same exponent ν and the same coupling constant λ for all the pairs of particles, $E_{\text{naïve}}$ and E_{improved} reduce respectively to

$$\begin{aligned} E_{\text{naïve}} &= |\lambda|^{\frac{2}{2+\nu}} \left(\frac{(N-1)(N-2)}{2} \left((N-1)m_1\right)^{\frac{-\nu}{2+\nu}} \right. \\ &\quad \left. + (N-1)\left(2(N-1)\tfrac{m_1 m_2}{m_1+m_2}\right)^{\frac{-\nu}{2+\nu}} \right) E^{(2)}(1,1,\nu) \end{aligned} \tag{4.10}$$

and

$$\begin{aligned} E_{\text{improved}} &= |\lambda|^{\frac{2}{2+\nu}} \left(\frac{(N-1)(N-2)}{2} \left(\tfrac{(N-1)m_1+m_2}{2}\right)^{\frac{-\nu}{2+\nu}} \right. \\ &\quad \left. + (N-1)\left(2m_1 m_2 \tfrac{(N-1)m_1+m_2}{(m_1+m_2)^2}\right)^{\frac{-\nu}{2+\nu}} \right) E^{(2)}(1,1,\nu) . \end{aligned} \tag{4.11}$$

Let us now consider the limit $m_2 \to \infty$. For $-2 < \nu < 0$ and thus $-\nu/(2+\nu) > 0$, it is easy to find out, if one bears in mind that $E^{(2)}(1,1,\nu)$ is negative for negative powers ν, that $E_{\text{improved}} \to -\infty$, while

$$\begin{aligned} E_{\text{naïve}} &\to |\lambda|^{\frac{2}{2+\nu}} \left(\tfrac{(N-1)(N-2)}{2} \left((N-1)m_1\right)^{\frac{-\nu}{2+\nu}} \right. \\ &\quad \left. + (N-1)\left(2(N-1)\, m_1\right)^{\frac{-\nu}{2+\nu}} \right) E^{(2)}(1,1,\nu) \end{aligned} \tag{4.12}$$

remains finite. Therefore,

$$E_{\text{naïve}} > E_{\text{improved}} . \tag{4.13}$$

In other words, the naïve lower bound is better than the improved one.

5. Optimized lower bound

Since the goal behind the introduction of the improved lower bound has been only partially reached, this has lead to the development of a new lower bound: the optimized lower bound [1–5]. The starting point is the following decomposition of the kinetic energy term

$$\sum_{i=1}^{N} \frac{1}{2m_i} \vec{p}_i^{\,2} = \left(\sum_{j=1}^{N} b_j \vec{p}_j \right) \left(\sum_{i=1}^{N} \vec{p}_i \right) + \sum_{i<j=1}^{N} a_{ij} \vec{p}_{ij}^{\,2} \,, \tag{5.1}$$

involving the parameters b_j and the necessary positive parameters a_{ij}, $i < j = 1, \ldots, N$. The $\vec{p}_{ij}$ are linear combinations of the momenta $\vec{p}_k$

$$\vec{p}_{ij} = \sum_{k=1}^{N} \frac{x_{ij,k}}{2} \vec{p}_k \,. \tag{5.2}$$

The factor $1/2$ in the expression of $\vec{p}_{ij}$ is a matter of convenience. Without loss of generality, one can take $x_{ij,i} = 1$. Then imposing to $\vec{p}_{ij}$ to be a conjugate momentum of $\vec{r}_{ij}$, one ends with $x_{ij,j} = -1$. The decomposition of the kinetic energy term thus involves N parameters b_k, $N(N-1)/2$ parameters a_{ij} and $N(N-1)(N-2)/2$ parameters $x_{ij,k}$. Identifying both sides of (5.1), one gets $N + N(N-1)/2$ constraints among the parameters, which one can consider as a system of $N + N(N-1)/2$ linear equations with the b_k and the a_{ij} as unknowns and the $x_{ij,k}$ as parameters. One can then express the a_{ij} and the b_k in terms of the $x_{ij,k}$ and the masses $m_1, \ldots, m_N$. From now on, the a_{ij} and the b_k should be considered as implicit functions of the parameters $x_{ij,k}$. To the decomposition of the kinetic energy term, (5.1), corresponds the following decomposition of the Hamiltonian of the system

$$H = \left(\sum_{j=1}^{N} b_j \vec{p}_j \right) \left(\sum_{i=1}^{N} \vec{p}_i \right) + \sum_{i<j=1}^{N} \left(a_{ij} \vec{p}_{ij}^{\,2} + V^{(ij)}(\vec{r}_{ij}) \right) . \tag{5.3}$$

Let $|\Psi\rangle$ denotes the normalized ground state of the system, with E the corresponding energy. Since $|\Psi\rangle$ is invariant under translations, then

$$\left(\sum_{i=1}^{N} \vec{p}_i \right) |\Psi\rangle = \mathbf{0} \,. \tag{5.4}$$

This on one hand. On the other hand, applying the variational principle results in

$$\langle \Psi | \left(a_{ij} \vec{p}_{ij}^{\,2} + V^{(ij)}(\vec{r}_{ij}) \right) |\Psi\rangle \geq E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})] \,, \tag{5.5}$$

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

$$H_{ij}^{(2)}[a_{ij}(x_{k\ell,m})] = a_{ij}\vec{p}_{ij}^{\,2} + V^{(ij)}(\vec{r}_{ij})\,. \tag{5.6}$$

It follows that

$$E \geq \sum_{i<j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})]\,. \tag{5.7}$$

We obtain in this way a family of lower bounds for E, a lower bound

$$\sum_{i<j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})]\,, \tag{5.8}$$

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

$$E_{\text{olb}} := \max_{\{x_{k\ell,m}\}} \sum_{i<j=1}^{N} E_{ij}^{(2)}[a_{ij}(x_{k\ell,m})]\,. \tag{5.9}$$

As for the two cases of naïve and improved lower bounds, let us consider the case of a two-body power law potential, (2.15). We have in this case, using scaling laws, (2.16),

$$E_{\text{olb}} = \max_{\{x_{k\ell,m}\}} \sum_{i<j=1}^{N} |\lambda_{ij}|^{\frac{2}{2+\nu_{ij}}} \left(a_{ij}(x_{k\ell,m})\right)^{\frac{\nu_{ij}}{2+\nu_{ij}}} E^{(2)}\left(1,1,\nu_{ij}\right)\,, \tag{5.10}$$

where $E^{(2)}(1,1,\nu_{ij})$ stands again for the ground state energy of the two-body Hamiltonian $H^{(2)}(\nu_{ij})$, (2.18). Let us consider, in turn, the mass configurations $(N\times m)$, $(n_1\times m_1, n_2\times m_2)$ and $(n_1\times m_1, n_2\times m_2, n_3\times m_3)$ with always the same assumptions on the exponents ν_{ij} and the coupling constants λ_{ij}.

5.1. Configuration $(N\times m)$

We have one parameter a_{ij}

$$a_{ij} = a\,, \qquad i<j=1,\ldots,N\,,$$

one parameter b_k

$$b_k = b\,, \qquad k=1,\ldots,N\,,$$

and all parameters $x_{ij,k}$ are equal to zero. The kinetic energy decomposition (5.1) reduces to

$$\sum_{i=1}^{N} \frac{1}{2m} \vec{p}_i^{\,2} = \left(\sum_{i=1}^{N} b \vec{p}_i \right) \left(\sum_{j=1}^{N} \vec{p}_j \right) + \sum_{i<j=1}^{N} \frac{a}{4} (\vec{p}_i - \vec{p}_j)^2 , \tag{5.11}$$

and the identification of both sides of (5.11) gives for the parameter a

$$a = \frac{2}{mN} , \qquad i < j = 1, \ldots, N . \tag{5.12}$$

One exponent $\nu_{ij} = \nu$ and one coupling constant $\lambda_{ij} = \lambda$ are involved, and the optimized lower bound reduces to

$$E_{\text{olb}} = \frac{N\,(N-1)}{2} |\lambda|^{\frac{2}{\nu+2}} \left(\frac{2}{mN} \right)^{\frac{\nu}{\nu+2}} E^{(2)}\,(1, 1, \nu) \tag{5.13}$$

which is identical to the improved lower bound for the same mass configuration, (3.14).

5.2. Configuration $(n_1 \times m_1,\, n_2 \times m_2)$

We have three values for the exponents, (2.24), three coupling constants, (2.23), three values for the parameter a_{ij},

$$\begin{aligned} a_{ij} &= a_{m_1 m_1} , && i < j = 1, \ldots, n_1 , \\ a_{ij} &= a_{m_2 m_2} , && i < j = n_1 + 1, \ldots, N , \\ a_{ij} &= a_{m_1 m_2} , && i = 1, \ldots, n_1 , \qquad j = n_1 + 1, \ldots, N , \end{aligned} \tag{5.14}$$

and two values of the parameters b_k,

$$\begin{aligned} b_k &= b_{m_1} , && k = 1, \ldots, n_1 , \\ b_k &= b_{m_2} , && k = n_1 + 1, \ldots, N . \end{aligned}$$

Two parameters $x_{ij,k}$ are involved in the optimized lower bound,

$$\begin{aligned} x_{ij,k} &= 0 , && i < j \le n_1 \qquad \text{or} \qquad n_1 < i < j \le N , \\ x_{ij,k} &= \ell , && i = 1, \ldots, n_1 , \quad j = n_1 + 1, \ldots, N , \quad 1 \le k \le n_1 \quad k \neq i , \\ x_{ij,k} &= p , && i = 1, \ldots, n_1 , \quad j = n_1 + 1, \ldots, N , \quad n_1 < k \le N \quad k \neq j . \end{aligned}$$

The kinetic energy decomposition, (5.1), then simplifies to

$$\sum_{i=1}^{n_1} \frac{1}{2m_1} \vec{p}_i^{\,2} + \sum_{i=n_1+1}^{N} \frac{1}{2m_2} \vec{p}_i^{\,2} = \left(\sum_{i=1}^{n_1} b_{m_1} \vec{p}_i + \sum_{i=n_1+1}^{N} b_{m_2} \vec{p}_i \right) \left(\sum_{j=1}^{N} \vec{p}_j \right)$$

$$+\frac{a_{m_1m_1}}{4}\sum_{i<j=1}^{n_1}(\vec{p}_i-\vec{p}_j)^2+\frac{a_{m_2m_2}}{4}\sum_{i<j=n_1+1}^{N}(\vec{p}_i-\vec{p}_j)^2$$
$$+\frac{a_{m_1m_2}}{4}\sum_{i=1}^{n_1}\sum_{j=n_1+1}^{N}\left(\vec{p}_i-\vec{p}_j+\ell\sum_{\substack{k=1\\k\neq i}}^{n_1}\vec{p}_k+p\sum_{\substack{k=n_1+1\\k\neq j}}^{N}\vec{p}_k\right)^2 . \tag{5.15}$$

Identifying both sides of equation (5.15), one gets a system of linear equations for the a_{ij} and b_k with ℓ and p as parameters. This system allows to express the a_{ij} in terms of the parameters ℓ and p with the result

$$a_{m_1m_1}(\ell,p)=\frac{2}{n_1m_1}-\frac{2n_2\,(n_2m_2+n_1m_1)\,(\ell-1)^2}{n_1m_1m_2\,(N-n_2\ell+n_1n_2\ell-n_1n_2p+n_1p)^2}\,, \tag{5.16}$$
$$a_{m_2m_2}(\ell,p)=\frac{2}{n_2m_2}-\frac{2n_1\,(n_1m_1+n_2m_2)\,(p+1)^2}{n_2m_1m_2\,(N-n_2\ell+n_1n_2\ell-n_1n_2p+n_1p)^2}\,, \tag{5.17}$$
$$a_{m_1m_2}(\ell,p)=2\frac{n_1m_1+n_2m_2}{m_1m_2\,(N-n_2\ell+n_1n_2\ell-n_1n_2p+n_1p)^2}\,. \tag{5.18}$$

The optimized lower bound, (5.9), then reduces to

$$E_{\rm olb} = \max_{\ell,p}\left(\frac{n_1\,(n_1-1)}{2}E^{(2)}\left[a_{m_1m_1}(\ell,p)\right]+\frac{n_2\,(n_2-1)}{2}E^{(2)}\left[a_{m_2m_2}(\ell,p)\right]\right.$$
$$\left.+n_1n_2E^{(2)}\left[a_{m_1m_2}(\ell,p)\right]\right), \tag{5.19}$$

which, in the case of power law potentials, (5.10) simplifies to

$$E_{\rm olb}=\max_{\ell,p}\left(\frac{n_1\,(n_1-1)}{2}|\lambda_{m_1m_1}|^{\frac{2}{\nu_{m_1m_1}+2}}\,(a_{m_1m_1})^{\frac{\nu_{m_1m_1}}{\nu_{m_1m_1}+2}}\,E^{(2)}\,(1,1,\nu_{m_1m_1})\right.$$
$$+\frac{n_2\,(n_2-1)}{2}|\lambda_{m_2m_2}|^{\frac{2}{\nu_{m_2m_2}+2}}\,(a_{m_2m_2})^{\frac{\nu_{m_2m_2}}{\nu_{m_2m_2}+2}}\,E^{(2)}\,(1,1,\nu_{m_2m_2})$$
$$\left.+n_1n_2|\lambda_{m_1m_2}|^{\frac{2}{\nu_{m_1m_2}+2}}\,(a_{m_1m_2})^{\frac{\nu_{m_1m_2}}{\nu_{m_1m_2}+2}}\,E^{(2)}\,(1,1,\nu_{m_1m_2})\right). \tag{5.20}$$

5.3. Configuration $(n_1\times m_1,\, n_2\times m_2,\, n_3\times m_3)$

We have six values of the exponent ν_{ij}, (2.27), and six coupling constants λ_{ij}, (2.28). The parameters b_k are in number of three,

$$b_k \;=\; b_{m_1}\,, \qquad k=1,\ldots,n_1\,,$$

$$
\begin{aligned}
b_k &= b_{m_2}\,, \qquad k = n_1+1,\ldots,n_2\,,\\
b_k &= b_{m_3}\,, \qquad k = n_2+1,\ldots,N\,,
\end{aligned}
$$

and six parameters a_{ij} are involved,

$$
\begin{aligned}
a_{ij} &= a_{m_1m_1}\,, \qquad i<j=1,\ldots,n_1\,,\\
a_{ij} &= a_{m_2m_2}\,, \qquad i<j=n_1+1,\ldots,n_1+n_2\,,\\
a_{ij} &= a_{m_3m_3}\,, \qquad i<j=n_1+n_2+1,\ldots,N\,,\\
a_{ij} &= a_{m_1m_2}\,, \qquad i=1,\ldots,n_1, j=n_1+1,\ldots,n_1+n_2\,,\\
a_{ij} &= a_{m_1m_3}\,, \qquad i=1,\ldots,n_1, j=n_1+n_2+1,\ldots,N\,,\\
a_{ij} &= a_{m_2m_3}\,, \qquad i=n_1+1,\ldots,n_1+n_2\,,\\
&\qquad\qquad\qquad j=n_1+n_2+1,\ldots,N\,.
\end{aligned}
\tag{5.21}
$$

The kinetic energy decomposition (5.1) reduces to

$$
\begin{aligned}
&\sum_{i=1}^{n_1}\frac{1}{2m_1}\vec{p}_i^{\,2}+\sum_{i=n_1+1}^{n_1+n_2}\frac{1}{2m_2}\vec{p}_i^{\,2}+\sum_{i=n_1+n_2+1}^{N}\frac{1}{2m_3}\vec{p}_i^{\,2}\\
&=\left(\sum_{i=1}^{n_1}b_1\vec{p}_i+\sum_{i=n_1+1}^{n_1+n_2}b_2\vec{p}_i+\sum_{i=n_1+n_2+1}^{N}b_3\vec{p}_i\right)\left(\sum_{i=1}^{N}\vec{p}_i\right)\\
&+\frac{a_{m_1m_1}}{4}\sum_{i<j=1}^{n_1}(\vec{p}_i-\vec{p}_j)^2+\frac{a_{m_2m_2}}{4}\sum_{i<j=n_1+1}^{n_1+n_2}(\vec{p}_i-\vec{p}_j)^2+\frac{a_{m_3m_3}}{4}\sum_{i<j=n_1+n_2+1}^{N}(\vec{p}_i-\vec{p}_j)^2\\
&+\frac{a_{m_1m_2}}{4}\sum_{i=1}^{n_1}\sum_{j=n_1+1}^{n_1+n_2}\left(\vec{p}_i-\vec{p}_j+c_1\sum_{k_1\neq i=1}^{n_1}\vec{p}_{k_1}+c_2\sum_{k_2\neq j=n_1+1}^{n_1+n_2}\vec{p}_{k_2}+c_3\sum_{k_3=n_1+n_2+1}^{N}\vec{p}_{k_3}\right)^2\\
&+\frac{a_{m_1m_3}}{4}\sum_{i=1}^{n_1}\sum_{j=n_1+n_2+1}^{N}\left(\vec{p}_i-\vec{p}_j+d_1\sum_{k_1\neq i=1}^{n_1}\vec{p}_{k_1}+d_2\sum_{k_2=n_1+1}^{n_1+n_2}\vec{p}_{k_2}+d_3\sum_{k_3\neq j=n_1+n_2+1}^{N}\vec{p}_{k_3}\right)^2\\
&+\frac{a_{m_2m_3}}{4}\sum_{i=n_1+1}^{n_1+n_2}\sum_{j=n_1+n_2+1}^{N}\left(\vec{p}_i-\vec{p}_j+e_1\sum_{k_1=1}^{n_1}\vec{p}_{k_1}+e_2\sum_{k_2\neq i=n_1+1}^{n_1+n_2}\vec{p}_{k_2}+|1e_3\sum_{k_3\neq j=n_1+n_2+1}^{N}\vec{p}_{k_3}\right)^2.
\end{aligned}
\tag{5.22}
$$

The optimized lower bound, (5.10), then reduces to

$$
\begin{aligned}
E_{\mathrm{olb}}=\max_{\substack{c_1,c_2,c_3\\ d_1,d_2,d_3\\ f_1,f_2,f_3}}\;&\frac{n_1\,(n_1-1)}{2}\,(a_{m_1m_1})^{\frac{-\nu_{m_1m_1}}{2+\nu_{m_1m_1}}}\,|\lambda_{m_1m_1}|^{\frac{2}{2+\nu_{m_1m_1}}}\,E^{(2)}(1,1,\nu_{m_1m_1})\\
&+\frac{n_2\,(n_2-1)}{2}\,(a_{m_2m_2})^{\frac{-\nu_{m_2m_2}}{2+\nu_{m_2m_2}}}\,|\lambda_{m_2m_2}|^{\frac{2}{2+\nu_{m_2m_2}}}\,E^{(2)}(1,1,\nu_{m_2m_2})\\
&+\frac{n_3\,(n_3-1)}{2}\,(a_{m_3m_3})^{\frac{-\nu_{m_3m_3}}{2+\nu_{m_3m_3}}}\,|\lambda_{m_3m_3}|^{\frac{2}{2+\nu_{m_3m_3}}}\,E^{(2)}(1,1,\nu_{m_3m_3})
\end{aligned}
$$

$$
\begin{aligned}
&+n_1n_2\left(a_{m_1m_2}\right)^{\frac{-\nu_{m_1m_2}}{2+\nu_{m_1m_2}}}\left|\lambda_{m_1m_2}\right|^{\frac{2}{2+\nu_{m_1m_2}}}E^{(2)}(1,1,\nu_{m_1m_2})\\
&+n_1n_3\left(a_{m_1m_3}\right)^{\frac{-\nu_{m_1m_3}}{2+\nu_{m_1m_3}}}\left|\lambda_{m_1m_3}\right|^{\frac{2}{2+\nu_{m_1m_3}}}E^{(2)}(1,1,\nu_{m_1m_3})\\
&+n_2n_3\left(a_{m_2m_3}\right)^{\frac{-\nu_{m_2m_3}}{2+\nu_{m_2m_3}}}\left|\lambda_{m_2m_3}\right|^{\frac{2}{2+\nu_{m_2m_3}}}E^{(2)}(1,1,\nu_{m_2m_3})\,,
\end{aligned}
\tag{5.23}
$$

where we have to adjust over nine parameters $x_{ij,k}$

$$
\begin{aligned}
x_{ij,k} &= c_1\,, && i=1,\ldots,n_1\,, \quad j=n_1+1,\ldots,n_1+n_2\,,\\
& && k\neq i=1,\ldots,n_1\,,\\
x_{ij,k} &= c_2\,, && i=1,\ldots,n_1\,, \quad j=n_1+1,\ldots,n_1+n_2\,,\\
& && k\neq j=n_1+1,\ldots,n_1+n_2\,,\\
x_{ij,k} &= c_3\,, && i=1,\ldots,n_1\,, \quad j=n_1+1,\ldots,n_1+n_2\,,\\
& && k=n_1+n_2+1,\ldots,N\,,\\
x_{ij,k} &= d_1\,, && i=1,\ldots,n_1\,, \quad j=n_2+1,\ldots,N\,,\\
& && k\neq i=1,\ldots,n_1\,,\\
x_{ij,k} &= d_2\,, && i=1,\ldots,n_1\,, \quad j=n_2+1,\ldots,N\,,\\
& && k=n_1+1,\ldots,n_1+n_2\,,\\
x_{ij,k} &= d_3\,, && i=1,\ldots,n_1\,, \quad j=n_2+1,\ldots,N\,,\\
& && k\neq j=n_2+1,\ldots,N\,,\\
x_{ij,k} &= e_1\,, && i=n_1+1,\ldots,n_1+n_2\,, \quad j=n_1+n_2+1,\ldots,N\,,\\
& && k=1,\ldots,n_1\,,\\
x_{ij,k} &= e_2\,, && i=n_1+1,\ldots,n_1+n_2\,, \quad j=n_1+n_2+1,\ldots,N\,,\\
& && k\neq i=n_1+1,\ldots,n_1+n_2\,,\\
x_{ij,k} &= e_3\,, && i=n_1+1,\ldots,n_1+n_2\,, \quad j=n_1+n_2+1,\ldots,N\,,\\
& && k\neq j=n_1+n_2+1,\ldots,N\,.
\end{aligned}
\tag{5.24}
$$

The a_{ij} are functions of the parameters c_1, c_2, $c_3,\ldots$, e_3 and their explicit dependence is obtained by inverting the matrix equation

$$
\widetilde{\boldsymbol{D}}\,\boldsymbol{A}=\boldsymbol{\alpha}\,,
\tag{5.25}
$$

where $\widetilde{\boldsymbol{D}}$ is a square 6×6 matrix given by

$$
\widetilde{\boldsymbol{D}}=\begin{pmatrix}
\frac{n_1}{2} & 0 & 0 & \frac{n_2(c_1-1)^2}{2} & \frac{n_3(d_1-1)^2}{2} & 0\\
0 & \frac{n_2}{2} & 0 & \frac{n_1(c_2+1)^2}{2} & 0 & \frac{n_3(e_2-1)^2}{2}\\
0 & 0 & \frac{n_3}{2} & 0 & \frac{n_1(d_3+1)^2}{2} & \frac{n_2(e_3+1)^2}{2}\\
\frac{n_1-1}{4} & \frac{n_2-1}{4} & 0 & \widetilde{\boldsymbol{D}}_{44} & \widetilde{\boldsymbol{D}}_{45} & \widetilde{\boldsymbol{D}}_{46}\\
\frac{n_1-1}{4} & 0 & \frac{n_3-1}{4} & \widetilde{\boldsymbol{D}}_{54} & \widetilde{\boldsymbol{D}}_{55} & \widetilde{\boldsymbol{D}}_{56}\\
0 & \frac{n_2-1}{4} & \frac{n_3-1}{4} & \widetilde{\boldsymbol{D}}_{64} & \widetilde{\boldsymbol{D}}_{65} & \widetilde{\boldsymbol{D}}_{66}
\end{pmatrix},
\tag{5.26}
$$

with

$$\widetilde{\boldsymbol{D}}_{54} = \frac{n_2\left(-2c_3 + c_3^2 n_1 + c_1\left(n_1-1\right)\left(c_1-2c_3\right)+1\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{64} = \frac{n_1\left(2c_3 + c_3^2 n_2 + c_2\left(n_2-1\right)\left(c_2-2c_3\right)+1\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{45} = \frac{n_3\left(-2d_2 + d_2^2 n_1 + 1 + d_1\left(d_1-2d_2\right)\left(n_1-1\right)\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{65} = \frac{n_1\left(2d_2 + d_2^2 n_3 + 1 + d_3\left(d_3-2d_2\right)\left(n_3-1\right)\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{46} = \frac{n_3\left(-2e_1 + e_1^2 n_2 + 1 + e_2\left(e_2-2e_1\right)\left(n_2-1\right)\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{56} = \frac{n_2\left(2e_1 + e_1^2 n_3 + 1 + e_3\left(e_3-2e_1\right)\left(n_3-1\right)\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{44} = \frac{n_1+n_2+2-2c_1c_2\left(n_1-1\right)\left(n_2-1\right)+c_1\left(n_1-1\right)\left(c_1n_2+2\right)+c_2\left(n_2-1\right)\left(c_2n_1-2\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{55} = \frac{n_1+n_3+\,v2-\,v2d_1d_3\left(n_1-1\right)\left(n_3-1\right)+d_1\left(n_1-1\right)\left(d_1n_3+2\right)+d_3\left(n_3-1\right)\left(d_3n_1-2\right)}{4},$$

$$\widetilde{\boldsymbol{D}}_{66} = \frac{n_2+n_3+2-2e_2e_3\left(n_2-1\right)\left(n_3-1\right)+e_2\left(n_2-1\right)\left(e_2n_3+2\right)+e_3\left(n_3-1\right)\left(e_3n_2-2\right)}{4}.$$

$\boldsymbol{A}$ and $\boldsymbol{\alpha}$ are 6×1 column matrices given by

$$\boldsymbol{A} := \begin{pmatrix} a_{m_1m_1} \\ a_{m_2m_2} \\ a_{m_3m_3} \\ a_{m_1m_2} \\ a_{m_1m_3} \\ a_{m_2m_3} \end{pmatrix}, \qquad \boldsymbol{\alpha} := \begin{pmatrix} \frac{1}{m_1} \\ \frac{1}{m_2} \\ \frac{1}{m_3} \\ \frac{1}{2m_1}+\frac{1}{2m_2} \\ \frac{1}{2m_1}+\frac{1}{2m_3} \\ \frac{1}{2m_2}+\frac{1}{2m_3} \end{pmatrix}. \tag{5.27}$$

The matrix equation (5.25) is obtained by identifying both sides of equation (5.22) taking into account the symmetry of the problem. One obtains in this way a linear system of 9 equations, with the bs: b_{m_1}, b_{m_2}, b_{m_3} and as: $a_{m_1m_1}$, $a_{m_2m_2}$, …, $a_{m_2m_3}$ as unknowns and c_1, c_2, …, e_3 as parameters. Eliminating the bs in favor of the as results in a linear system of 6 equations with the 6 as as unknowns, which may be written in matrix form as in (5.25).

The optimization problem implied by (5.23) may be greatly simplified if one takes into account that the values of the parameters c_1, …, e_3 corresponding to the optimized lower bound are constrained by four relations, which are independent of the particular form of the potential and of dynamical nature, the so-called universal dynamical constraints

$$d_1 = \frac{c_1 - c_3 - c_1 d_2 + d_2}{1-c_3}, \tag{5.28}$$

$$e_2 = -\frac{c_2 - c_2 d_2 + c_3 d_2 - d_2}{1 - c_3 d_2}\,, \tag{5.29}$$

$$d_3 = \frac{c_3 - c_3 d_2 - c_3 d_2 e_3 + e_3}{1 - c_3}\,, \tag{5.30}$$

$$e_1 = -\frac{c_3 - d_2}{1 - c_3 d_2}\,. \tag{5.31}$$

More details of the derivation of those constraints will be given in a forthcoming paper.

This allows us to reduce the number of parameters over which we optimize from 9 to 5: c_1, c_2, c_3, d_2 and e_3, resulting in a great simplification.

Note that for configurations $(n_1 \times m_1, n_2 \times m_2, n_3 \times m_3)$, we have considered implicitly the cases where $n_1 > 1$, $n_2 > 1$, $n_3 > 1$. The cases where one or more of the n_i, $i = 1, 2, 3$ equals 1 may be obtained from the results corresponding to $n_1 > 1$, $n_2 > 1$, $n_3 > 1$ by appropriate replacements in the final result for $E_{\text{naïve}}$ and E_{improved}. For E_{olb}, there are additional subtleties: The optimization problem becomes less involved since a part of the parameters disappear. For $n_1 > 1$, $n_2 > 1$, $n_3 = 1$, the number of parameters decreases from 9 to 7: the parameters d_3 and e_3 no longer exist. The universal dynamical constraints are in number of 3, Eqs. (5.28), (5.29) and (5.31), and if we take into account these constraints, we have to optimize over 4 parameters, which we may choose to be c_1, c_2, c_3 and d_2. When $n_1 > 1$, $n_2 = 1$, $n_3 = 1$, we have only 5 parameters c_1, c_3, d_1, d_2 and e_1, 2 universal dynamical constraints, Eqs. (5.28), (5.31), which allow to reduce the problem to an optimization over 3 parameters, that one may choose to be c_1, c_3, and d_2. In the case of $n_1 = 1$, $n_2 = 1$, $n_3 = 1$, *i.e.*, the three-body case, there are only 3 parameters: c_3, d_2 and e_1 which are related by (5.31), and thus we have to optimize over two parameters, for instance c_3 and d_2.

6. Numerical results

The following tables illustrate our numerical results for mass configurations up to three distinct masses. We have considered the six-body system with power-law potentials in Table I, where four representative powers ν_{ij} are considered: $\nu = 2$, $\nu = 1$, $\nu = 0.1$ and $\nu = -1$. We have also considered some non power-law potentials: the Coulomb + Linear $V_{ij} = r_{ij} - 1/r_{ij}$ and the Coulomb + Harmonic $V_{ij} = r_{ij}^2 - 1/r_{ij}$ potentials, also in the case of the six-body system, Table II.

It is worthwhile to notice that for non power-law potentials, and since there is no scaling laws at our disposal, the reduced mass μ cannot be extracted from the ground state energy of the two-body Hamiltonian as in (2.16) with $2\mu = 1/a$. Technically, we need to inject the algorithm of the

TABLE I

Lower bounds for six-body systems with power-law potentials: $V_{ij} = r_{ij}^2$, $V_{ij} = r_{ij}$, $V_{ij} = r_{ij}^{0.1}$ and $V_{ij} = -1/r_{ij}$.

	Harmonic potential $V_{ij} = r_{ij}^2$			Linear potential $V_{ij} = r_{ij}$		
$m_1, \ldots, m_6$	$E_{\text{naïve}}$	E_{improved}	E_{olb}	$E_{\text{naïve}}$	E_{improved}	E_{olb}
1,1,1,1,1,1	20.12	25.98	25.98	20.51	24.32	24.32
1,1,1,1,1,3	18.89	23.66	24.25	19.65	22.83	23.20
1,1,1,1,1,0.5	21.63	27.68	27.82	21.50	25.37	25.43
1,1,1,1,2,2	18.29	23.23	23.51	19.23	22.57	22.73
1,1,1,1,0.5,0.5	23.09	29.38	29.65	22.45	26.39	26.52
1,1,1,2,2,2	17.33	21.99	22.24	18.54	21.75	21.90
1,1,1,1,2,3	17.95	22.46	22.99	18.97	22.06	22.38
1,1,1,1,2,0.5	20.77	26.19	26.61	20.91	24.44	24.67
1,1,1,2,2,0.5	19.87	24.86	25.37	20.28	23.60	23.88
1,1,1,2,2,3	16.96	21.29	21.71	18.27	21.29	21.54
1,1,2,2,3,3	15.56	19.53	19.88	17.23	20.10	20.30
1,1,2,2,0.5,0.5	21.41	26.44	27.23	21.30	24.58	25.02
1,1,1,1,1,∞	18.16	10.61	22.91	19.10	9.279	22.28
1,1,1,1,2,∞	16.17	9.985	21.57	18.38	8.896	21.40
1,1,1,2,2,∞	16.13	9.364	20.24	17.62	8.513	20.49

	Martin potential $V_{ij} = r_{ij}^{0.1}$			Coulomb potential $V_{ij} = -1/r_{ij}$		
$m_1, \ldots, m_6$	$E_{\text{naïve}}$	E_{improved}	E_{olb}	$E_{\text{naïve}}$	E_{improved}	E_{olb}
1,1,1,1,1,1	17.17	17.59	17.59	−18.75	−11.25	−11.25
1,1,1,1,1,3	17.06	17.43	17.47	−21.88	−13.75	−13.07
1,1,1,1,1,0.5	17.28	17.70	17.70	−16.67	−9.931	−9.921
1,1,1,1,2,2	17.01	17.40	17.42	−23.33	−14.11	−13.90
1,1,1,1,0.5,0.5	17.39	17.80	17.81	−14.79	−8.819	−8.774
1,1,1,2,2,2	16.92	17.31	17.33	−26.25	−15.75	−15.58
1,1,1,1,2,3	16.97	17.35	17.38	−24.67	−15.21	−14.63
1,1,1,1,2,0.5	17.21	17.60	17.62	−18.50	−11.17	−10.95
1,1,1,2,2,0.5	17.13	17.51	17.54	−20.75	−12.45	−12.17
1,1,1,2,2,3	16.88	17.26	17.28	−27.88	−16.88	−16.46
1,1,2,2,3,3	16.74	17.12	17.14	−33.67	−20.09	−19.77
1,1,2,2,0.5,0.5	17.25	17.61	17.65	−18.38	−11.09	−10.67
1,1,1,1,1,∞	16.98	5.978	17.36	−25.00	$-\infty$	−15.60
1,1,1,1,2,∞	16.88	5.939	17.26	−29.17	$-\infty$	−17.22
1,1,1,2,2,∞	16.78	5.900	17.15	−33.75	$-\infty$	−19.76

TABLE II

Lower bounds for six-body systems with some non power-law potentials: The Coulomb + Linear and the Coulomb + Harmonic potentials.

	Potential $V_{ij} = r_{ij} - 1/r_{ij}$			Potential $V_{ij} = r_{ij}^2 - 1/r_{ij}$		
$m_1,\ldots,m_5$	$E_{\text{naïve}}$	E_{improved}	E_{olb}	$E_{\text{naïve}}$	E_{improved}	E_{olb}
1,1,1,1,1,1	−10.67	0.883	0.883	−13.42	−0.740	−0.740
1,1,1,1,1,3	−14.59	−3.232	−2.192	−17.39	−5.381	−4.236
1,1,1,1,1,0.5	−7.544	3.389	3.450	−10.03	2.256	2.369
1,1,1,1,2,2	−16.45	−3.896	−3.533	−19.27	−6.162	−5.737
1,1,1,1,0.5,0.5	−4.660	5.675	5.839	−6.867	5.076	5.341
1,1,1,2,2,2	−19.98	−6.394	−6.100	−22.80	−8.890	−8.542
1,1,1,1,2,3	−17.99	−5.519	−4.649	−20.80	−7.913	−6.952
1,1,1,1,2,0.5	−9.951	1.101	1.541	−12.51	−0.445	0.117
1,1,1,2,2,0.5	−12.79	−1.101	−0.574	−15.39	−2.977	−2.315
1,1,1,2,2,3	−21.82	−7.998	−7.368	−24.61	−10.59	−9.890
1,1,2,2,3,3	−28.46	−12.41	−11.93	−31.16	−15.19	−14.67
1,1,2,2,0.5,0.5	−9.363	1.359	2.172	−11.72	−0.092	0.949
1,1,1,1,1,∞	−18.16	−∞	−5.244	−20.88	−∞	−7.559
1,1,1,1,2,∞	−22.93	−∞	−8.353	−25.63	−∞	−10.88
1,1,1,2,2,∞	−28.13	−∞	−11.81	−30.79	−∞	−14.50

resolution of the two-body Schrödinger equation inside the optimization process which makes the numerical calculation of the optimized lower bound more complicated.

A variational calculation allows us to determine an upper bound for the ground state energy of an N-body system, which when combined with the optimized lower bound determine a frame for the ground state energy lying between. The following figure, Fig. 1, shows the variation of lower bounds: the naïve bound, $E_{\text{naïve}}$, the improved bound, E_{improved}, and the optimized bound E_{olb} as functions of the particle mass. We have considered a 5-body system with Coulombian interactions $V^{(ij)} = -1/r_{ij}$, where we have fixed the masses of all particles with the exception of one mass, m_5, which we leave variable. We have also plotted in the same figure an upper bound, $E_{\text{variational}}$, obtained, by a variational calculation using a trial wave function of Gaussian form

$$\Psi(\boldsymbol{\rho_1},\boldsymbol{\rho_2},\boldsymbol{\rho_3},\boldsymbol{\rho_4}) = B\exp\left(-\sum_{i=j=1}^{4} A_{ij}\boldsymbol{\rho_i}\boldsymbol{\rho_j}\right), \tag{6.1}$$

where $\boldsymbol{\rho_1}$, $\boldsymbol{\rho_2}$, $\boldsymbol{\rho_3}$ and $\boldsymbol{\rho_4}$ are Jacobi coordinates, B is a normalized constant and A_{ij} are variational parameters determined by minimizing the expectation value of the Hamiltonian for the trial wave function.

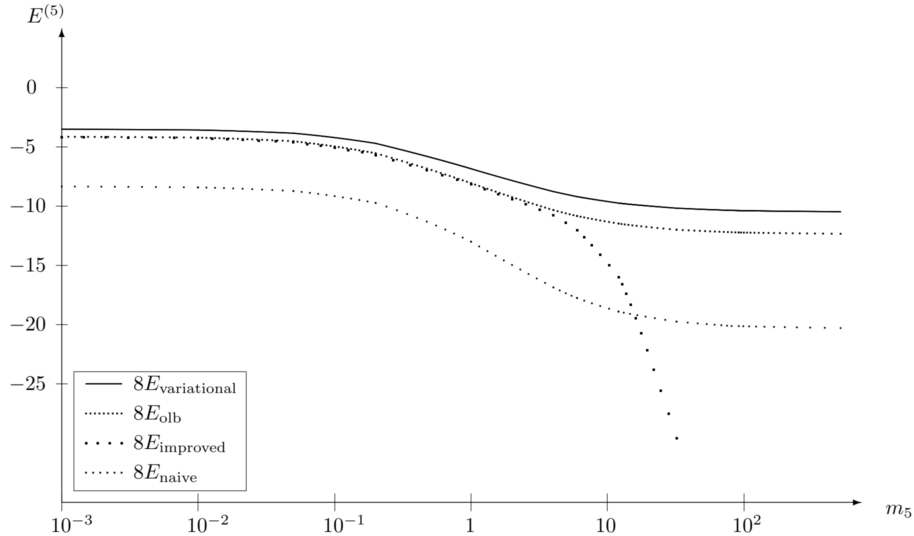

Fig. 1. Lower and upper bounds for 5-body system with Coulombian interactions $V^{(ij)} = -1/r_{ij}$: $m_1 = m_2 = 1$, $m_3 = m_4 = 2$ and m_5 variable.

7. Conclusion

An optimized lower bound derived initially for the ground state energies of three-body [1] and four-body [2] Hamiltonians, has been generalized recently for the ground state energy of an N-body Hamiltonian with arbitrary N [4], with particular emphasis on the five-body case [3]. The procedure applies under the two conditions of non-relativistic kinematics and translationally invariant two-body forces. In this paper, we have compared this optimized lower bound with other lower bounds, namely the so-called naïve [6–11] and improved lower bounds [14–16]. We have considered various mass configurations, various forms of the interaction potential and different values of N, the number of bodies. In the case of harmonic interactions, the optimized lower bound becomes saturated, *i.e.*, equal to the ground state energy, for all mass configurations and all values of N we have considered. This is not the case for the naïve lower bound which is never saturated. For the improved lower bound the saturation occurs only for equal mass configurations. In the case of other forms of interactions, the optimized lower bound is always better, *i.e.*, gives greater values, than both the naïve and improved lower bounds. Thus the optimized lower bound is always better than the two other bounds naïve and improved (there is, however, the situation in the equal mass case where the optimized and improved lower bounds give identical values) for all mass configurations, all forms of the potential and all values of N we have considered. Our investigations are sufficiently intensive to allow us to make a conclusion: the optimized lower bound is better than both the naïve and the improved lower bounds.

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