OPTIMIZED LOWER BOUND ON FOUR-BODY HAMILTONIANS

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Abstract

Generalizing a method elaborated for three-body systems, we derive a new lower bound on four-body ground-state energies in terms of two-body binding energies in the unequal-mass case. For simple power-law potentials, this bound is compared to variational calculations, and is shown to be very close to the exact result. In particular, it gives the exact answer for harmonic interactions.

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I. INTRODUCTION

The question of obtaining lower bounds on the ground state energy of many-particle systems is of great importance [1]. In recent years, we have proposed [2] a method which provides lower bounds on three-body energies in terms of two-body energies with a dramatic improvement, in comparison to what has been done previously [1,3]. An important aspect is that they become exact in the case of harmonic forces, and therefore are in some sense optimal. Moreover, these bounds are often so accurate that they can be used as reliable estimates of the three-body ground-state energy.

In this paper, this method is generalized to the case of four and more particles of unequal masses, a problem which remained open up to now. We obtain a lower bound expressed as a sum of two-body binding energies. The bound is again optimal in the sense it gives the exact result for harmonic forces.

The paper is organized as follows. In Sec. II, we present the method. Sec. III is devoted to numerical results. In Sec. IV we sketch the strategy to extend the method for systems made of an arbitrary number of particles.

II. THE METHOD

Consider a system of N non-relativistic particles interacting pairwise via a potential $\sum v_{ij}(\mathbf{r}_{ij})$, where the two-body interaction v_{ij} may depend on the pair $\{i,j\}$. We shall hereafter denote by $|\Omega\rangle$ the ground-state of the system and E_0 the corresponding energy. Before presenting the method, we shall recall what is meant by "naïve" and "improved" lower bounds, since they will be compared to our optimized lower bound.

A. Naïve bounds

We start from the following decomposition of the kinetic energy

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

Then the Hamiltonian $H^{(N)}$ of the system is recast in the form of a sum of non-commuting two-body Hamiltonians $H_{ij}^{(2)}$

$$H^{(N)} = \sum_{i < j=1}^N H_{ij}^{(2)}, \quad (2.2)$$

where

$$H_{ij}^{(2)} = \frac{1}{N-1} \left\{ \frac{\mathbf{p}_i^2}{2m_i} + \frac{\mathbf{p}_j^2}{2m_j} \right\} + v_{ij}(\mathbf{r}_{ij}). \quad (2.3)$$

Taking the expectation value of both sides of Eq. (2.2) in $|\Omega\rangle$ yields to the so-called "naïve" lower bound

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$$E_0 \geq \sum_{i < j=1}^N E^{(2)}[\alpha_{ij}]. \quad (2.4)$$

To obtain Eq. (2.4), we make use of the variational principle. $E^{(2)}[\alpha]$ denotes the ground-state energy of the two-body Hamiltonian $\alpha \mathbf{p}^2 + v(\mathbf{r})$, and the inverse reduced masses are given by

$$\alpha_{ij} = \frac{m_i + m_j}{2(N-1)m_i m_j}. \quad (2.5)$$

B. Improved lower bounds

The above bound [1,3] is not very accurate. The energy of each $\{i,j\}$ pair is replaced by the ground energy of $H_{ij}^{(2)}$ without accounting for the overall motion of this pair within the N -body system. An improvement [4] consists of separating the center-of-mass kinetic energy from the relative kinetic energy using the identity

$$\sum_{i=1}^N \frac{\mathbf{P}_i^2}{2m_i} = \frac{\mathbf{P}^2}{2M} + \sum_{i < j=1}^N \frac{(m_j \mathbf{P}_i - m_i \mathbf{P}_j)^2}{2m_i m_j M}, \quad (2.6)$$

where M is the total mass and $\mathbf{P}$ the total momentum

$$M = \sum_{i=1}^N m_i, \quad \mathbf{P} = \sum_{i=1}^N \mathbf{P}_i. \quad (2.7)$$

This leads to a decomposition

$$H^{(N)} = \frac{\mathbf{P}^2}{2M} + \sum_{i < j} \tilde{H}_2(\tilde{\alpha}_{ij}) \quad (2.8)$$

of the Hamiltonian in terms of reduced (translation invariant) two-body Hamiltonians

$$\tilde{H}_2(\alpha) = \alpha \mathbf{p}^2 + v_{ij}(\mathbf{r}), \quad (2.9)$$

with inverse reduced mass

$$\tilde{\alpha}_{ij} = \frac{(m_i + m_j)^2}{2m_i m_j M}. \quad (2.10)$$

Taking the expectation value within $|\Omega\rangle$ and applying the variational principle leads to the “improved bound”

$$E_0 \geq \sum_{i < j=1}^N E^{(2)}[\tilde{\alpha}_{ij}], \quad (2.11)$$

where $E^{(2)}[\alpha]$ is the ground state of $\tilde{H}_2(\alpha)$. In the equal-mass case, we remark that

$$\tilde{\alpha}_{ij} = \frac{2}{Nm} > \alpha_{ij} = \frac{1}{(N-1)m}, \quad (2.12)$$

and thus

$$\sum_{i < j=1}^N E^{(2)}[\tilde{\alpha}_{ij}] > \sum_{i < j=1}^N E^{(2)}[\alpha_{ij}], \quad (2.13)$$

which means that the improved lower bound is more accurate than the naive one. However, we have pointed out [2] that for unequal masses the “improved” bound is sometimes smaller, i.e., less efficient than the “naive” one.

C. Optimized lower bounds for three particles

Let us briefly review the method used to derive an optimized bound for $N = 3$ particles [2]. As compared to Ref. [2], we use slightly different notations, which are more easily generalized for $N > 3$.

The basic idea is that the ground-state $\Omega(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)$ is a function of the relative coordinates only. Therefore

$$\mathbf{B} \cdot \mathbf{P} |\Omega\rangle = 0, \quad (2.14)$$

if $\mathbf{P}$ is the total-momentum operator and $\mathbf{B}$ any vector. This suggests writing the kinetic energy as

$$\sum_{i=1}^3 \frac{\mathbf{P}_i^2}{2m_i} = \left(\sum_{i=1}^3 b_i \mathbf{P}_i \right) \cdot \mathbf{P} + a_{12} (\mathbf{P}_1 - \mathbf{P}_2 + x_{12} \mathbf{P}_3)^2 / 4 + \dots \quad (2.15)$$

The identification gives 6 relations which enable us to eliminate the coefficients b_i and express the inverse reduced masses a_{ij} in terms of parameters $\{x_{12}, x_{23}, x_{31}\}$. The Hamiltonian is thus decomposed as

$$H^{(3)} = \left(\sum_{i=1}^3 b_i \mathbf{P}_i \right) \cdot \mathbf{P} + \sum_{\{i,j\}} \tilde{H}_{ij}^{(2)}(\alpha_{ij}), \quad (2.16)$$

where the second sum extends to pairs $\{1,2\}$, $\{2,3\}$ and $\{3,1\}$. As $(\mathbf{P}_1 - \mathbf{P}_2 + x_{12} \mathbf{P}_3)/2$ has canonical commutation relations with $\mathbf{r}_1 - \mathbf{r}_2$, a_{12} is the reduced mass appropriate to $H_{12}^{(2)}$. Taking the expectation value within $|\Omega\rangle$ and applying the variational principle gives

$$E_0 \geq \sup_{\{x_{kl}\}} \sum_{\{i,j\}} E_{ij}^{(2)}[a_{ij}(\{x_{kl}\})]. \quad (2.17)$$

The maximum in Eq. (2.17) happens when all partial derivatives with respect to the x_{ij} are equal to zero, that is to say,

$$\sum_{\{i,j\}} \frac{\partial E_{ij}^{(2)}}{\partial a_{ij}} \cdot \frac{\partial a_{ij}}{\partial x_{kl}} = 0. \quad (2.18)$$

Hence the determinant of the Jacobian matrix $[\partial a_{ij}/\partial x_{kl}]$ must vanish. As shown in [2], this gives the rather simple relation

$$y_1 y_2 y_3 = 1, \quad (2.19)$$

where $y_3 = (1 + x_{12}) / (1 - x_{12})$, etc.

The optimization requires varying at most two parameters. If $m_1 = m_2$, then $x_{12} = 0$, and we have a single parameter to adjust. In the equal-mass case $m_1 = m_2 = m_3$, we have $x_{12} = x_{23} = x_{31} = 0$, and the optimized bound coincides with the improved bound of Eq. (2.11).

We have shown [2] the remarkable fact that the optimized bound Eq. (2.17) is saturated in the case of harmonic interaction $v_{ij}(r) \propto r^2$, whatever the masses or strength factors, equal or unequal.

Physically, this procedure is similar to Eq. (2.11) except that the kinetic energy is now distributed among the $N(N-1)/2 = 3$ pairs in an optimal way.

D. Optimized lower bounds for four particles

In Ref. [2], the decomposition of the 3-body kinetic-energy operator was written as

$$\sum_{i=1}^3 \frac{\mathbf{P}_i^2}{2m_i} = \left(\sum_{i=1}^3 b_i \mathbf{P}_i \right) \cdot \mathbf{P} + a_{12} \left(\frac{\mathbf{P}_1 - y_3 \mathbf{P}_2}{1 + y_3} \right)^2 + \dots \quad (2.20)$$

which is completely equivalent to our Eq. (2.15). This above writing suggests a naive generalization to $N = 4$ particles

$$\sum_{i=1}^4 \frac{\mathbf{P}_i^2}{2m_i} = \left(\sum_{i=1}^4 b_i \mathbf{P}_i \right) \cdot \mathbf{P} + \sum_{i < j}^4 a_{ij} \left(\frac{\mathbf{P}_i - y_{ij} \mathbf{P}_j}{1 + y_{ij}} \right)^2, \quad (2.21)$$

which involves only genuine two-body operators $\mathbf{P}_i - y_{ij} \mathbf{P}_j$. This gives a reasonable decomposition of the four-body Hamiltonian $H^{(4)}$ and hence a lower bound, which can be optimized by varying the y_{ij} coefficients. Results obtained that way are good, but not fully satisfactory. In particular, saturation is *not* obtained for *harmonic forces*, except for particular configurations of masses. One should then elaborate a more general decomposition of the kinetic energy. Indeed there are $N(N-1)/2 = 6$ potential terms whereas there are only $N = 4$ momenta. Our method will consist in distributing the kinetic energy over the $N(N-1)/2 = 6$ subsystems in an optimal way. One first writes

$$\sum_{i=1}^4 \frac{\mathbf{P}_i^2}{2m_i} = \left(\sum_{i=1}^4 b_i \mathbf{P}_i \right) \cdot \mathbf{P} + \sum_{i < j}^4 \frac{a_{ij}}{4} \left(\sum_{k=1}^4 x_{ij,k} \mathbf{P}_k \right)^2. \quad (2.22)$$

If one identifies both sides of this equation and eliminates the b_i coefficients, one can express the inverse masses a_{ij} in terms of the $x_{ij,k}$ coefficients by solving

$$N \begin{bmatrix} a_{12} \\ \vdots \\ a_{34} \end{bmatrix} = \begin{pmatrix} 2/m_1 + 2/m_2 \\ \vdots \\ 2/m_3 + 2/m_4 \end{pmatrix}, \quad (2.23)$$

where $N_{kl,ij} = (x_{ij,k} - x_{ij,l})^2$. One can add an arbitrary vector proportional to $\mathbf{P}$ to each combination $\sum x_{ij,k} \mathbf{P}_k$, and transfer the overall normalization to a rescaling of a_{ij} , so one can choose

$$x_{ij,i} = +1, \quad x_{ij,j} = -1, \quad (2.24)$$

without loss of generality. Hence $(\sum x_{ij,k} \mathbf{P}_k) / 2$ is conjugate to $(\mathbf{r}_i - \mathbf{r}_j)$. We are then left with 12 parameters.

The identity (2.22) leads to a decomposition of the Hamiltonian

$$H^{(4)} = (\mathbf{B} \cdot \mathbf{P}) + \sum_{i < j} \left[\frac{a_{ij}}{4} \left(\sum_{k=1}^4 x_{ij,k} \mathbf{P}_k \right)^2 + v_{ij}(\mathbf{r}_{ij}) \right], \quad (2.25)$$

where $\mathbf{B} = \sum_i b_i \mathbf{P}_i$, and an inequality

$$E_0 \geq \sup_{\{x_{mn,k}\}} \sum_{i < j} E_{ij}^{(2)} [a_{ij} (x_{12,3}, \dots, x_{34,2})]. \quad (2.26)$$

The optimization requires the vanishing of the derivatives

$$\sum_{i < j} E_{ij}^{(2)} \frac{\partial a_{ij}}{\partial x_{mn,k}} = 0, \quad (2.27)$$

for $m < n$, $k \neq m$ and $k \neq n$. Here $E_{ij}^{(2)}$ denotes the derivatives of $E_{ij}^{(2)}$ with respect to its single variable a_{ij} . As these derivatives do not vanish (they are actually positive), the matrix $[\partial a_{ij}/\partial x_{mn,k}]$ should be of rank at most 5. This gives seven conditions and allows us to express seven parameters in terms of the five others. The corresponding expressions are given in Appendix A. So in the most general case (unequal masses and/or different potentials), the best bound is obtained by varying only five independent parameters.

In some special cases, for example for equal masses $m_1 = m_2$ and $m_3 = m_4$, the cumbersome relations between the parameters become simpler. In particular, the number of independent parameters is reduced. More details are provided in Appendix A.

Implicit in Eq. (2.26) is the existence of a ground-state energy $E_{ij}^{(2)}$. If the potential v_{ij} does not bind, one can set $E_{ij}^{(2)} = 0$, but the bound will not be expected to be very accurate. In particular, the bound for a repulsive v_{12} potential would be the same as for the companion problem with $v_{12} = 0$.

III. NUMERICAL RESULTS

We have considered the case of power-law potentials

$$v_{ij}(r) = \text{sgn}(\beta) r^\beta, \quad (3.1)$$

taken for simplicity to be the same for all pairs. Here sgn is the sign function. This choice of potentials is motivated by their simple scaling properties, for instance for the energy

$$E^{(2)}[\alpha] = (2\alpha)^{3/(2+\beta)} E^{(2)}[1/2]. \quad (3.2)$$

Then Eq. (2.26) reduces to

$$\frac{E_0}{E^{(2)}[1/2]} \geq \sup_{\{x_{ij}\}} R(\{x_{ij}\}, \beta) \quad \text{if } \beta > 0, \quad (3.3)$$

or

$$\frac{E_0}{E^{(2)}[1/2]} \leq \inf_{\{x_{ij}\}} R(\{x_{ij}\}, \beta) \quad \text{if } \beta < 0, \quad (3.4)$$

where

$$R(\{x_{ij}\}, \beta) = \sum_{i < j=1}^4 (2a_{ij} \{x_{ij}\})^{\beta/(3+\beta)}. \quad (3.5)$$

We have considered various powers $\beta = -1, 0, 1, 1$ and 2 , corresponding to Coulomb, Martin [5], linear and quadratic potentials, respectively. The results are displayed in Tables I to IV for the case where $m_1 = m_2 = m_3 = 1$ and m_4 is variable, and in Tables V to VIII for $m_1 = m_2 = 1$ and $m_3 = m_4$ variable. The last Tables (IX to XII) correspond to $m_1 = m_2 = 1$, $m_3 = 2$ fixed and m_4 variable. Also shown in these Tables are the values obtained from the naive and improved lower bounds and those from a variational calculation based on an expansion on correlated Gaussian functions, namely

$$\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \sum_{k=1}^G k_k \left\{ \exp \left[-\frac{1}{2} (a_{11}^k \mathbf{x}_1^2 + 2a_{12}^k \mathbf{x}_1 \cdot \mathbf{x}_2 + \dots + a_{33}^k \mathbf{x}_3^2) \right] + \dots \right\}. \quad (3.6)$$

In each of the G generations, the dots at the end mean at most five terms deduced by permutation to make it properly symmetrized. The $\mathbf{x}_i$ are Jacobi relative coordinates. The parameters are optimized numerically. For further details, the reader is referred to the abundant literature on the subject [6]. The results presented in the Tables correspond to $G = 7$ generations of Gaussians. A good convergence is already achieved, except for $\beta = -1$.

In all cases, the optimized lower bound is better than the naive and improved ones. Sometimes the naive bound becomes better than the improved one, when m_4 is greater than a critical value which is an increasing function of β . In most cases, the optimized lower bounds are not very far from the variational results. This means we have a reasonable approximation to the ground state energy.

The harmonic-oscillator case deserves a special attention. The optimized inequality $E_N \geq \sum E^{(2)}[\alpha_{ij}]$ becomes saturated whatever masses and strength coefficients are adopted in the Hamiltonian.

The comparison of the various lower bounds and variational upper bound is illustrated in Figs. 1 to 3, for selected cases. We have somewhat restricted the range of variation of the mass ratio m_4 to try to get distinguishable curves. We have clearly a very good approximation of the ground-state energy.

For the $(1, 1, 1, m_4)$ and $(1, 1, 2, m_4)$ mass configurations studied in Tables I to IV and IX to XII, respectively, the limit $m_4 \rightarrow \infty$ corresponds to three light particles in a static field. For the $(1, 1, m_4, m_4)$ configuration of Tables V to VIII, the limit $m_4 \rightarrow \infty$ is that of a 2-body bound state (m_4, m_4) (with infinite energy in the case $\beta = -1$ of a Coulomb potential) entering as a point-like constituent of a 3-body bound state $(1, 1, \infty)$.

In the limit $m_4 \rightarrow 0$, any particle of mass m_4 goes to infinite distances, with a vanishing ($\beta = -1$) or infinite ($\beta > 0$) energy. It can be checked that once this energy is subtracted out, the remainder is just the naive, improved or optimized lower bound for the particles with finite mass.

IV. CONCLUSION

We have derived a lower bound on the energy of four-body systems in terms of two-body binding energies. We have investigated numerically some representative power-law potentials, in cases involving up to three different values for the masses.

When compared to the previously obtained naive and improved lower bounds, the optimized lower bound proves to be better in all cases. This optimized lower bound when combined with variational calculations, gives an interval in which lies the energy of the four-body system. In all examples that have been studied, the optimized lower bounds are not very far from the variational estimates, and then can be used as approximate estimates to the ground state energies of the four-body systems. There are, however, other cases where the present lower bound may be inaccurate, an example being the repulsive potential already mentioned in Sec. II D. The optimized lower bound becomes exact for the harmonic oscillator. A direct analytic proof of saturation is unfortunately not available.

It is obvious that similar optimized lower bounds can also be obtained in the case of five or more particles, using the same techniques as in the three and four-body cases. For N particles, we have $N' = N(N-1)/2$ pairs, thus the Hamiltonian is decomposed in N' terms, with $n = N'(N-2)$ coefficients generalizing our $x_{ij,k}$. The Jacobian conditions will, however, reduce them to at most $n' = N' - 1$ independent terms ($n' = 9$ for the 5-body problem, for instance).

In summary, we get a lower bound to the few-body ground-state energy by a simple optimization of a sum of simple two-body energies. This lower bound turns out to be a good approximation when all pair potentials are attractive.

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APPENDIX A

Here some details are provided on the weight coefficients $x_{ij,k}$ and inverse reduced masses a_{ij} entering the optimized bound derived in Sec. IID.

For later convenience we note $x_{12,3} = a$, $x_{12,4} = b$, $x_{13,1} = c$, $\dots$, $x_{34,1} = k$ and $x_{34,2} = l$. Similarly, we simplify $a_{12} = a_1$, $\dots$, $a_{34} = a_6$.

Now to clarify more our parametrization we write the kinetic energy in the most general case of four unequal masses and/or six different potential functions $v_{ij}(r)$:

$$\sum_{i=1}^4 \frac{\mathbf{P}_i^2}{2m_i} = \left(\sum_{i=1}^4 b_i \mathbf{P}_i \right) \cdot \mathbf{P} + a_1 (\mathbf{P}_1 - \mathbf{P}_2 + a \mathbf{P}_3 + b \mathbf{P}_4)^2 / 4 + a_2 (\mathbf{P}_1 - \mathbf{P}_3 + c \mathbf{P}_2 + d \mathbf{P}_4)^2 / 4 + a_3 (\mathbf{P}_1 - \mathbf{P}_4 + e \mathbf{P}_2 + f \mathbf{P}_3)^2 / 4 + a_4 (\mathbf{P}_2 - \mathbf{P}_3 + g \mathbf{P}_1 + h \mathbf{P}_4)^2 / 4 + a_5 (\mathbf{P}_2 - \mathbf{P}_4 + i \mathbf{P}_1 + j \mathbf{P}_3)^2 / 4 + a_6 (\mathbf{P}_3 - \mathbf{P}_4 + k \mathbf{P}_1 + l \mathbf{P}_2)^2 / 4. \quad (\text{A1})$$

To find the inverse masses a_k in terms of the coefficients a , b , $\dots$, l , we follow the procedure discussed above. Let us define

$$\alpha_1 = 2/m_1 + 2/m_2, \dots, \alpha_6 = 2/m_3 + 2/m_4. \quad (\text{A2})$$

By identifying the terms in $\mathbf{P}_i^2$ and $\mathbf{P}_i \cdot \mathbf{P}_j$ in both sides of Eq. (A1) and eliminating the coefficients b_i , we obtain the matrix equation (2.23), $N\mathbf{a} = \boldsymbol{\alpha}$, where N is the matrix

$$N = \begin{bmatrix} 4 & (c-1)^2 & (e-1)^2 & (g-1)^2 & (i-1)^2 & (k-1)^2 \\ (a-1)^2 & 4 & (f-1)^2 & (g+1)^2 & (i-j)^2 & (k-1)^2 \\ (b-1)^2 & (d-1)^2 & 4 & (g-h)^2 & (i+1)^2 & (k+1)^2 \\ (a+1)^2 & (c+1)^2 & (e-f)^2 & 4 & (j-1)^2 & (l-1)^2 \\ (b+1)^2 & (c-d)^2 & (e+1)^2 & (h-1)^2 & 4 & (l+1)^2 \\ (a-b)^2 & (d+1)^2 & (f+1)^2 & (h+1)^2 & (j+1)^2 & 4 \end{bmatrix}. \quad (\text{A3})$$

By inverting the matrix N we obtain the inverse masses a_i in terms of a , b , $\dots$, l . At this stage we are left with 12 parameters which are however not independent.

The optimization of the bound $\sum E_{ij}^{(2)}[a_{ij}\{x_{mn,k}\}]$ implies that the 6×12 Jacobian matrix $\partial a_{ij}/\partial x_{mn,k}$ is of rank at most 5.

From $N\mathbf{a} = \boldsymbol{\alpha}$, we get, for instance, $\partial \mathbf{a}/\partial a = -N^{-1}(\partial N/\partial a)\mathbf{a}$, where $\partial N/\partial a$ has non-zero elements in the first column only. Similarly, each $\partial N/\partial x_{ij,k}$ has a single non-vanishing column. This gives

$$\left[\frac{\partial a_{ij}}{\partial x_{mn,k}} \right] = -2N^{-1}M', \quad (\text{A4})$$

The first and second column of the 6×12 matrix M' contains an overall factor a_1 , the third and fourth, a_2 , etc., that is to say, $M'_{ij} = M_{ij}a_k$ for $j = 2k-1$ and $j = 2k$. Each 6×6 determinant of M' contains unessential a_k^6 factors, with $a_k > 0$. Thus, it is equivalent to impose a rank at most 5 to

$$M = \begin{bmatrix} 0 & 0 & c-1 & 0 & e-1 & 0 & g-1 & 0 & i-1 & 0 & k-l & l-k \\ a-1 & 0 & 0 & 0 & 0 & f-1 & g+1 & 0 & i-j & j-i & k-1 & 0 \\ 0 & b-1 & 0 & d-1 & 0 & 0 & g-h & h-g & i+1 & 0 & k+1 & 0 \\ a+1 & 0 & c+1 & 0 & e-f & f-e & 0 & 0 & j-1 & 0 & l-1 & 0 \\ 0 & b+1 & c-d & d-c & e+1 & 0 & 0 & h-1 & 0 & 0 & l+1 & 0 \\ a-b & b-a & 0 & d+1 & 0 & f+1 & 0 & h+1 & 0 & j+1 & 0 & 0 \end{bmatrix} \quad (\text{A5})$$

The columns such as (1,2) or (3,4), etc., are clearly associated, for they involve the same parameters. The 6×6 determinants including only such pairs have relatively simple expressions. For instance, taking the first six columns gives

$$\Delta_{123456} = (a-b-c+bc+d-ad+e-ae-de+ade-f+bf+cf-bcf) \quad (\text{A6}) \\ (-4-a-b-c+2ac-bc-d-ad-e-ae+2bc-de+ade-f-bf-cf+bcf+2df),$$

whose vanishing leads to two possible values for f in terms of $a, \dots, e$. Only one of those is consistent with the vanishing of the other 6×6 determinants and gives the correct limiting behavior $f=0$ for equal masses and identical potentials.

Similarly, the simultaneous vanishing of Δ_{123478} and Δ_{345678} provides a system of equations to express g and h in terms of $a, b, \dots, e$ and f . There are four sets of solution, but only one of those is acceptable.

One can proceed similarly for i and j , and for k and l . The result is

$$f = \frac{a-b-c+d+e+bc-ad-e-ae-de+ade}{1-b-c+bc}, \quad (\text{A7}) \\ g = \frac{c-a}{1-ac}, \\ h = \frac{d-b+bc-ad}{1-ac}, \\ i = \frac{e-b}{1-be}, \\ j = \frac{d+e-b-c+ac+bc-ad-de-ace+ade}{1-c-be+ace}, \\ k = \frac{a-b-c+d+bc-ad-de+ade}{1-b-c+e+bc-ac}, \\ l = \frac{e-c-be+ac+bc-ace}{1-b-c+d+bc-ad-de+ade},$$

where the last parameters are expressed in terms of the first ones. There are, of course, many other relations deduced by permutations, for instance $i = (e-b)/(1-be)$.

Let us now see how these relations simplify when $v_{ij}(r_{ij}) = v(r_{ij})$ and some masses are equal.

1. Four equal masses (m, m, m, m)

$a = b = \dots = l = 0$, there is no parameter to be adjusted.

2. Three equal masses (m, m, m, M)
 $a = b = c = d = 0$, and $e \neq 0$, one checks that $f = e$, $g = h = 0$, $i = j = k = l = e$.
 We have one parameter to adjust.
3. Two sets of equal masses (m, m, M, M)
 $a = b = 0$, $e = c$, $f = h = j = d$, $g = i = c$, and $k = l = 0$. Two parameters are
 needed.
4. Two equal masses (m, m, m_3, m_4)
 $a = b = 0$, and one checks that $f = (c - d - e + ed) / (c - 1)$, $g = c$, $h = d$, $i = e$,
 $j = f$, and $k = l = (e - c) / (1 - c + d - ed)$. Then c , d , and e can be chosen as free
 parameters.

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TABLES

TABLE I. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the Coulomb potential with $m_1=m_2=m_3=1$ and m_4 variable

variable	m_4	naive	improved	optimized	variational
0.01	0.01	4.58910	2.34603	2.34565	2.21657
0.1	0.1	5.31818	3.09359	3.08334	2.91603
0.5	0.5	7.50000	4.95833	4.95235	4.57714
1.0	1.0	9.00000	6.00000	6.00000	5.57524
3.0	3.0	11.2500	7.87500	7.46333	6.91106
10.0	10.0	12.6818	12.9731	8.41754	7.81651
100.0	100.0	13.4109	80.2791	8.93460	8.30862
500.0	500.0	13.4820	380.256	8.98677	8.35828
∞	∞	13.5000	∞	9.00000	8.38517

TABLE II. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the Martin potential with $m_1=m_2=m_3=1$ and m_4 variable

variable	m_4	naive	improved	optimized	variational
0.01	0.01	6.48950	6.58887	6.58933	6.59210
0.1	0.1	6.13411	6.23762	6.24093	6.24492
0.5	0.5	5.94263	6.05525	6.05692	6.06184
1.0	1.0	5.88526	6.00000	6.00000	6.00483
3.0	3.0	5.82899	5.92585	5.93960	5.94442
10.0	10.0	5.80267	5.82603	5.90764	5.91232
100.0	100.0	5.79107	5.56867	5.89208	5.89668
500.0	500.0	5.79000	5.38283	5.89057	5.89517
∞	∞	5.78972	3.00000	5.89019	5.89474

TABLE III. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the linear potential with $m_1=m_2=m_3=1$ and m_4 variable

variable	m_4	naive	improved	optimized	variational
0.01	0.01	12.3077	13.0067	13.0871	13.0947
0.1	0.1	7.24681	7.98952	8.07072	8.07920
0.5	0.5	5.62074	6.39869	6.41725	6.42522
1.0	1.0	5.24148	6.00000	6.00000	6.00745
3.0	3.0	4.91017	5.50524	5.59668	5.60362
10.0	10.0	4.76797	4.95443	5.39804	5.40464
100.0	100.0	4.70774	4.00628	5.30476	5.31117
500.0	500.0	4.70221	3.59682	5.29582	5.30222
∞	∞	4.70081	3.00000	5.29357	5.30000

TABLE IV. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the quadratic potential with $m_1=m_2=m_3=1$ and m_4 variable

variable	m_4	naive	improved	optimized	variational
0.01	0.01	19.8564	20.9230	21.3493	21.3493
0.1	0.1	8.19405	9.33475	9.56776	9.56776
0.5	0.5	5.44949	6.60882	6.64575	6.64575
1.0	1.0	4.89898	6.00000	6.00000	6.00000
3.0	3.0	4.44949	5.27792	5.41421	5.41421
10.0	10.0	4.26608	4.55839	5.14018	5.14018
100.0	100.0	4.19018	3.57675	5.01489	5.01489
500.0	500.0	4.18327	3.26455	5.00300	5.00300
∞	∞	4.18153	3.00000	5.00000	5.00000

TABLE V. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the Coulomb potential with $m_1=m_2=1$ and $m_3=m_4$ variable

variable	m_4	naive	improved	optimized	variational
0.001	0.001	1.51349	1.00899	0.51114	0.50984
0.002	0.002	1.52695	1.01797	0.52228	0.51970
0.005	0.005	1.56720	1.04480	0.55561	0.54920
0.010	0.010	1.63381	1.08921	0.61093	0.64806
0.050	0.050	2.14643	1.43095	1.03927	1.01006
0.100	0.100	2.74091	1.82727	1.52878	1.46160
0.200	0.200	3.80000	2.53333	2.35843	2.21950
0.500	0.500	6.25000	4.16667	4.12853	3.83733
0.800	0.800	8.03333	5.35556	5.35104	4.96187
1.000	1.000	9.00000	6.00000	6.00000	5.57473

TABLE VI. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the Martin potential with $m_1=m_2=1$ and $m_3=m_4$ variable

variable	m_4	naive	improved	optimized	variational
0.001	0.001	7.61877	7.44482	7.72590	7.72870
0.002	0.002	7.40346	7.27034	7.47280	7.51186
0.005	0.005	7.12993	7.04858	7.23396	7.23684
0.010	0.010	6.93144	6.88751	7.03478	7.03478
0.050	0.050	6.50051	6.53623	6.60552	6.60942
0.100	0.100	6.33072	6.39601	6.43830	6.44262
0.200	0.200	6.17412	6.26408	6.28527	6.28994
0.500	0.500	5.99467	6.10557	6.10954	6.11444
0.800	0.800	5.91781	6.03256	6.03297	6.03788
1.000	1.000	5.88526	6.00000	6.00000	6.00482

TABLE VII. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the linear potential with $m_1=m_2=1$ and $m_3 = m_4$

m_4 variable	naive	improved	optimized	variational
0.001	37.3531	34.1776	39.9431	39.9727
0.002	29.8347	27.7334	31.9981	32.0226
0.005	22.2285	21.1129	23.9683	23.9877
0.010	17.8444	17.2966	19.3461	19.3628
0.050	10.8966	11.2382	12.0362	12.0362
0.100	8.92374	9.50174	9.96094	9.97197
0.200	7.40707	8.14026	8.35793	8.36774
0.500	5.97422	6.78014	6.81782	6.82623
0.800	5.44886	6.23166	6.23533	6.24310
1.000	5.24148	6.00000	6.00000	6.00745

TABLE VIII. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the quadratic potential with $m_1=m_2=1$ and $m_3 = m_4$

m_4 variable	naive	improved	optimized	variational
0.001	99.7026	92.3145	109.989	109.989
0.002	70.7654	66.1345	78.3758	78.3758
0.005	45.1048	42.9211	50.3340	50.3340
0.010	32.1907	31.2397	36.2126	36.2126
0.050	15.0510	15.7218	17.4250	17.4250
0.100	11.0579	12.0776	13.0149	13.0149
0.200	8.29909	9.51019	9.93623	9.93623
0.500	5.9712	7.20838	7.27791	7.27791
0.800	5.19347	6.35083	6.35738	6.35738
1.000	4.89898	6.00000	6.00000	6.00000

TABLE IX. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the Coulomb potential with $m_1=m_2=1$, $m_3 = 2$ and m_4 variable

m_4 variable	naive	improved	optimized	variational
0.01	5.58925	2.88321	2.85662	2.68888
0.1	6.33117	3.71085	3.59270	3.41014
0.5	8.70000	5.84500	5.69402	5.28086
1.0	10.5000	7.08333	6.97834	6.45405
3.0	13.6000	9.16611	8.92845	8.28250
10.0	15.9545	13.9807	10.3526	9.64941
100.0	17.3229	76.2605	11.2044	10.4725
500.0	17.4641	354.008	11.2944	10.5596
∞	17.5000	∞	11.3174	10.5990

TABLE X. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the Martin potential with $m_1=m_2=1$, $m_3 = 2$ and m_4 variable

m_4 variable	naive	improved	optimized	variational
0.01	6.46253	6.54932	6.55845	6.56312
0.1	6.10506	6.19689	6.20922	6.21297
0.5	5.90730	6.01017	6.01882	6.02362
1.0	5.84523	5.95328	5.95782	5.96271
3.0	5.78101	5.88193	5.89040	5.89513
10.0	5.74886	5.79185	5.85249	5.85703
100.0	5.73398	5.54421	5.83300	5.83741
500.0	5.73257	5.35898	5.83104	5.83548
∞	5.73222	2.96753	5.83055	5.83492

TABLE XI. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the linear potential with $m_1=m_2=1$, $m_3 = 2$ and m_4 variable

m_4 variable	naive	improved	optimized	variational
0.01	12.1426	12.6528	12.8629	12.8716
0.1	7.06332	7.67565	7.82830	7.83622
0.5	5.40202	6.07722	6.14763	6.15519
1.0	5.00184	5.68142	5.71437	5.72149
3.0	4.63975	5.22382	5.28364	5.29014
10.0	4.47727	4.73493	5.06160	5.06771
100.0	4.40628	3.82066	4.95269	4.95858
500.0	4.39968	3.40544	4.94202	4.94787
∞	4.39802	2.79370	4.93932	4.94516

TABLE XII. The ratio $E^{(4)}/E^{(2)}[1/2]$ for the quadratic potential with $m_1=m_2=1$, $m_3 = 2$ and m_4 variable

m_4 variable	naive	improved	optimized	variational
0.01	19.6232	20.3024	20.9773	20.9773
0.1	7.93125	8.83791	9.18406	9.18406
0.5	5.14358	6.12132	6.24090	6.24090
1.0	4.57081	5.52933	5.58114	5.58114
3.0	4.09109	4.87676	4.96993	4.96993
10.0	3.88898	4.24489	4.67332	4.67332
100.0	3.80348	3.30016	4.53267	4.53267
500.0	3.79563	2.98121	4.51907	4.51907
∞	3.79365	2.70711	4.51564	4.51564

APPENDIX: List of Figures

- 1 Four-body system with constituent masses $(1, 1, 1, m)$. Comparison of the variational upper bound to the ground-state energy $E^{(4)}$ and the naive, improved and optimized lower bounds. The quantity displayed is the ratio of $E^{(4)}$ to the 2-body energy $E^{(2)}$ with unit masses. The binding potential is $v_{ij}(r) = \text{sgn}(\beta)r^\beta$, with $\beta = -1, 0.1, 1$ and 2 17
- 2 Same as Fig. 1 for masses $(1, 1, m, m)$ 18
- 3 Same as Fig. 1 for masses $(1, 1, 2, m)$ 19

FIGURES

FIG. 1. Four-body system with constituent masses $(1, 1, 1, m)$. Comparison of the variational upper bound to the ground-state energy $E^{(4)}$ and the naive, improved and optimized lower bounds. The quantity displayed is the ratio of $E^{(4)}$ to the 2-body energy $E^{(2)}$ with unit masses. The binding potential is $v_{ij}(r) = \text{sgn}(\beta)r^\beta$, with $\beta = -1, 0.1, 1$ and 2 .

FIG. 2. Same as Fig. 1 for masses (1, 1, m , m).

FIG. 3. Same as Fig. 1 for masses (1, 1, 2, m).