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A set of inequalities between the ground state energies of many-body systems

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The energy E_N of a system of N identical pairwise-interacting particles of mass M is shown to satisfy the inequalities

$$E_N(M) \geqslant \frac{N(N-1)}{n(n-1)} E_n\left(\frac{N}{n} M\right),$$

where $N > n \geqslant 2$. These inequalities generalize the Stenschke result $E_3(M) \geqslant 3E_2(3M/2)$. They hold for Bose or Fermi systems in any number of dimensions, and are shown to be the strongest possible of this type. Further extensions are made to the case where the potential is varied instead of the mass, or where both are varied together.

In this note we shall give various generalizations of the Stenschke [1] inequality

$$E_3(M) \geqslant 3E_2(3M/2), \tag{1}$$

which relates the ground state energy of three particles of mass M to that of two particles (with the same pairwise interaction) of mass $3M/2$. One generalization of (1) has already been given by Etters *et al.* [2] :

$$E_N(M) \geqslant \tfrac{1}{2}N(N-1)E_2(NM/2). \tag{2}$$

Inequalities of this type are a useful complement to the usual variational upper bound $E_N^{\text{var}} \geqslant E_N$, and have been applied to the question of the existence of bound states of small molecules of helium [1, 2]. However, when N gets large, (2) reduces to the trivial statement that an N-body system will not bind if the two-body system does not bind in the classical limit, i.e. that a necessary condition for binding is that the interaction potential must be negative at some point. Our first task therefore is to try to relate E_N to E_{N-1} rather than to E_2.

We consider systems of N identical particles with hamiltonian

$$H_N = -\frac{\hbar^2}{2M} \sum_{i \leqslant N} \nabla_i^2 + \sum_{1 \leqslant i < j \leqslant N} V_{ij}. \tag{3}$$

The interactions are assumed to be pairwise but may be non-central or spin-dependent : the only property we need is $V_{ij} = V_{ji}$. We work in the coordinate frame where the total momentum of the system is zero. There any power of

$(\Sigma\nabla_i)$ gives zero when operating on the exact wavefunction, and thus the centre-of-mass kinetic energy

$$-\frac{\hbar^2}{2NM}(\Sigma\nabla_i)^2 \tag{4}$$

may be subtracted from the hamiltonian. (One can obtain similar inequalities without working in the rest frame, but these are weaker, for example $E_3(M) \geqslant 3E_2(2M)$ in the three-body case). The resulting hamiltonian is

$$\begin{aligned}\tilde{H}_N &= -\frac{\hbar^2}{2M}\{\Sigma\nabla_i^2 - N^{-1}(\Sigma\nabla_i)^2\} + \sum_{i<j}\sum V_{ij} \\ &= -\frac{\hbar^2}{2M}\left\{\frac{N-1}{N}\Sigma\nabla_i^2 - \frac{2}{N}\sum_{i<j}\sum \nabla_i \cdot \nabla_j\right\} + \sum_{i<j}\sum V_{ij} \\ &= -\frac{\hbar^2}{2MN}\sum_{i<j}\sum\{\nabla_i^2 + \nabla_j^2 - 2\nabla_i \cdot \nabla_j\} + \sum_{i<j}\sum V_{ij} \\ &= -\frac{\hbar^2}{2MN}\sum_{i<j}\sum(\nabla_i - \nabla_j)^2 + \sum_{i<j}\sum V_{ij}.\end{aligned} \tag{5}$$

Instead of the spatial coordinates $\mathbf{r}_i$, $\mathbf{r}_j$ we can transform to

$$\left.\begin{aligned}\mathbf{r}_{ij} &= \mathbf{r}_i - \mathbf{r}_j, \\ \bar{\mathbf{r}}_{ij} &= \mathbf{r}_i + \mathbf{r}_j\end{aligned}\right\} \tag{6}$$

in terms of which

$$(\nabla_i - \nabla_j)^2 = 4\nabla_{ij}^2 \tag{7}$$

where $\bar{\mathbf{r}}_{ij}$ and all $\mathbf{r}_k$ with $k \neq i, j$ are kept constant in the differentiation.

Thus
$$\tilde{H}_N = \sum_{1 \leqslant i<j \leqslant N}\sum\left\{-\frac{2\hbar^2}{NM}\nabla_{ij}^2 + V_{ij}\right\}. \tag{8}$$

The hamiltonian is thus written as the sum over $\frac{1}{2}N(N-1)$ pair hamiltonians. Taking the expectation value of (8) with an exact wavefunction of the N-particle system, and using the fact that this wavefunction is symmetric or antisymmetric with respect to the interchange of any two sets of particle coordinates, we have

$$E_N(M) = \tfrac{1}{2}N(N-1)\left\langle -\frac{2\hbar^2}{NM}\nabla_{12}^2 + V_{12}\right\rangle. \tag{9}$$

The hamiltonian of the relative motion of two particles of mass M is

$$\tilde{H}_2 = -\frac{\hbar^2}{M}\nabla_{12}^2 + V_{12}$$

and the expectation value of $\tilde{H}_2$ taken with any wavefunction is $\geqslant E_2$ by the variational theorem. Thus we obtain (2).

To get a relation between E_N and E_{N-1} we need to re-arrange the right side of (8) into clusters of $N-1$ particles. There are N such clusters, of which $N-2$ contain a given pair (i, j). Thus

$$E_N(M) = \frac{N}{N-2} \left\langle \sum_{1 \leqslant i < j \leqslant N-1} \left\{ -\frac{2\hbar^2}{NM} \nabla_{ij}{}^2 + V_{ij} \right\} \right\rangle, \tag{10}$$

where again the expectation value is taken with an exact wavefunction of the N-body system. On comparison with (8) the variational principle yields

$$E_N(M) \geqslant \frac{N}{N-2} E_{N-1} \left(\frac{NM}{N-1} \right). \tag{11}$$

Iteration then gives the complete set of inequalities for $N > n \geqslant 2$:

$$E_N(M) \geqslant \frac{N(N-1)}{n(n-1)} E_n \left(\frac{N}{n} M \right). \tag{12}$$

We note that the proof holds for any number of dimensions and for any symmetric pair interaction.

Instead of comparing the energies of systems of different masses, one might be interested in the energies of systems with different interaction strength. Relations generalizing (12) may be obtained for pair interactions of the form

$$V_{ij} = vu(r_{ij}/a), \tag{13}$$

where v is a potential strength and a is a length characterizing the potential shape. A familiar example is the 6–12 potential

$$V(r) = v \left\{ \left(\frac{a}{r} \right)^{12} - 2 \left(\frac{a}{r} \right)^6 \right\}. \tag{14}$$

As in the two-body case [3], the N-body system is then completely characterized by the dimensionless coupling parameter

$$\alpha = Ma^2 v/\hbar^2. \tag{15}$$

The hamiltonian for relative motion becomes

$$\frac{Ma^2}{\hbar^2} \tilde{H}_N = \sum_{1 \leqslant i < j \leqslant N} \left\{ -\frac{2}{N} \nabla_{ij}{}^2 + \alpha u(X_{ij}) \right\} \tag{16}$$

where now the differentiation in the laplacian is to be carried out with respect to $\mathbf{X}_i = \mathbf{r}_i/a$. We write

$$\epsilon_N = Ma^2 E_N/\hbar^2. \tag{17}$$

Then taking the expectation value of (16) with an exact eigenstate of $\tilde{H}_N$ as before, we have

$$\epsilon_N(\alpha) = \frac{1}{N} \left\langle \sum_{1 \leqslant i < j \leqslant N} \{ -2\nabla_{ij}{}^2 + N\alpha u(X_{ij}) \} \right\rangle \geqslant \frac{N-1}{N-2} \epsilon_{N-1} \left(\frac{N\alpha}{N-1} \right). \tag{18}$$

The general expression in terms of the coupling parameter α is therefore

$$\epsilon_N(\alpha) \geqslant \frac{N-1}{n-1}\,\epsilon_n\left(\frac{N}{n}\,\alpha\right). \tag{19}$$

An interesting set of relations follows readily for the critical value $\alpha_0(N)$ of the coupling parameter, for which the N-body system is just bound (e.g. $\alpha_0(2)=7{\cdot}04$ for the 6–12 potential [3]). We note first that

$$\frac{\partial E_N}{\partial M} < 0 \tag{20}$$

because M^{-1} multiplies an operator with positive definite expectation value in the hamiltonian. Thus from (17) and (15)

$$\frac{\partial \epsilon_N}{\partial \alpha} < 0 \tag{21}$$

provided $\epsilon_N < 0$, i.e. the reduced bound state energy decreases monotonically with increasing α. Since $\epsilon_N = 0$ for $\alpha = \alpha_0(N)$, we therefore always have binding for $\alpha > \alpha_0$. From (19) we see that for the N-body system to bind we need

$$\frac{N}{n}\,\alpha(N) \geqslant \alpha_0(n)$$

so that, for all $n < N$,

$$N\alpha_0(N) \geqslant n\alpha_0(n). \tag{22}$$

We expect the critical coupling parameter to decrease with N because on adding the Nth particle one adds *one* kinetic energy term but *several* potential energy terms (roughly equal to the number of possible nearest neighbours). The above relation shows that α_0 cannot decrease with N faster than N^{-1}.

We turn finally to the question of whether the sets of inequalities derived above are as strong as they could be. The answer is *yes*: the inequalities cannot be strengthened further because there exists a system for which the equality holds, namely bosons interacting with harmonic forces. Consider N bosons in d dimensions, with pair interactions

$$V_{ij} = v\{1 + (r_{ij}/a)^2\}. \tag{23}$$

In terms of the reduced variables $\mathbf{X}_{ij} = \mathbf{r}_{ij}/a$, Schrödinger's equation reads

$$\left[-\tfrac{1}{2}\Sigma\nabla_i^2 + \alpha \sum_{i<j}\sum X_{ij}^2\right]\Psi = [\epsilon - \tfrac{1}{2}N(N-1)\alpha]\Psi. \tag{24}$$

We look for a solution of the form

$$\Psi = \exp\left[-\tfrac{1}{2}\beta \sum_{i<j}\sum X_{ij}^2\right]. \tag{25}$$

Direct differentiation and use of the identities

$$2\mathbf{X}_{ik}\,.\,\mathbf{X}_{jk} = X_{ik}^2 + X_{jk}^2 - X_{ij}^2$$

shows that (25) is a solution if $\beta=(2\alpha/N)^{1/2}$, and has the reduced energy

$$\epsilon_N(\alpha)=\tfrac{1}{2}N(N-1)\alpha+d(N-1)(N\alpha/2)^{1/2}. \tag{26}$$

Since Ψ has no nodes, it is the ground state wavefunction. The energy (26) is in agreement with the known result for N bosons in three dimensions [4, 5].

On substituting (26) in (19) we find that the latter is satisfied as an equality. The inequalities therefore cannot be improved upon without additional restrictions being made on the pair potential.

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