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BOUNDS ON RADII AND KINETIC ENERGIES OF N PARTICLE SYSTEMS

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ABSTRACT

Within non-relativistic quantum mechanics we derive simple bounds on the kinetic energy and the mean square radius of a system of N particles in the ground state. These bounds hold if no symmetry requirement is imposed on the wave-function.

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1. INTRODUCTION

In a previous paper¹⁾ we presented bounds on the kinetic energy and the mean square radius of a two-body system. For the ground state the results are

$$\langle T \rangle_0 \geq \frac{3}{4} (E_1 - E_0) \quad (1)$$

and

$$\langle r^2 \rangle_0 \leq \frac{3}{2\mu(E_1 - E_0)} \quad (2)$$

where E_0 is the ground state energy, E_1 the first $L = 1$ excitation, and μ the reduced mass of the system. These bounds which we derived from Thomas-Reiche-Kuhn (TRK) sum rules [for a different approach see Ref. 2)] are exact results valid for any potential, and they are optimal being saturated by the harmonic oscillator. For simple power potentials they are accurate estimates (the bounds deviate from the exact values by some per cent only); for singular potentials like the Coulomb potential the error is 25 per cent. Because of this high saturation we could estimate the kinetic energy of the $c\bar{c}$ system (J/ψ) rather accurately in a model independent way.

In this paper we are concerned with a generalization of (1) and (2) to N -body systems and derive the results within a non-relativistic Schrödinger theory. In N -body theory, however, we are faced with the problem of statistics, a question which does not arise in the two-body case. As we unfortunately did not succeed in involving statistics in our proof (the reason will become clear in the text), our final results hold for N particles which are not subjected to any symmetry requirement. We consider first N interacting particles moving in the field of a fixed centre, and remove afterwards that infinitely heavy centre, so that they only interact with each other.

2. N PARTICLES WITH A FIXED CENTRE

Given N particles with equal mass m interacting with each other and in addition with some infinitely heavy centre, the Hamiltonian will be

$$H = T + V \quad (3)$$

with

$$T = \sum_{i=1}^{3N} \frac{p_i^2}{2m} \quad (4)$$

the kinetic part, and

$$V = V(x_1, x_2, \dots, x_{3N}), \quad (5)$$

the interaction part which generates at least 2 (non-degenerate) bound states. Apart from this V is totally arbitrary.

Bound on $\langle r^2 \rangle_0$

For the mean square radius we begin with the commutator

$$\frac{1}{2} [[x_i, H], x_i] = x_i H x_i - \frac{1}{2} H x_i^2 - \frac{1}{2} x_i^2 H. \quad (6)$$

Since

$$[x_i, H] = \frac{1}{2m} [x_i, p_i^2] = \frac{p_i}{m}, \quad (7)$$

one easily gets

$$\frac{1}{2} [[x_i, H], x_i] = \frac{1}{2m} \quad (8)$$

Evaluating (6) in the N body ground state

$$\begin{aligned} & \langle 0 | \frac{1}{2} [[x_i, H], x_i] | 0 \rangle = \\ & = \sum_n \left[\langle 0 | x_i H | n \rangle \langle n | x_i | 0 \rangle - \frac{1}{2} \langle 0 | H x_i | n \rangle \langle n | x_i | 0 \rangle \right. \\ & \quad \left. - \frac{1}{2} \langle 0 | x_i | n \rangle \langle n | x_i H | 0 \rangle \right] \end{aligned} \quad (9)$$

$$= \sum_n (\epsilon_n - \epsilon_0) \langle 0 | x_i | n \rangle \langle n | x_i | 0 \rangle, \quad (10)$$

where we inserted the complete set of energy eigenstates without any symmetry requirements

$$\sum |n\rangle \langle n| = \mathbb{1} \quad (11)$$

Note that in a restriction to symmetric or antisymmetric states $x_i |0\rangle$ destroys this symmetry and (11) is no longer true.

Combining (8) with (10) gives the well-known TRK sum rule

$$2m \sum_n (\epsilon_n - \epsilon_0) |\langle 0 | x_i | n \rangle|^2 = 1 \quad (12)$$

which we minimize by the lowest intermediate n state possible, and respecting (11),

$$2m (\epsilon_1 - \epsilon_0) \langle 0 | x_i^2 | 0 \rangle \leq 1. \quad (13)$$

Now summing over all $3N$ degrees of freedom and defining the mean square radius of the N body system

$$r^2 = \frac{1}{N} \sum_{i=1}^{3N} x_i^2 \quad (14)$$

we obtain the final result

$$\langle r^2 \rangle_0 \leq \frac{3}{2m(E_1 - E_0)} \quad (15)$$

Bound on $\langle T \rangle_0$

Here we can assume that particles have different masses, m_i . We calculate

$$\langle 0 | [T, x_i] | n \rangle = \langle 0 | [H, x_i] | n \rangle \quad (16)$$

which is

$$-\frac{i}{m_i} \langle 0 | p_i | n \rangle = (E_0 - E_n) \quad (17)$$

After squaring and summation over all energy eigenstates, again without any symmetry requirement, we get

$$\langle 0 | \frac{\hat{p}_i^2}{2m_i} | 0 \rangle = \frac{1}{4} 2m_i \sum_n (E_n - E_0)^2 |\langle 0 | x_i | n \rangle|^2 \quad (18)$$

which is

$$\geq \frac{1}{4} (E_1 - E_0) \quad (19)$$

using the analogue of (12)

$$2m_i \sum (E_n - E_0) |\langle 0 | x_i | n \rangle|^2 = 1.$$

A summation over all indices i gives the bound on the kinetic energy (4) of N bodies in the ground state

$$\langle T \rangle_0 \geq \frac{3N}{4} (E_1 - E_0) \quad (20)$$

(20) and (15) demonstrate that the kinetic energy increases at least proportional

to N the number of particles, whereas the mean radius has an upper bound independent of N.

3. N PARTICLES WITHOUT A FIXED CENTRE

Now we treat N particles interacting only with each other by some general potential. They certainly always have a centre of mass which can be removed since it describes just the global motion of the system, whereas the reduced co-ordinates are responsible for the internal motion we are interested in. In such a transformation to centre of mass co-ordinates, we reduce 3N degrees of freedom by three, leaving the internal dynamics unchanged, thus suggesting only a substitution of N by N-1 in (15) and (20). A specific example, the one-dimensional three-body system, will illustrate this idea in more detail.

The kinetic energy

$$T(x_1, x_2, x_3) = -\frac{1}{2m} \left[\left(\frac{\partial}{\partial x_1} \right)^2 + \left(\frac{\partial}{\partial x_2} \right)^2 + \left(\frac{\partial}{\partial x_3} \right)^2 \right] \quad (21)$$

with m the common mass, transforms under the change of variables

$$\begin{aligned} X &= \frac{1}{3} (x_1 + x_2 + x_3) \\ u &= x_1 - x_2 \\ v &= -\frac{1}{2} (x_1 + x_2) + x_3 \end{aligned} \quad (22)$$

to

$$T_R(u, v) = -\frac{1}{2m} \left[2 \left(\frac{\partial}{\partial u} \right)^2 + \frac{3}{4} \left(\frac{\partial}{\partial v} \right)^2 \right] \quad (23)$$

where the centre of mass motion is already separated. For the expectation of T in the ground state we have to evaluate

$$\langle 0 | \left(\frac{\partial}{\partial u} \right)^2 | 0 \rangle = \sum_n \langle 0 | \frac{\partial}{\partial u} | n \rangle \langle n | \frac{\partial}{\partial u} | 0 \rangle \quad (24)$$

with the relation

$$-\frac{1}{2m} \times 4 \langle 0 | \frac{\partial}{\partial u} | n \rangle = (E_0 - E_n) \langle 0 | u | n \rangle \quad (25)$$

The second variable v is treated analogously and we get

$$\langle T \rangle_0 = 2m \sum_n (E_n - E_0)^2 \left[\frac{1}{8} |\langle 0|u|n \rangle|^2 + \frac{1}{6} |\langle 0|v|n \rangle|^2 \right] \quad (26)$$

As before we minimize

$$\langle T \rangle_0 \geq 2m(E_1 - E_0) \left[\sum_n (E_n - E_0) \left[\frac{1}{8} |\langle 0|u|n \rangle|^2 + \frac{1}{6} |\langle 0|v|n \rangle|^2 \right] \right] \quad (27)$$

and use TRK sum rules for u and v, and get

$$\langle T \rangle_0 \geq (E_1 - E_0) \left(\frac{1}{4} + \frac{1}{4} \right) = \frac{2}{4} (E_1 - E_0), \quad (28)$$

just what we claimed.

This procedure could be applied to all higher N. But what we do instead is to give a general proof avoiding an explicit choice of relative co-ordinates for arbitrary N by adapting a trick once used some time ago by Lipkin in nuclear physics³⁾. We split the Hamiltonian into the centre of mass motion and the reduced part H_{red} , one-dimensional to begin with

$$H = H_{red} + \frac{P_x^2}{2(\sum m_i)} \quad (29)$$

and now we add a fictitious harmonic oscillator in the centre of mass co-ordinate X, thus trapping all N particles by a heavy centre. The total Hamiltonian is

$$H' = H_{red} + H_{osc} \quad (30)$$

where

$$H_{osc} = \frac{P_x^2}{2(\sum m_i)} + \omega^2 X^2 \quad (31)$$

and

$$X = \frac{\sum_{i=1}^N m_i x_i}{\sum m_i} \quad (32)$$

By this trick we obtain exactly the situation we had before where the N particles interact in addition with some common potential. Applying bounds (15) and (20) to the total system and subtracting the known contribution of the oscillator, we shall get the desired result for the reduced part. We denote the energies of the various systems by

$$H' \rightarrow E'_0, E'_1, E'_2 \quad (33)$$

$$H_{red} \rightarrow E_0, E_1, E_2 \quad (34)$$

$$H_{osc} \rightarrow \Delta, 3\Delta, 5\Delta, \dots \quad (35)$$

The ground state energy of the total system is

$$E'_0 = E_0 + \Delta \quad (36)$$

and the first excited energy

$$E'_1 = E_1 + \Delta \quad (37)$$

or

$$E'_1 = E_0 + 3\Delta \quad (38)$$

depending on which combination is lower. Since there is still ω free to be chosen, we adjust it such that (37) and (38) become equal, yielding

$$E'_1 - E'_0 = E_1 - E_0 = 2\Delta \quad (39)$$

and show later on that this choice is the best.

Bound on $\langle T \rangle_0$

The kinetic energy of the reduced system in the ground state is

$$\langle T \rangle_0 = \langle T' \rangle_0 - \langle T_{osc} \rangle_0 \quad (40)$$

We apply for the total system the bound we know already, (20), and use for the oscillator the virial theorem

$$\langle T_{osc} \rangle_0 = \frac{\Delta}{2} \quad (41)$$

then (40) becomes

$$\langle T \rangle_0 \geq \frac{1}{4} [N(\epsilon'_1 - \epsilon'_0) - 2\Delta] \quad (42)$$

and by our choice (39)

$$\langle T \rangle_0 \geq \frac{N-1}{4} (\epsilon_1 - \epsilon_0) . \quad (43)$$

Finally, in three dimensions, the result has to be multiplied by a factor 3

$$\langle T \rangle_0 \geq \frac{3(N-1)}{4} (\epsilon_1 - \epsilon_0) . \quad (44)$$

It remains to show that our choice (39) is the best.

Proof:

i) If $\epsilon_1 - \epsilon_0 > 2\Delta$ the lower total energy difference is

$$\epsilon'_1 - \epsilon'_0 = 2\Delta \quad (45)$$

then the kinetic energy is bounded by

$$\langle T \rangle_0 \geq \frac{N-1}{4} \times 2\Delta \quad (46)$$

Since by assumption $2\Delta < E_1 - E_0$ the inequality is all right but worse than the one we have got before (43)

ii) If $E_1 - E_0 < 2\Delta$, then the lower total energy difference is

$$E'_1 - E'_0 = E_1 - E_0 \quad (47)$$

and the kinetic energy

$$\langle T \rangle_0 \geq \frac{1}{4} (N(E_1 - E_0) - 2\Delta) \quad (48)$$

or

$$\langle T \rangle_0 \geq \frac{N-1}{4} (E_1 - E_0) - \frac{1}{4} (2\Delta - (E_1 - E_0)) \quad (49)$$

Since by assumption the second term is positive, the inequality is again worse than (43).

Bound on $\langle r^2 \rangle$

Here we assume that all masses are equal to m . The mean square radius is

$$N \langle r^2 \rangle_0 = N \langle r'^2 \rangle_0 - \langle R_{\text{ox}}^2 \rangle_0 \quad (50)$$

For the total system we apply bound (15),

$$\langle r'^2 \rangle_0 \leq \frac{3}{2m(E'_1 - E'_0)} \quad (51)$$

$$\langle R_{\text{ox}}^2 \rangle_0 = \frac{3}{2m \times 2\Delta} \quad (52)$$

This gives

$$N \langle r^2 \rangle_0 \leq \frac{3N}{2m(E'_1 - E'_0)} - \frac{3}{2m \times 2\Delta} \quad (53)$$

and respecting our choice (39) the final answer is

$$\langle r^2 \rangle_0 \leq \frac{3(N-1)}{2Nm(E_1 - E_0)} \quad (54)$$

Notice that here our definition of r^2 does not agree with the two body case.

4. CONCLUDING REMARKS

We derived simple bounds on the kinetic energy and the mean square radius of an N body system in terms of the energy difference $E_1 - E_0$. These bounds being optimal, hold if no symmetry requirement is imposed on the spatial wave function. But we believe that they are also true for symmetric states - Bose-Einstein statistics^{*)}. For antisymmetric states - Fermi-Dirac statistics - there exists the bound of Lieb and Thirring^{4,2)} on the product $\langle r^2 \rangle \cdot \langle T \rangle$ [for atoms (Coulomb interaction!) the bound on each of them] but we see in fact no way of writing an inequality (valid for general potentials) by using the antisymmetric (physical!) levels only.

We even know that inequality (15) is definitely false for fermions. A simple example is the one-dimensional harmonic oscillator with, say, two independent particles ($2m = 1$). Then the antisymmetric ground state is

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} [\varphi(x_1) \chi(x_2) - \varphi(x_2) \chi(x_1)] \quad (55)$$

with

$$\varphi(x) = N_1 e^{-x^2/2}$$

and

$$\chi(x) = N_2 x e^{-x^2/2} \quad (56)$$

and the energies are

$$E_0 = 1 + 3 = 4$$

and

$$E_1 = 1 + 5 = 6 \quad (57)$$

This gives

$$(E_1 - E_0) \langle \frac{1}{2}(x_1^2 + x_2^2) \rangle_0 = 2 \times \frac{1}{2} \left(\frac{1}{2} + \frac{3}{2} \right) = 2$$

and N for N particles, whereas from our bound (15), we always have 1. (The kinetic energy bound in this example is all right).

*) It is clear that the ground state of the system can be symmetrized. One should also show that the first excited state is symmetric.

Finally, we want to mention that numerical calculations⁵⁾ for a system of three quarks (symmetric spatial wave-function!) show that bound (44) is a good estimate. For a linear potential, (44) is saturated up to 0.7 per cent, for the Coulomb potential up to 36 per cent, and for superpositions of both, the error is just in between, very much like in the two-body case.

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- 5) These calculations using the hypercentral method were performed by J.M. Richard. We want to thank him for providing us with his results.