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Is Energy Increasing with Angular Momentum?

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We submit to the community of physicists and mathematical physicists the following problem: prove that the ground-state energy of a system of N particles without spin, without statistics, and interacting by central forces increases with angular momentum. For two particles, this is obvious. For more than two we give a number of arguments which support our conjecture.

KEY WORDS: Many-body systems; Regge trajectories; energy dependence on angular momentum; comparison between classical and quantum mechanics; multidimensional harmonic oscillators.

It is a great pleasure to dedicate this paper to Philippe Choquard, who deserves our admiration as a researcher, a teacher, and a leader in research in theoretical physics. I have chosen a subject which is rather a question: something I believe to be true, but that I have not been able to prove and that many of my friends have not been able to prove either. Maybe the referee will find a proof and reject my paper! The best would probably be if Philippe, after reading it, would find the proof himself.

The problem is this: take a quantum mechanical system of N spinless particles (to simplify your life), do not impose any symmetry requirement on the wave function (although Bose statistics would not hurt!), and make these particles interact through two-body potentials depending only on the distance. Such a system admits J, the total relative angular momentum of the system, as a good quantum number. For any given J it has a ground-state energy $E(J)$. Is $E(J)$ an increasing function of J? That is the question.

Perhaps I should explain my motivation. I was having discussions in Calcutta, after giving the Memorial Saha Lecture there, with an Indian

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physicist, Prof. Anjan Kundu, who pointed out that there existed models of nuclei as q-deformed rotators, where the energy, as a function of the angular momentum, would reach some maximum.[1] I replied that this was impossible, but later realized that there is no proof—to my knowledge—of my statement, except for two-body systems, for which it is *obvious* because the centrifugal term is explicit in the Schrödinger equation. In that case the set of ground-state energies for increasing J and their interpolation forms what is called a "Regge trajectory."[2] I still believe that it is impossible, and I want to present here the convergent indications that I have collected so far.

1. THEOREM

If $E(J)$ designates the ground-state energy of an N-particle system with angular momentum J, then

$$E(J) > E(0) \qquad \text{for} \quad J \geqslant 1$$

This is obvious: the state with angular momentum J has a $2J+1$ degeneracy, with magnetic quantum numbers running from $M = -J$ to $M = +J$. Hence, since the overall ground state (for arbitrary J) is non-degenerate and has a positive wave function under our assumptions (no spin, no statistics), $E(J)$ for $J \geqslant 1$ cannot be the absolute ground-state energy.

2. EXAMPLES

2.1. *Harmonic oscillator forces* (I thank J.-M. Richard for help in this case). We take a Hamiltonian

$$H = \sum \frac{\mathbf{p}_i^2}{2m_i} + \sum_{i>j} a_{ij} \mathbf{r}_{ij}^2 \tag{1}$$

where $\sum a_{ij} \mathbf{r}_{ij}^2$ is a positive-definite quadratic form. Let us restrict ourselves to the three-body case. Then we can define Jacobi coordinates

$$\begin{aligned} \boldsymbol{\rho} &\simeq \mathbf{r}_2 - \mathbf{r}_1 \\ \boldsymbol{\lambda} &= \mathbf{r}_2 - \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2} \end{aligned} \tag{2}$$

and the relative Hamiltonian, with the center-of-mass motion removed, becomes

$$H = \frac{\mathbf{p}_\rho^2}{2m_\rho} + \frac{\mathbf{p}_\lambda^2}{2m_\lambda} + A\boldsymbol{\rho}^2 + B\boldsymbol{\lambda}^2 + 2C\boldsymbol{\rho}\boldsymbol{\lambda} \tag{3}$$

There is a *linear transformation* in $\mathbf{\rho}$, $\boldsymbol{\lambda}$ space which diagonalizes the interaction. With the new variables $\mathbf{\rho}'$, $\boldsymbol{\lambda}'$ we get

$$H = \mathbf{p}_{\rho'}^2 + \mathbf{p}_{\lambda'}^2 + k_1 \boldsymbol{\rho}'^2 + k_2 \boldsymbol{\lambda}'^2 \tag{4}$$

and the energy is

$$E = 2\sqrt{k_1}\,(3 + 2n_{\rho'} + l_{\rho'}) + 2\sqrt{k_2}\,(3 + 2n_{\lambda'} + l_{\lambda'}) \tag{5}$$

where n_ρ and n_λ are the numbers of nodes of the wave functions of the subHamiltonians. Then one has to minimize this expression for given $\mathbf{J} = \mathbf{L}_{\rho'} + \mathbf{L}_{\lambda'}$.

Obviously we must take

$$\begin{gathered} j = l_{\rho'} + l_{\lambda'} \\ n_{\rho'} = n_{\lambda'} = 0 \end{gathered} \tag{6}$$

and minimize in $l_{\rho'}$. Clearly, if $k_1 < k_2$, we get

$$E(J) = 6\sqrt{k_2} + 2\sqrt{k_1}\,(3 + J) \tag{7}$$

which can be generalized to N bodies.

2.2. Particles 1 and 2, with equal masses, interact by an *arbitrary* potential, but 13 and 23 forces are equal-strength harmonic oscillator forces.

Then using again the Jacobi variables (2), we have that the Hamiltonian is still separable

$$H = \frac{p_\rho^2}{2m_\rho} + V(\rho) + g\,\frac{\rho^2}{2} + \frac{p_\lambda^2}{2m_\lambda} + 2g\lambda^2 \tag{8}$$

The energy levels are given by

$$E(l_\rho, n_\rho) + C[2n_\lambda + l_\lambda + 3] \tag{9}$$

where $E(l_\rho, n_\rho)$ is an increasing function of l_ρ for fixed n_ρ. To get the ground state we must take $n_\rho = n_\lambda = 0$. Furthermore, among the possible choices of l_ρ and l_λ, for

$$|l_\lambda - l_\rho| \leqslant J \leqslant l_\lambda + l_\rho$$

it is clear that the only possible choice is $J = l_\lambda + l_\rho$, for otherwise one could decrease the energy by diminishing l_λ or l_ρ. This still leaves a number of possibilities, among which there is at least one minimizing choice:

$$J = l_\lambda^o + l_\rho^o \tag{10}$$

We assume $J \geqslant 1$. Consider now the case $J' = J - 1$. One state of the system will have the quantum numbers

$$l'_\lambda = l^o_\lambda - 1, \qquad l'_\rho = l^o_\rho \qquad \text{if} \quad l^o_\lambda \geqslant 1$$
$$l'_\lambda = l^o_\lambda, \qquad l_\rho = l^o_\rho - 1 \qquad \text{if} \quad l^o_\rho \geqslant 1$$

In the first case the energy of this state will be

$$C(l^o_\lambda + 2) + E(l^o_\rho, 0) < C(l^o_\lambda + 3) + E(l^o_\rho, 0) = E(J)$$

and, in the second case,

$$C(l^o_\lambda + 3) + E(l^o_\rho - 1, 0) < C(l^o_\lambda + 3) + E(l^o_\rho, 0) = E(J)$$

Here the monotonicity of the energy of a two-body system with respect to angular momentum has been used. Now this particular state has an energy superior or equal to $E(J-1)$, which proves our statement.

2.3. Another rather extreme example is that of two particles with no interaction between them, while they interact with the third one, which is infinitely heavy, i.e.,

$$H = \frac{p_1^2}{2m_1} + V(r_1) + \frac{p_2^2}{2m_2} + W(r_2) \tag{11}$$

Then the energy levels are characterized by (l_1, n_1) and (l_2, n_2). It is now obvious that one must take

$$n_1 = n_2 = 0; \qquad J = l_1 + l_2$$

Then, following the same lines as in the previous subsection and using the monotonicity of the individual energies in l_1 and l_2, one gets the desired result.

3. THE CLASSICAL CASE

If the potential energy is lower bounded, which is guaranteed if all two-body potentials are lower bounded, the energy of a classical system of N particles has a lower bound $E_c(J)$ for any given angular momentum J. This lower bound $E_c(J)$ is not only an infimum, but a minimum, since one can restrict oneself to a compact region of phase space to find it. The energy is

$$\sum \frac{p_i^2}{2m_i} + \sum V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) \tag{12}$$

The relative angular momentum is given by

$$\mathbf{J} = \sum \mathbf{r}_i \times \mathbf{p}_i \tag{13}$$

with the condition that the center of mass is at the origin

$$\sum m_i \mathbf{r}_i = 0 \tag{14}$$

Now we have the chain of inequalities

$$|\mathbf{J}| \leqslant \sum |\mathbf{r}_i \times \mathbf{p}_i| \leqslant \sum |r_i p_i| \leqslant \left[\left(\sum m_i r_i^2\right)\left(\sum \frac{p_i^2}{m_i}\right)\right]^{1/2} \tag{15}$$

which is saturated at a time t if all $\mathbf{r}_i$ are in a plane perpendicular to $\mathbf{J}$ going through the origin, and if the motion is a global rotation around this axis. Combining (11) and (14), we get

$$E \geqslant \frac{J^2}{2 \sum m_i \mathbf{r}_i^2} + \sum V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) \tag{16}$$

If in addition all forces are attractive, i.e.,

$$\frac{dV_{ij}(r)}{dr} > 0, \qquad \forall r > 0 \tag{17}$$

the minimizing configuration is *certainly* in a plane perpendicular to $\mathbf{J}$ and is a global rotation, since one saturates (15), and, by projecting the $\mathbf{r}_i$'s on a plane one reduces the distances between them.

Anyway, minimizing (16) with respect to the various $\mathbf{r}_i$'s, constrained with $\sum m_i \mathbf{r}_i = 0$, will give a lower bound to $E_c(J)$, but this lower bound may coincide with $E_c(J)$ only if the $\mathbf{r}_i$ are in a plane perpendicular to $\mathbf{J}$.

If the forces are not purely attractive, it is not clear that the minimizing configuration will be in a plane, but one can use another argument to show that again it is necessarily a rotation around the $\mathbf{J}$ axis. We can replace (14) by another chain of inequalities:

$$|\mathbf{J}| \leqslant \sum |\mathbf{r}_i \times \mathbf{p}_i| \leqslant \sum |d_i p_i| \leqslant \left[\left(\sum m_i d_i^2\right)\left(\sum \frac{p_i^2}{m_i}\right)\right]^{1/2} \tag{18}$$

where the d_i represent the distances of the $\mathbf{r}_i$ to the J axis. Then

$$E_c(J) \geqslant \frac{1}{2} \frac{\mathbf{J}^2}{\sum m_i d_i^2} + \sum V_{ij}(\mathbf{r}_i - \mathbf{r}_j) \tag{19}$$

and the inequality (18) is saturated at a given time if the motion is a global rotation around the axis.

One can minimize (19) with respect to the $\mathbf{r}_i$, taking into account the center-of-gravity constraint. Then one gets indeed $E_c(J)$ since the energy cannot go below that.

Let us now show that $E_c(J)$ is *increasing*. Let r_i^J, d_i^J be a set of equilibrium positions for an angular momentum J. For an angular momentum $J-\varepsilon$ the energy can certainly be as small as

$$\frac{1}{2}\frac{(J-\varepsilon)^2}{\sum m_i (d_i^J)^2}+\sum V_{ij}(|\mathbf{r}_i^J-\mathbf{r}_j^J|) \tag{20}$$

because the lower bound (18) on the kinetic energy can be saturated for the angular momentum $J-\varepsilon$ by adjusting the impulsions. Therefore $E_c(J-\varepsilon)$ is certainly less than $E_c(J)$.

4. A LOWER BOUND ON THE QUANTUM ENERGY FOR THREE- AND *N*-BODY SYSTEMS

Here we repeat an argument that was already presented years ago.[3] The idea is to find an operator lower bound on the kinetic energy. To do this, we are allowed to use the basis generated by the Jacobi variables (2), i.e., to expand any state as a sum of components $|l_\lambda, l_\rho\rangle$. For simplicity we restrict ourselves to equal masses. Then we can look at the diagonal elements of T since the off-diagonal elements will disappear. Hence we get

$$\langle T\rangle = -\frac{1}{m}\frac{d^2}{d\rho^2}+\frac{1}{m}\frac{l_\rho(l_\rho+1)}{\rho^2}+-\left(\frac{1}{m}+\frac{1}{2m}\right)\frac{d^2}{d\lambda^2}+\frac{3}{2m}\frac{l_\lambda(l_\lambda+1)}{\lambda^2} \tag{21}$$

and, using the standard inequality

$$-\frac{d^2}{dr^2}>\frac{1}{4r^2} \tag{22}$$

we get

$$\langle T\rangle \geqslant \frac{1}{m}\frac{(l_\rho+1/2)^2}{\rho^2}+\frac{3}{2m}\frac{(l_\lambda+1/2)^2}{\lambda^2}$$

and since $|l_\rho - l_\lambda| < J < l_\rho + l_\lambda$ we minimize with respect to l_ρ, making the obvious choice $J = l_\rho + l_\lambda$ and get

$$T \geqslant \frac{(J+1)^2}{m}\frac{1}{\rho^2+2\lambda^2/3}$$

which can be reexpressed as

$$T \geqslant \frac{3}{2}\frac{(J+1)^2}{m(r_{12}^2+r_{23}^2+r_{13}^2)} \tag{23}$$

and hence

$$E(J) \geqslant \inf\left[\frac{3}{2}\frac{(J+1)^2}{m(r_{12}^2+r_{23}^2+r_{13}^2)}+\sum V_{ij}(r_{ij})\right] \tag{24}$$

It is interesting to compare this lower bound with $E_c(J)$. In the case where the V_{ij} are *attractive*, $E_c(J)$ is indeed given by the *infimum* of (15):

$$\frac{J^2}{2m\sum \mathbf{r}_i^2}+\sum V_{ij}(\mathbf{r}_i-\mathbf{r}_j)$$

but

$$\sum \mathbf{r}_i^2 = \frac{1}{3}\sum_{i>j} \mathbf{r}_{ij}^2 \tag{25}$$

if one takes into account the center-of-gravity constraint (14).

Then (15) and (23) coincide.

So, at least for *purely attractive* forces we have

$$E(J) > E^c(J) \tag{26}$$

This agrees with the Golden–Symanzik theorem on the comparison of the quantum and classical energies[4] of a system, but the *new* element is that this is constrained to a *given* angular momentum.

Therefore, even if we are not able to prove that $E(J)$ is increasing, we are able to find an increasing lower bound. In ref. 3 we also find lower bounds that can be used for singular potentials, for instance,

$$T > \frac{1}{12m}\left(\frac{1}{r_{12}^2}+\frac{1}{r_{13}^2}+\frac{1}{r_{23}^2}\right)+\frac{3}{2m}\frac{(J+1/2)^2}{r_{12}^2+r_{13}^2+r_{23}^2} \tag{27}$$

which shows that, as in the two-body case, the energy is lower bounded for two-body potentials less singular than r^{-2}.

5. POWER POTENTIALS AND ASYMPTOTIC BEHAVIOR FOR LARGE J IN THE THREE-BODY CASE

In ref. 3 we prove that at least for two-body potentials of the form r^ν, $\nu > 0$, the ratio of the quantum and classical energies tends to unity for $J \to \infty$. Depending on whether $\nu < 2$ or $\nu > 2$, the minimizing classical configurations are either two particles coinciding and the other one further away, or an equilateral triangle, respectively. In both cases one finds that the energy increases as a positive power of J.

6. CONCLUSION

All these indications are not a substitute for a serious proof, but we are convinced that the energy increases with angular momentum. Presumably, the proof is easier than that of Fermat's last theorem and will be given some day.

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