PHYSICAL REVIEW A VOLUME 40, NUMBER 12 DECEMBER 15, 1989

Impossibility of the ground-state total angular momentum taking any value

I. V. Komarov* and R. Tarrach
Departament d'Estructura i Constituents de la Matèria, Universitat de Barcelona,† Barcelona, Spain
(Received 4 January 1989)

We prove that for any nonrelativistic rotationally invariant two-particle quantum system whose interaction is velocity independent the total angular momentum of the ground state is bounded by the sum of the spins; i.e., $j_{\max}=s_1+s_2$.

There are basic (and old) questions in nonrelativistic quantum mechanics which, surprisingly, seem to not have been answered in its 60-plus years of existence. A survey of the literature and an oral sampling indicate that one of them is the following: what are the possible ground-state total angular momentum values j of a system of two particles of spin s_1 and s_2? It is known that if the interaction is velocity-dependent j can take any value. We therefore restrict ourselves to velocity-independent potentials. For $s_i=s_2=0$ one knows the answer: due to the centrifugal barrier $l=0$ and thus $j=0$. For $s_1=0$, $s_2=\frac{1}{2}$ the answer is $j=\frac{1}{2}$.[1] For $s_1=s_2=\frac{1}{2}$ the answer is, restricting oneself to parity and time-reversal invariant interactions, $j=0,1$.[1] One might think that this is what one expects for $l=0$ but, of course, neither is l a good quantum number nor, as shown in Ref. 1, does the ground state necessarily have a component with $l=0$. Indeed, the ground state can be a pure $l=1$ state.

In this paper we do three things. We streamline the proof of Ref. 1 very much by working in a suitable basis. We extend the proof for $s_1=s_2=\frac{1}{2}$ to any type of velocity-independent interactions. The result remains the same: $j=0$ or 1. And, most importantly, we generalize the proof to any values of the spin of the particles. The result is $j_{\max}=s_1+s_2$.

Consider the most general rotationally invariant Hamiltonian describing the velocity-independent interaction between two spin-$\frac{1}{2}$ particles,

$$H=p_r^2+\frac{\mathbf{L}^2}{r^2}+V_c(r)+V_\sigma(r)A_\sigma+V_T(r)A_T+V_p(r)A_p+V_s(r)A_s+V_d(r)A_d\ , \tag{1}$$

where

$$\begin{aligned}&A_s=(\mathbf{S}_1+\mathbf{S}_2)\cdot\hat{\mathbf{r}}\equiv\mathbf{S}\cdot\hat{\mathbf{r}}\equiv S_r=\mathbf{J}\cdot\hat{\mathbf{r}}\ ,\\&A_\sigma=\mathbf{S}_1\cdot\mathbf{S}_2=(2\mathbf{S}^2-3)/4\ ,\\&A_T=3\mathbf{S}_1\cdot\hat{\mathbf{r}}\mathbf{S}_2\cdot\hat{\mathbf{r}}-\mathbf{S}_1\cdot\mathbf{S}_2=(3S_r^2-\mathbf{S}^2)/2\ ,\\&A_p=\mathbf{S}_1\times\mathbf{S}_2\cdot\hat{\mathbf{r}}\ ,\\&A_d=(\mathbf{S}_1-\mathbf{S}_2)\cdot\hat{\mathbf{r}}\ ,\end{aligned}\tag{2}$$

with $\mathbf{S}_i=\sigma_i/2$. No parity or time-reversal invariance has been assumed. Consider the set of mutually commuting operators

$$\mathbf{J}^2, J_3, \mathbf{S}^2, S_r \tag{3}$$

with common eigenstates

$$\begin{aligned}&\mathbf{J}^2|j,m;s,h\rangle=j(j+1)|j,m;s,h\rangle,\quad j=0,1,2,\ldots\\&J_3|j,m;s,h\rangle=m|j,m;s,h\rangle,\quad m\in[-j,j]\\&\mathbf{S}^2|j,m;s,h\rangle=s(s+1)|j,m;s,h\rangle,\quad s=0,1\\&S_r|j,m;s,h\rangle=h|j,m;s,h\rangle,\\&\qquad h\in[-s,s],\quad j>0,\quad h=0,\quad j=0\ .\end{aligned}\tag{4}$$

As

$$[H,\mathbf{J}^2]=[H,J_3]=0 \tag{5}$$

it is enough to consider the m-independent matrix elements

$$\langle j,m;s',h'|H|j,m;s,h\rangle=\langle j,m;s,h|H|j,m;s',h'\rangle^* \tag{6}$$

which for $j>0$ correspond to a 4×4 and for $j=0$ to a 2×2 matrix. Now, the five operators given in (2) form a closed algebra. Indeed

$$\begin{aligned}&[S_r,A_d]=0\ ,\\&[S_r,A_p]=0\ ,\\&[\mathbf{S}^2,A_d]=4iA_p\ ,\\&[\mathbf{S}^2,A_p]=-iA_d\ ,\\&[A_p,A_d]=i(S_r^2-\mathbf{S}^2+1)\ .\end{aligned}\tag{7}$$

The important point is that $\mathbf{J}^2$ commutes with all these operators and does not appear in the algebra. In fact, it cannot. Thus the matrix elements of these operators are j independent (with the proper choice of phases). Let us see this explicitly.

The first four commutators of (7) imply, in a simplified notation,

$$\begin{aligned}&(h'-h)\langle s'h'|A_d|sh\rangle=0\ ,\\&[s'(s'+1)-s(s+1)]\langle s'h'|A_d|sh\rangle=4i\langle s'h'|A_p|sh\rangle\ ,\\&(h'-h)\langle s'h'|A_p|sh\rangle=0\ ,\\&[s'(s'+1)-s(s+1)]\langle s'h'|A_p|sh\rangle=-i\langle s'h'|A_d|sh\rangle\ ,\end{aligned}\tag{8}$$

from which it follows that there is only one independent nonvanishing matrix element

$$\langle 10|A_d|00\rangle = 2i\langle 10|A_p|00\rangle \ , \tag{9}$$

The last commutator of (7) finally leads to

$$|\langle 10|A_d|00\rangle| = 1 \tag{10}$$

so that absorbing the possible j-dependent phase of the matrix element (9) into $|j,m;0,0\rangle$ no j dependence enters through the spin part of H. Thus the whole j dependence comes from $\mathbf{L}^2$. It is not difficult to study the matrix elements of $\mathbf{L}^2$ in the basis (3). This is best done with the help of

$$\begin{aligned}&[\mathbf{L}^2,\mathbf{S}^2]=0 \ ,\\ &[S_r,[S_r,\mathbf{L}^2]]=\mathbf{L}^2-\mathbf{J}^2-\mathbf{S}^2+2S_r^2 \ ,\\ &[\mathbf{L}^2,[\mathbf{L}^2,S_r]]=2\{\mathbf{L}^2,S_r\} \ ,\end{aligned} \tag{11}$$

which imply

$$\begin{aligned}&[s'(s'+1)-s(s+1)]\langle s'h'|\mathbf{L}^2|sh\rangle=0 \ ,\\ &[(h'-h)^2-1]\langle s'h'|\mathbf{L}^2|sh\rangle\\ &\qquad=[-j(j+1)-s(s+1)+2h^2]\delta_{s,s'}\delta_{h,h'} \ ,\\ &(h+h')\langle s'h'|(\mathbf{L}^2)^2|sh\rangle-2\langle s'h'|\mathbf{L}^2S_r\mathbf{L}^2|sh\rangle\\ &\qquad=2(h+h')\langle s'h'|\mathbf{L}^2|sh\rangle \ .\end{aligned} \tag{12}$$

From here one readily obtains the only nonvanishing matrix elements

$$\begin{aligned}&\langle 00|\mathbf{L}^2|00\rangle=j(j+1) \ ,\\ &\langle 1h|\mathbf{L}^2|1h\rangle=j(j+1)+2-2h^2 \ ,\\ &|\langle 1h\pm 1|\mathbf{L}^2|1h\rangle|^2=2j(j+1) \ .\end{aligned} \tag{13}$$

Thus, with a particular choice of phases of, say, $|j,m;1,1\rangle$ and $|j,m;1,0\rangle$ and the ordering $|00\rangle$, $|11\rangle$, $|10\rangle$, and $|1-1\rangle$, we find for $j>0$,

$$H_j=p_r^2+V_c+\frac{j(j+1)}{r^2}+\frac{V_\sigma}{4}+\begin{pmatrix}-V_\sigma & 0 & V_d+i\frac{V_p}{2} & 0\\ 0 & \frac{V_T+V_s}{2} & \frac{\sqrt{2j(j+1)}}{r^2} & 0\\ V_d-i\frac{V_p}{2} & \frac{\sqrt{2j(j+1)}}{r^2} & \frac{2}{r^2}-V_T & \frac{\sqrt{2j(j+1)}}{r^2}\\ 0 & 0 & \frac{\sqrt{2j(j+1)}}{r^2} & \frac{V_T-V_s}{2}\end{pmatrix} \tag{14}$$

from which it follows, using the Hellmann-Feynman theorem,[2] that

$$H_1<H_2<H_3<\cdots \ . \tag{15}$$

This is seen immediately from the derivative of H_j with respect to j,

$$H_j'=\frac{2j+1}{r^2}+\frac{2j+1}{\sqrt{2j(j+1)}}\frac{1}{r^2}\begin{pmatrix}0&0&0&0\\0&0&1&0\\0&1&0&1\\0&0&1&0\end{pmatrix} \tag{16}$$

which is non-negative (recall $j>0$) for $j=1$ and positive for $j>1$ because

$$(H_j')_{ii}\geq \sum_{k\,(\neq i)}|(H_j')_{ki}|, \quad j\geq 1 \tag{17}$$

with strict noninequality for $j>1$.[3]

One can extend this proof to any spin. Consider two particles of spin s_1 and s_2. The Hamiltonian will be more complicated than in (1), as products of spin matrices do not linearize as for spin $\frac{1}{2}$. Still, there is only a finite number of spin-dependent operators and they can all be written as monomials in S_r, $\mathbf{S}^2$, A_d, and A_p. Thus, the generalization of (7) to arbitrary spins suffices for generating the whole algebra

$$\begin{aligned}&[S_r,A_d]=0 \ ,\\ &[S_r,A_p]=0 \ ,\\ &[\mathbf{S}^2,A_d]=4iA_p \ ,\\ &[\mathbf{S}^2,A_p]=i[s_1(s_1+1)-s_2(s_2+1)]S_r-i\{A_d,\mathbf{S}^2\}/2 \ ,\\ &[A_p,A_d]=i[s_1(s_1+1)+s_2(s_2+1)]\\ &\qquad -i(2\mathbf{S}^2-S_r^2+A_d^2)/2 \ .\end{aligned} \tag{18}$$

Again, $\mathbf{J}^2$ does not appear. The first four commutators lead to the following expressions for the only nonvanishing matrix elements of A_p and A_d:

$$\langle sh|A_d|sh\rangle=\frac{s_1(s_1+1)-s_2(s_2+1)}{s(s+1)}h\ ,$$
$$\langle s+1h|A_d|sh\rangle=\frac{2i}{s+1}\langle s+1h|A_p|sh\rangle\ . \tag{19}$$

With the help of (19) the last equation of (18) leads to

$$(2s+3)|\langle sh|A_d|s+1h\rangle|^2-(2s-1)|\langle sh|A_d|s-1h\rangle|^2$$
$$=2[s_1(s_1+1)+s_2(s_2+1)-s(s+1)]+h^2$$
$$-h^2\left[\frac{s_1(s_1+1)-s_2(s_2+1)}{s(s+1)}\right]^2 . \tag{20}$$

This allows an easy computation of $|\langle sh|A_d|s+1h\rangle|$ which of course is j independent.

Equations (11) and (12) hold for any values of s_1 and s_2. They lead to the following generalization of (13):

$$\langle sh|\mathbf{L}^2|sh\rangle=j(j+1)+s(s+1)-2h^2\ ,$$
$$|\langle sh|\mathbf{L}^2|sh-1\rangle|$$
$$=\sqrt{[j(j+1)-h(h-1)][s(s+1)-h(h-1)]}\ . \tag{21}$$

Let us choose the states $|j,m;s,h\rangle$ with $h\neq -s$ such that the phase of $\langle sh|\mathbf{L}^2|sh-1\rangle$ is zero, so that the right-hand side of the second equation of (21) is the matrix element (not its modulus). There are now only $2s_2+1$ (with $s_1\geq s_2$) states with unfixed phase left. This is not enough for fixing the phases of all $\langle sh|A_d|s+1h\rangle$ and thus to ensure that no j dependence creeps in through these phases. In order to solve this problem consider the double commutator

$$[\mathbf{L}^2,[\mathbf{L}^2,A_d]]=2\{\mathbf{L}^2,A_d\}\ . \tag{22}$$

Using (21), with the above mentioned phase convention, one obtains from (22), after a certain amount of algebra,

$$\langle s+1h|A_d|sh\rangle=\left[\frac{(s+1)^2-h^2}{(s+1)^2-(h-1)^2}\right]^{1/2}$$
$$\times\langle s+1h-1|A_d|sh-1\rangle\ , \tag{23}$$

which allows to fix the phases of all $\langle s+1h|A_d|sh\rangle$ in such a way that no j dependence enters by taking the phase of $\langle s+1-s|A_d|s-s\rangle$ to be zero. This requires an appropriate choice of the phase of the states $|j,m;s,-s\rangle$ for all $s<s_1+s_2$. Incidentally all matrix elements of A_d can now be obtained from (20) and (23).

The upshot of this study is that all the j dependence is contained in (21). The final stages of the proof go through as before in (16) and (17). The equivalent to (17) now reads

$$1\geq\frac{\sqrt{s(s+1)-h(h-1)}}{2\sqrt{j(j+1)-h(h-1)}}+\frac{\sqrt{s(s+1)-h(h+1)}}{2\sqrt{j(j+1)-h(h+1)}} \tag{24}$$

which holds for $j=s_1+s_2$ and holds strictly for $j>s_1+s_2$.

Thus $j_{\max}=s_1+s_2$.

One of us (R.T.) would like to thank Alberto Galindo for pointing out that the proof was not complete. He has given recently a different proof of the same theorem (Ref. 3). This collaboration has taken place within the University of Barcelona–University of Leningrad exchange agreement. Financial support by CICYT (Spain) Contract No. AEN-88-0016 is acknowledged.

*Permanent address: Department of Computational Physics, University of Leningrad, Leningrad, Union of Soviet Socialist Republics.

†Mailing address: Faculty of Physics, Diagonal 647, 08028 Barcelona, Spain.

[1] A. Galindo and R. Tarrach, Ann. Phys. (N.Y) **173**, 430 (1987).

[2] H. Hellmann, Acta Physicochim. URSS **6**, 913 (1935); R. P. Feynman, Phys. Rev. **56**, 340 (1939).

[3] A. Galindo, J. Phys. A **22**, L593 (1989).