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LETTER TO THE EDITOR

Spin of the ground state

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Abstract. The following theorem is proved. The spin J_g of the ground state of a system of any two particles of spins s_1, s_2 interacting through rotationally invariant but otherwise arbitrarily spin-dependent potentials fulfils the inequality $J_g \leqslant s_1 + s_2$.

The non-degeneracy of the ground state (GS) of two-body systems with spinless particles follows from the classical Perron–Frobenius argument and the positivity improving property of the dynamical semigroup $\exp(-tH)$, $H := -\Delta + V$, $t > 0$, for quite general potentials V [1]. Nevertheless, the simplicity of the ground energy may be lost for spinning particles; recall, for instance, that the deuteron has multiplicity three. The question was recently addressed [2] as to which possible values may be taken on by the GS intrinsic total angular momentum and the degeneracy for rotationally invariant systems of two particles with spins s_1, s_2. The analysis therein was limited to the cases $s_i \leqslant \frac{1}{2}$, $i = 1, 2$. The present paper removes this restriction and a proof is provided of the following theorem. The spin (i.e. intrinsic total angular momentum) J_g of the GS of a system of any two particles of spins s_1, s_2 interacting through rotationally invariant but otherwise arbitrarily spin-dependent potentials fulfils the inequality $J_g \leqslant s_1 + s_2$.

The Hilbert space $\mathscr{H}$ of the state vectors for the relative motion of two elementary particles of spins s_1, s_2 is of the form [3, 4]

$$\mathscr{H} = L^2(\mathbb{R}^+, \mathrm{d}r) \otimes \mathscr{K} \qquad \mathscr{K} := L^2(S^2, (4\pi)^{-1}\,\mathrm{d}\Omega) \otimes \mathbb{C}^{N(s_1, s_2)} \tag{1}$$

where S^2 stands for the unit 2-sphere with normalised measure $(4\pi)^{-1}\,\mathrm{d}\Omega$ and $N(s_1, s_2) := (2s_1 + 1)(2s_2 + 1)$. The (reduced) radial part of the wavefunction lies in the first factor $L^2(\mathbb{R}^+, \mathrm{d}r)$ of $\mathscr{H}$, whereas its dependence on the angular variables and third components of spin is respectively reflected in the two factors of $\mathscr{K}$.

The (universal covering SU(2) of the) rotation group acts unitarily in $\mathscr{K}$. This representation $\mathrm{SU}(2) \ni A \mapsto \mathrm{U}(A)$ decomposes into a direct sum of irreducible actions $D^j(A)$:

$$U = \bigoplus_{j \in j_{\min} + \mathbb{Z}^+} \mu_j(s_1, s_2) D^j \tag{2}$$

where $j_{\min} := 0$ if $s_1 + s_2 \in \mathbb{Z}$, and $j_{\min} := \frac{1}{2}$ otherwise. The multiplicity $\mu_j(s_1, s_2)$ of D^j is given by

$$\mu_j(s_1, s_2) = \sum_{s \in S_1 + S_2} [2\min(j, s) + 1] \tag{3}$$

where S_1 and S_2 are the spin operators of the intervening particles. The sum in (3) runs over all possible values of the total spin, the symbol $s \in S_1 + S_2$ indicating that D^s

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enters the Clebsch-Gordan series of $D^{s_1} \otimes D^{s_2}$. The subspaces $\mathcal{K}_j$ on which the $\mu_j(s_1, s_2) D^j$ act have dimension $(2j+1)\mu_j(s_1, s_2)$. Associated with (2) we thus have a decomposition

$$\mathcal{H} = \bigoplus_{j \in j_{\min} + \mathbb{Z}^+} \mathcal{H}_j := \bigoplus_{j \in j_{\min} + \mathbb{Z}^+} L^2(\mathbb{R}^+, \mathrm{d}r) \otimes \mathcal{K}_j \tag{4}$$

into subspaces $\mathcal{H}_j$ of total angular momentum $J := L + S$ $(S := S_1 + S_2)$ equal to j.

Let H be the self-adjoint Hamiltonian which generates the inner dynamics of our system. The space isotropy allows one to assume H to be invariant under rotations. Therefore the spaces $\mathcal{H}_j$ are dynamically invariant and so will be their subspaces $\mathcal{H}_{j,m}$ with $m = -j, -j+1, \ldots, j-1, j$ for J_z. We shall denote by $\mathcal{K}_{j,m}$ the factor space of $\mathcal{H}_{j,m}$ associated with the angular and spin variables. For a given j, the $(2j+1)$ restrictions $H_{j,m}$ of H to $\mathcal{H}_{j,m}$ are all unitarily equivalent to each other.

We will suppose H of the form $H = -\Delta + V$ in appropriate units, where V is a self-adjoint potential $N(s_1, s_2) \times N(s_1, s_2)$ matrix, invariant under rotations (i.e. under the action $\int_{\mathbb{R}^+}^{\oplus} \mathbb{1} \otimes U(A)\, \mathrm{d}r$) and with entries, say, in $L^{3/2}(\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3)$, to ensure a good quantum dynamics [5]. Let P_H denote the spectral family of H. The existence of a discrete ground level $E_g := \inf \sigma(H) \in \sigma_{\mathrm{disc}}(H)$ will be taken for granted. Finally J_g will stand for the greatest of all angular momenta in the subspace $\mathcal{H}_g := P_H(\{E_g\})\mathcal{H}$ spanned by all the GS.

The familiar techniques [6] of the angular momentum formalism allow any of the above-mentioned potential matrices to be written as

$$V(\boldsymbol{r}) = \sum_{t_1 t_2 l} v_{t_1 t_2 l}(r) V_{t_1 t_2 l}(\boldsymbol{\Omega}) \tag{5}$$

$$V_{t_1 t_2 l}(\boldsymbol{\Omega}) := \mathrm{i}^{t_1 + t_2 + l} \sum (-1)^{l-m} (2l+1)^{-1/2} C(t_1, t_2, l; m_1, m_2, m) \times Y^l_{-m}(\boldsymbol{\Omega}) T(1)^{t_1}_{m_1} \otimes T(2)^{t_2}_{m_2} \tag{6}$$

where $\boldsymbol{\Omega}$ is the unit vector along $\boldsymbol{r}$. The summation in (5) runs over all t_1, t_2, l such that $t_1 \in S_1 + S_1$, $t_2 \in S_2 + S_2$, $l \in t_1 + t_2$, whereas that in (6) ranges through all possible values of m, m_1, m_2. $T(1)^{t_1}_{m_1}$ and $T(2)^{t_2}_{m_2}$ are the following irreducible tensor operators with angular momenta t_1, t_2 and third components m_1, m_2, which act in the spin spaces of the particles 1, 2, respectively:

$$T(i)^t_m := [(t+m)!/(2t)!(t-m)!]^{1/2} C^{t-m}_{i_-} S^t_{i_+} \tag{7}$$

$$S_{i_\pm} := S_{ix} \pm \mathrm{i} S_{iy} \qquad C_{i_-} A := [S_{i_-}, A]. \tag{8}$$

The operator $T(1)^{t_1}_{m_1} \otimes T(2)^{t_2}_{m_2}$ in (6) is properly coupled to the spherical harmonic $Y^l_{-m}(\boldsymbol{\Omega})$ to produce a rotationally invariant operator $V_{t_1 t_2 l}(\boldsymbol{\Omega})$ in $\mathcal{K}$. The number $M(s_1, s_2)$ of such basic $V_{t_1 t_2 l}(\boldsymbol{\Omega})$ is

$$M(s_1, s_2) = \sum (2 \min(t_1, t_2) + 1) = \sigma_<[\sigma_<(3\sigma_> - \sigma_<) + 1]/3 \tag{9}$$

with $\sigma_< := \min(2s_1 + 1, 2s_2 + 1)$, $\sigma_> := \max(2s_1 + 1, 2s_2 + 1)$. Thus, $M(0, \frac{1}{2}) = 2$, $M(0, 1) = 3$, $M(\frac{1}{2}, \frac{1}{2}) = 6$, $M(\frac{1}{2}, 1) = 10$, $M(1, 1) = 19$, etc.

The matrix elements of $V_{t_1 t_2 l}(\boldsymbol{\Omega})$ in the physically natural orthonormal basis $|sLjm\rangle$ of $\mathcal{K}_j$ which diagonalises $(S := S_1 + S_2)^2$, L^2, J^2, J_z are explicitly computable in terms of Clebsch-Gordan, Racah and Rosen coefficients, but their dependence in j is buried in a Racah W coefficient and this makes the spectral comparison between the different Hamiltonians $H_{j,m}$ look formidable. Hence the interest in an alternative analysis.

Given a rotation R, the action of SU(2) unitarily transforms the rotationally invariant matrix $V(\boldsymbol{r})$ into $V(R\boldsymbol{r})$. Therefore, the spectral decomposition of $V(\boldsymbol{r})$ will be of the form

$$V(\boldsymbol{r}) = \sum_{1 \leqslant n \leqslant N(s_1, s_2)} v_n(\boldsymbol{r}) P_n(\boldsymbol{r}) \tag{10}$$

where $P_n(\boldsymbol{r})$ are, for a fixed $\boldsymbol{r}$, mutually orthogonal projections of rank 1. Being polynomials in $V(\boldsymbol{r})$, the matrices $P_n(\boldsymbol{r})$ inherit the rotational invariance of $V(\boldsymbol{r})$, and thus are determined by $P_n(re_3)$, $e_3 := (0, 0, 1)$. These projections $P_n(re_3)$ must commute with the generator $S_z := S_{1z} + S_{2z}$ of the little group (or stabiliser) of re_3; the cardinal of a maximal orthogonal system of such projections is precisely $M(s_1, s_2)$.

The analysis via (10) of the matrix elements of $V(r\boldsymbol{\Omega})$, r fixed, in $\mathscr{H}_J$ suggests the convenience of introducing the following orthonormal basis of $\mathscr{H}_J$:

$$|J; smM\rangle := \sum_L (-1)^L C(sJL; -mm0)|sLJM\rangle \tag{11}$$

where $M \in \{-J, -J+1, \ldots, J-1, J\}$, $s \in \{|s_1 - s_2|, |s_1 - s_2| + 1, \ldots, s_1 + s_2\}$, and m, either integer or half-integer as s, satisfies $|m| \leqslant \min(s, J)$. The peculiarity of this strange and unexpected basis lies in the fact that the matrix representing the operator $V_{t_1 t_2 l}(\boldsymbol{\Omega})$ in such a basis depends trivially on J. That is:

$$\langle J; \bar{s}_2 m_2 M_2 | V_{t_1 t_2 l} | J; \bar{s}_1 m_1 M_1 \rangle = \delta_{M_2 M_1} \{\bar{s}_2 m_2 | V_{t_1 t_2 l} | \bar{s}_1 m_1\} \tag{12}$$

with

$$\begin{aligned} \{\bar{s}_2 m_2 | V_{t_1 t_2 l} [\bar{s}_1 m_1\} &:= \delta_{m_2 m_1} (-1)^{l + \bar{s}_1 + 2\bar{s}_2 + m_1} (2\bar{s}_1 + 1)^{1/2} (2\bar{s}_2 + 1)^{1/2} f(s_1 s_2 t_1 t_2) \\ &\quad \times C(\bar{s}_1 \bar{s}_2 l; m_1 - m_1 0) X(s_1 s_2 \bar{s}_1 : s_1 s_2 \bar{s}_2 : t_1 t_2 l) \end{aligned} \tag{13}$$

$$\begin{aligned} f(s_1 s_2 t_1 t_2) &:= [(2s_1 + t_1 + 1)!(t_1!)^2 (2s_2 + t_2 + 1)!(t_2!)^2]^{1/2} \\ &\quad \times [(2s_1 - t_1)!(2t_1)!(2s_2 - t_2)!(2t_2)!]^{-1/2}. \end{aligned} \tag{14}$$

This essential independence of J will render straightforward the comparison between different $H_{J,M}$. The simplicity of L^2 in this basis is also helpful:

$$\langle J; \bar{s}_2 m_2 M_2 | L^2 | J; \bar{s}_1 m_1 M_1 \rangle = \delta_{M_2 M_1} \delta_{\bar{s}_1 \bar{s}_2} B(J, \bar{s}_1)_{m_2 m_1} \tag{15}$$

$$\begin{aligned} B(J, \bar{s}_1)_{m_2 m_1} &:= [J(J+1) + \bar{s}_1(\bar{s}_1 + 1) - 2m_1^2] \delta_{m_2 m_1} \\ &\quad + [(J - m_1)(J + m_1 + 1)(\bar{s}_1 - m_1)(\bar{s}_1 + m_1 + 1)]^{1/2} \delta_{m_2, m_1 + 1} \\ &\quad + [(J + m_1)(J - m_1 + 1)(\bar{s}_1 + m_1)(\bar{s}_1 - m_1 + 1)]^{1/2} \delta_{m_2, m_1 - 1}. \end{aligned} \tag{16}$$

With the previous notation we claim the following results.

Lemma 1. The matrices $B(J, \bar{s})$ (16) appearing in the representation of L^2 in the basis (11) of $\mathscr{H}_J$ are strictly increasing operator-valued functions of J for $J \geqslant s_1 + s_2$.

Proof. Note first that for $J \geqslant s_1 + s_2$ all these matrices are of the same order $(2\bar{s} + 1)$. We must prove that $\Delta(J, \bar{s}) := B(J+1, \bar{s}) - B(J, \bar{s}) > 0$. But it is easy to convince oneself that if a self-adjoint matrix A satisfies $A_{ii} > \Sigma_{j \neq i} |A_{ij}|$, $\forall i$, then $A > 0$. (Just take into account that if $|z_k| = \max\{|z_i|, \forall i\}$, then $\Sigma_{ij} z_i^* A_{ij} z_j \geqslant |z_k|^2 (A_{kk} - \Sigma_{i \neq k} |A_{ki}|)$.) In our case ($A :=$ Jacobi matrix $\Delta(J, \bar{s})$) it is quite simple to check the fulfillment of such inequalities. □

Lemma 2. Up to unitary equivalence, the partial Hamiltonians $J_{J,M}$ also increase strictly with J for $J \geqslant s_1 + s_2$.

Proof. Since all partial Hamiltonians with the same J are unitarily equivalent, it will suffice to prove the lemma for the subfamily $H_J := H_{J,j_{\min}}$. For $J_1, J_2 \geqslant s_1 + s_2$, define an isometric bijection $T(J_1 \to J_2) := \mathbb{1} \otimes t(J_1 \to J_2)$: $\mathcal{H}_{J_1, j_{\min}} \to \mathcal{H}_{J_2, j_{\min}}$ by the identity on the radial factor and such that $t(J_1 \to J_2)|J_1; smj_{\min}\rangle = |J_2; smj_{\min}\rangle$ (note that both dimensions $\mu_{J_1}(s_1, s_2)$, $\mu_{J_2}(s_1, s_2)$ of $\mathcal{H}_{J_1, j_{\min}}$ and $\mathcal{H}_{J_2, j_{\min}}$ equal $N(s_1, s_2)$). And now let $\bar{H}_J := T(J \to s_1 + s_2) H_J T(s_1 + s_2 \to J)$. We claim that $J_2 > J_1 \Rightarrow \bar{H}_{J_2} > \bar{H}_{J_1}$. In fact, remembering [3, 4] that $H = p_r^2 (:= -\partial^2/\partial r^2) + L^2 r^{-2} + V(r)$ for (1) and using (5), (12), (15), the expectation value of $\bar{H}_J$ in the state unit vector

$$\Phi := \sum_{sm} f_{sm}(r) |s_1 + s_2; smj_{\min}\rangle \in \mathcal{H}_{s_1+s_2, j_{\min}} \cap D(|H|^{1/2}) \tag{17}$$

is given by:

$$\langle \Phi | \bar{H}_J | \Phi \rangle = \langle \Phi | p_r^2 | \Phi \rangle + \langle \Phi | L^2 r^{-2} | \Phi \rangle + \langle | V | \Phi \rangle \tag{18}$$

with

$$\langle \Phi | p_r^2 | \Phi \rangle = \sum_{sm} \int_{\mathbb{R}^+} |\partial f_{sm}(r)/\partial r|^2 \, \mathrm{d}r \tag{19}$$

$$\langle \Phi | L^2 r^{-2} | \Phi \rangle = \sum_{s} \int_{\mathbb{R}^+} \langle f_s(r) | B(J, s) | f_s(r) \rangle r^{-2} \, \mathrm{d}r \tag{20}$$

$$\langle \Phi | V | \Phi \rangle = \sum_{t_1 t_2 l \bar{s}_2 \bar{s}_1 m} \int_{\mathbb{R}^+} f^*_{\bar{s}_2 m}(r) v_{t_1 t_2 l}(r) f_{\bar{s}_1 m}(r) \{\bar{s}_2 m | V_{t_1 t_2 l} | \bar{s}_1 m\} \, \mathrm{d}r. \tag{21}$$

By $f_s(r)$ we abbreviate in (20) the vector in $\mathbb{C}^{2s+1}$ with components $f_{sm}(r)$.

In view of lemma 1, and using (18)-(21), lemma 2 is now evident. □

Theorem. Let $E_g := \inf \sigma(H) \in \sigma_{\mathrm{disc}}(H)$, $\mathcal{H}_g := P_H(\{E_g\})\mathcal{H}$ be the ground energy and the associated eigensubspace for a quantum system consisting of two particles with spins s_1, s_2 interacting through a rotationally invariant potential matrix. Then $\mathcal{H}_g \subset \bigoplus_{J \leqslant s_1 + s_2} \mathcal{H}_J$, i.e. the maximum intrinsic total angular momentum J_g of this system in any of its ground states satisfies $J_g \leqslant s_1 + s_2$.

Proof. It is a clear consequence of lemma 2 that the lowest point $E_{0,J} := \inf \sigma(H | \mathcal{H}_J)$ in the spectrum of the restriction of H to $\mathcal{H}_J$ is a function strictly increasing with J for $J \geqslant s_1 + s_2$. And as $E_g = \inf_J E_{0,J}$, the conclusion plainly follows. □

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