Bases for the hydrogenic quadratic Zeeman effect

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A simple relationship between the two spherical bases $|n\lambda m\rangle$ and $|nlm\rangle$ is presented and is used to deduce the relative parity and the large-n behavior of the former. Approximate energy levels obtained in these bases from perturbation theory are compared with the eigenvalues obtained by diagonalizing the first-order perturbation matrix.

Motivated by the approximate symmetry[1,2] of the quadratic Zeeman effect, Labarthe[3] introduced the $|n\lambda m\rangle$ basis, where λ is associated with the operator $\Lambda=(A_x,A_y,L_z)$, and found them useful at low magnetic fields. Herrick[4] explored this approximate symmetry by utilizing the elliptic cylindrical coordinates on a sphere in four-dimensional momentum space and concluded that the $O(3)_\lambda$ symmetry is strong at all levels but breaks down for low value of m and λ. Zimmerman, Hulet, and Kleppner[5] made comparisons of the $|n\lambda m\rangle$ basis and the Clark basis[6] with their M basis by evaluating overlapping integrals. Their results revealed that the Labarthe and M bases provide better approximations to the exact eigenstates than the Clark basis. As a continuing effort in the study of quadratic Zeeman effect, we first present in this report a simple relationship between the $|n\lambda m\rangle$ and $|nlm\rangle$ bases in position space, from which their relative parity and large-n behavior can be deduced. We then compare the first-order Rayleigh-Shcrödinger expansion coefficient E_1 for the energy levels in these bases with the exact coefficient obtained from the degenerate perturbation theory by diagonalizing the first-order perturbation matrix.[7]

We begin by giving the following matrix elements of L^2 and A^2, which can be calculated in terms of the SO(4,2) generators in the oscillator representation:[8]

$$\langle N_1N_2m|A_x^2+A_y^2|N_1N_2m\rangle=\langle N_1N_2m|L_x^2+L_y^2|N_1N_2m\rangle=\tfrac{1}{2}(n^2-q^2-m^2-1)\ , \tag{1}$$

$$\langle N_1N_2m|A_z^2|N_1N_2m\rangle=q^2\ , \tag{2}$$

$$\langle N_1N_2m|L_z^2|N_1N_2m\rangle=m^2\ , \tag{3}$$

$$\begin{aligned}\langle N_1N_2m|A_x^2+A_y^2|N_1\pm 2N_2\mp 2m\rangle &= -\langle N_1N_2m|L_x^2+L_y^2|N_1\pm 2N_2\mp 2m\rangle\\ &=\tfrac{1}{2}[(N_1\pm 1)^2-m^2]^{1/2}[(N_2\mp 1)^2-m^2]^{1/2}\ ,\end{aligned} \tag{4}$$

where $n=n_1+n_2+|m|+1$, $N_1=2n_1+|m|+1=n+q$, $N_2=2n_2+|m|+1=n-q$, and $q=\frac{1}{2}(N_1-N_2)=n_1-n_2$. It is important to note in connection with the operator Λ^2 that the replacement of $L_x^2+L_y^2$ by $A_x^2+A_y^2$ changes the sign of the off-diagonal matrix elements but leaves the diagonal matrix elements invariant. Next we expand the two spherical bases in terms of the parabolic basis as follows:

$$|nlm\rangle=\sum_i a_{li}|Mq_i\rangle\ , \tag{5}$$

$$|n\lambda m\rangle=\sum_i a_{\lambda i}|Mq_i\rangle\ , \tag{6}$$

where a_{li} and $a_{\lambda i}$ are the Clebsch-Gordon coefficients, $|Mq\rangle=|n_1n_2m\rangle$ with $M=n-|m|$ and $q=n_1-n_2$. The sum in Eqs. (5) and (6) is taken over all possible values of $q_i=0,\pm 2,\pm 4,\ldots,\pm(M-1)$ for odd values of M and $q_i=\pm 1,\pm 3,\pm 5,\ldots,\pm(M-1)$ for even values of M. For given n and m, M is a constant and in each M manifold there are M states.[9] Using these expansions, we can write down the following matrix elements:

$$\langle nlm|L^2|nlm\rangle=l(l+1)=\sum a_{li}^2\langle Mq_i|L^2|Mq_i\rangle+\sum a_{li}a_{lj}\langle Mq_i|L^2|Mq_j\rangle\ , \tag{7}$$

$$\langle n\lambda m|\Lambda^2|n\lambda m\rangle=\lambda(\lambda+1)=\sum a_{\lambda i}^2\langle Mq_i|\Lambda^2|Mq_i\rangle+\sum a_{\lambda i}a_{\lambda j}\langle Mq_i|\Lambda^2|Mq_j\rangle\ , \tag{8}$$

where $q_j=q_i\pm 2$. The matrix elements in Eqs. (7) and (8) are those given in Eqs. (1)–(4), which indicate that the matrix elements in the second sum of these equations differ in sign only. It becomes evident by letting l and λ taken on the same numerical values that the coefficients are related as follows:

$$a_{\lambda i}=a_{li},\quad i=1,3,5,\ldots\ , \tag{9}$$

$$a_{\lambda i}=-a_{li},\quad i=2,4,6,\ldots\ . \tag{10}$$

Thus, we have established the simple relationship between the two spherical bases, namely, the signs of the their expansion coefficients in Eqs. (5) and (6) change alternately as the value of q_i goes from $-(M-1)$ to $+(M-1)$. As a consequence, the sign changes give rise to a mixing of states with l values differing by ± 2, which is the characteristic of the quadratic Zeeman effect. As examples, we give below the relationship explicitly for states in the $M=3$ and $M=4$ manifolds. For $M=3$,

$$|nn-3n-3\rangle_\lambda=(2n-3)^{-1}[|nn-3n-3\rangle+2(n-1)^{1/2}(n-2)^{1/2}|nn-1n-3\rangle]\ , \tag{11}$$

$$|nn-2n-3\rangle_\lambda=|nn-2n-3\rangle\ , \tag{12}$$

$$|nn-1n-3\rangle_\lambda=(2n-3)^{-1}[2(n-1)^{1/2}(n-2)^{1/2}|nn-3n-3\rangle+|nn-1n-3\rangle]\ , \tag{13}$$

and for $M=4$,

$$|nn-4n-4\rangle_\lambda=(2n-3)^{-1/2}(2n-5)^{-1/2}[3^{1/2}|nn-3n-4\rangle+2(n-1)^{1/2}(n-3)^{1/2}|nn-1n-4\rangle] , \quad (14)$$

$$|nn-3n-4\rangle_\lambda=(2n-3)^{-1/2}(2n-5)^{-1/2}[3^{1/2}|nn-4n-4\rangle+2(n-1)^{1/2}(n-3)^{1/2}|nn-2n-4\rangle] , \quad (15)$$

$$|nn-2n-4\rangle_\lambda=(2n-3)^{-1/2}(2n-5)^{-1/2}[2(n-1)^{1/2}(n-3)^{1/2}|nn-3n-4\rangle-3^{1/2}|nn-1n-4\rangle] , \quad (16)$$

$$|nn-1n-4\rangle_\lambda=(2n-3)^{-1/2}(2n-5)^{-1/2}[2(n-1)^{1/2}(n-3)^{1/2}|nn-4n-4\rangle-3^{1/2}|nn-2n-4\rangle] . \quad (17)$$

The above is valid for all values of $n\geq3$ or $n\geq4$ for $M=3$ or $M=4$, respectively. The results show that the parity remains the same for even values of M while the parity is reversed for odd values of M. It is also seen as is evident in the examples that the l mixing diminishes as n increases and as $n\rightarrow\infty$ the $|n\lambda m\rangle$ basis states tend to be hydrogenic with the order in l and the order in λ in the manifold reversed. This property is shared by the exact eigenstates that diagonalize the first-order perturbation matrix.[7] The Clark states, however, do not have this property. Their l-mixing remains significant as $n\rightarrow\infty$. This provides a plausible explanation for the reason why the Labarthe basis better approximates the exact eigenstates than the Clark basis as concluded in Ref. 5.

To compare the approximate energy levels, we compute the first Rayleigh-Schrödinger expansion coefficient E_1 for the energy. This is done by using the diagonal matrix elements, which are the expectation values of the perturbation, given by Gallas[10] and Herrick[11] and the first-order eigenvalues $\lambda^{(1)}$ for $M\leq4$ in Ref. 7 together with the relationship $E_1=n\lambda^{(1)}/8$. For $n=5$, $m=0$, and $M=5$ we solve the following secular equations for the eigenvalues.

Doublet:

$$\lambda^2-1520\lambda+385\,200=0 . \quad (18)$$

Triplet:

$$\lambda^3-2780\lambda^2+183\,960\lambda-273\,384\,000=0 . \quad (19)$$

The three sets of E_1 are given in Table I. It can be seen that for all singlet levels in the manifolds $M=1$ and $M=3$ the three approaches give identical results. In fact, it can be shown that for $M=1$, $l=\lambda=m=n-1$,

$$E_1=n^2(4n^4-7n^2-3n)/(4n^2-4n-3)=n\lambda^{(1)}/8 , \quad (20)$$

where[12]

$$\lambda^{(1)}=8n^2(n+1) , \quad (21)$$

and for $M=3$, $l=\lambda=n-2$, $m=n-3$,

$$E_1=n^2(4n^4-71n^2+135n-50)/(4n^2-12n+5)=n\lambda^{(1)}/8 , \quad (22)$$

where[13]

$$\lambda^{(1)}=8n(n+5)(n-2) . \quad (23)$$

In the case of the doublets in $M=2,3,4$ and the triplets in $M=5$, the order of l and the order of λ are reversed as mentioned earlier and the Labarthe basis gives remarkably good results for all values of M included in this report regardless of the values of m and λ. Except for the singlet levels, the $|nlm\rangle$ basis yields poor results[14] for small values of n. As n becomes large, say $n=20$, the results become equally good. This is consistent with the related facts that the quadratic perturbation can be scaled according to $1/n^4$ and as $n\rightarrow\infty$ the $|n\lambda m\rangle$ basis tends to be hydrogenic and the off-diagonal matrix elements in Eq. (4) becomes much smaller than the diagonal matrix elements in Eq. (1). This seems to suggest that the expectation values become almost identical because the wave functions become almost identical for highly excited states. For the singlet levels, the expectation values are identical because the wave functions are exactly identical.

We believe that the conclusions based upon our findings are valid in general for the quadratic Zeeman effect in hydrogen.

TABLE I. Comparisons of the first Rayleigh-Schrödinger expansion coefficient for the energy.

M	nlm	E_1	$n\lambda m$	E_1	Exact E_1
2	200	28	210	28	28
	210	12	200	12	12
1	211	24	211	24	24
3	300	138	320	156	157
	310	72	310	72	72
	320	60	300	42	41
2	311	144	321	144	144
	321	72	311	72	72
1	322	108	322	108	108
4	400	432	432	522	523
	410	240	420	304	309
	420	240	410	150	149
	430	176	400	112	107
3	411	406	431	499	500
	421	288	421	288	288
	431	192	411	173	172
2	422	432	432	432	432
	432	240	422	240	240
1	433	320	433	320	320
5	500	1050	540	1321	1173
	510	600	530	870	749
	520	643	520	529	427
	530	550	510	280	201
	540	407	500	250	131
4	511	1200	541	1286	1287
	521	771	531	840	845
	531	600	521	514	513
	541	429	511	360	355
3	522	1157	542	1179	1179
	532	750	532	750	750
	542	492	522	371	471
2	533	1000	543	1000	1000
	543	600	533	600	600
1	544	750	544	750	750
4	201 616	230 229	201 916	230 432	230 440
	201 716	199 038	201 816	199 234	199 243
	201 816	170 571	201 716	170 568	170 360
	201 916	144 162	201 616	143 565	143 958

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[9]The symbol $M = n - |m|$ is not related to the M basis of Ref. 5.
[10]Equation (9e) of J. A. C. Gallas, Phys. Rev. A **29**, 132 (1984).
[11]The diagonal matrix element in Eq. (17) of Ref. 4.
[12]Equation (3) is the second of Ref. 7.
[13]Equation (11) is the second of Ref. 7.
[14]The "remnant" degeneracy mentioned in Ref. 10 is perhaps of very rare occurrence. It can be shown more straightforwardly by using the expansion in Eq. (5) and the relevant matrix elements $M_{ij}^{(1)}$ in the second of Ref. 7 that the only case of remnant degeneracy in the manifolds $M = 2, 3, 4$ concerns the states $|410\rangle$ and $|420\rangle$ listed in the second column of Table I.