Supersymmetric Factorization for Rydberg Atoms in Parallel Electric and Magnetic Fields

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Some peculiarities of the energy diagram of Rydberg atoms in parallel electric and magnetic fields are interpreted by making use of a supersymmetric approach to these systems. The expression of the supercharge operator is given as a function of the generators of the SO(4) symmetry group. Some applications to analytical determinations of the spectrum and eigenfunctions are discussed and agree with previous experimental observations.

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The purpose of the present paper is to present evidence for an unexpected supersymmetric behavior in Rydberg atoms experiencing parallel magnetic and electric fields, in the limit where both the diamagnetic interaction and the linear Stark effect are small perturbations to the Coulomb field. Manifestations of such a property have been recently experimentally and numerically recorded in the lithium and hydrogen spectra, although the origin and consequences were elusive.[1,2]

Symmetry considerations have played an key role in the past years for understanding the physics of perturbed Rydberg systems in external fields, in particular, their diamagnetic and crossed-field behaviors.[3] They also led to the design of an efficient scheme for building atomic circular states[4,5] and to the definition of elliptic atomic states with appropriate semiclassical behavior.[6] Although the present investigations are based on the same concept, the one of symmetry group, our goal here is not to establish what the symmetries of a given system are, but rather to establish how they relate to the ones of seemingly different Hamiltonian systems. Bridging between the dynamical properties of two such different systems is the main concern of supersymmetry. More precisely, they share the same spectrum and their eigenstates are interrelated. Our purpose here is to use this supersymmetry formalism in its general sense and not in its high-energy context for bosons and fermions.

The Hamiltonian of a Rydberg atom in parallel electric and magnetic fields (along the z axis) is (in atomic units)

$$H=\frac{p^2}{2}-\frac{1}{r}+\frac{B}{2}L_z+\frac{B^2}{8}(x^2+y^2)+Fz\ ,$$

where B and F are measured respectively in units of $B_c=2.35\times10^5$ T and $F_c=5.14\times10^9$ V/cm. At low fields, when Bn^3 and $En^4\ll 1$, the energy levels are given by the restriction of H to a given n shell, which can be conveniently expressed as a function of the generators $(\mathbf{L},\mathbf{A})$ of the SO(4) symmetry group [$\mathbf{L}$ is the angular momentum, and $\mathbf{A}=n\{(\mathbf{p}\times\mathbf{L}-\mathbf{L}\times\mathbf{p})/2-\mathbf{r}/r\}$ the scaled Lenz vector; $\mathbf{L}^2+\mathbf{A}^2+1=n^2$]:

$$H_n=-\frac{1}{2n^2}+\frac{B}{2}L_z+\frac{B^2n^2}{16}W(\alpha)\ ,$$

where $W(\alpha)$ stands for[3]

$$W(\alpha)=n^2+3+L_z^2+4A^2-5A_z^2-2\sqrt{5}\alpha A_z\ , \qquad (1)$$

with $\alpha=12F/\sqrt{5}nB^2$ (a dimensionless parameter).[7] An alternate form of $W(\alpha)$ can be obtained by making use of the SO(3)⊗SO(3) description of SO(4), introducing the 3D angular momenta $\mathbf{j}_{1,2}=\frac{1}{2}(\mathbf{L}\mp\mathbf{A})$ such that $j_1=j_2=(n-1)/2$.[8] $L_z=j_{1z}+j_{2z}$ commutes with the effective Hamiltonian W which thus mixes $n-|M|$ ($L_z=M$) states among the n^2 degenerate ones of the shell. Being unessential, the paramagnetic term $BL_z/2$ is dropped in the following. Even in this low-field limit, the problem cannot be solved analytically.

Equation (1) can be cast under a supersymmetric form (or factorized) by introducing the supercharge operator Q:[9]

$$Q=cL_-+dA_-\ , \qquad (2)$$

where $\pm$ refers to the standard components of the vectorial operators. It fulfills the commutation relations

$$[L_z,Q]=-Q,\ \ [L_z,Q^\dagger]=Q^\dagger\ , \qquad (3)$$

which means that Q and $Q^\dagger$ are lowering and raising operators, respectively, for L_z, although they do not coincide with the ladder operators $L_\pm$ of the angular momentum $\mathbf{L}$ (see below).

By considering the supersymmetric partners $QQ^\dagger$ and $Q^\dagger Q$ and identifying with W, one obtains the solution $c=1$, $d=\sqrt{5}$, leading to[8]

$$W(\alpha)=Q^\dagger Q+2(L_z-1)(L_z-2)+2\sqrt{5}A_z(L_z-1-\alpha)\ , \qquad (4a)$$

$$W(\alpha)=QQ^\dagger+2(L_z+1)(L_z+2)+2\sqrt{5}A_z(L_z+1-\alpha)\ . \qquad (4b)$$

The operators W, $QQ^\dagger$, and $Q^\dagger Q$ commute with L_z. W and $Q^\dagger Q$ commute with each other when choosing $\alpha = L_z - 1$. They have then the same spectrum to within a constant.

Equation (4) indicates that, although the system is not supersymmetric, two different parallel-field situations can be associated with, respectively, $QQ^\dagger$ and $Q^\dagger Q$. These factorizations actually suggest that the action of the supercharge results in some connections between the angular momentum $L_z = M$ values and specific values of the field $\mathbf{F}$ in the parallel-field energy diagram. This can be established from the following operatorial identity:

$$W(\alpha)Q^{\dagger p} = Q^{\dagger p}[W(\alpha+p) - 4p^2 - 8pL_z] + 2\sqrt{5}pQ^{\dagger(p-1)}P^\dagger(L_z - \alpha)\,, \tag{5}$$

where

$$P^\dagger = [A_z, Q^\dagger] = A_+ + \sqrt{5}L_+\,, \quad [Q^\dagger, P^\dagger] = 0\,. \tag{6}$$

After projecting on a given $L_z = M$ subspace, Eq. (5) simplifies if one chooses field values such that $\alpha = M$. The substitution $k = M + p$ restores the quite symmetrical role played by M and k. In particular, k is an integer such that $0 \le M \le k \le n-1$. Finally, one obtains

$$W^k(\alpha = M)Q^{\dagger(k-M)} = Q^{\dagger(k-M)}\{W^M(\alpha = k) + 4M^2 - 4k^2\}\,. \tag{7}$$

Although this equation is not exactly of the supersymmetric style, the interpretation is similar. Let us introduce the spectrum $\{\epsilon^M(k)\}$ and eigenfunctions $\{|\Psi^M(k)\rangle\}$ of the Hamiltonian in parallel fields for $L_z = M$ and the field value $\alpha = k$. Then Eq. (7) implies that $Q^{\dagger(k-M)}|\Psi^M(k)\rangle$ is either (i) an eigenfunction of the same Hamiltonian for $L_z = k$ and a different electric field value $\alpha = M$, for the same energy (to within a constant term), that is,

$$\epsilon^k(\alpha = M) = \epsilon^M(\alpha = k) + 4(M^2 - k^2)\,;$$

or (ii) $Q^{\dagger(k-M)}|\Psi^M(\alpha = k)\rangle = 0$, which defines the states of $W^M(\alpha = k)$ having no supersymmetric partner in $W^k(\alpha = M)$. There are $k - M$ such states (which is the difference of the dimensions of W^k and W^M) which build a "ground-state ensemble" for the operation $Q^{\dagger(k-M)}$.

Equation (7) thus implies that the parallel-field energy diagram and wave functions have subtle interconnections, allowing one to deduce the spectrum and eigenfunctions by knowing only one of the supersymmetric conjugate situations ($L_z = M$, $\alpha = k$) or ($L_z = k$, $\alpha = M$). They are linked by the $Q^{\dagger(k-M)}$ operator which raises L_z by $k - M$ units and lowers α by the same amount. These "quantized" electric-field values and the angular momentum thus play the astounding role of conjugate variables as shown in Fig. 1.

Some consequences of Eq. (7) are even more striking,

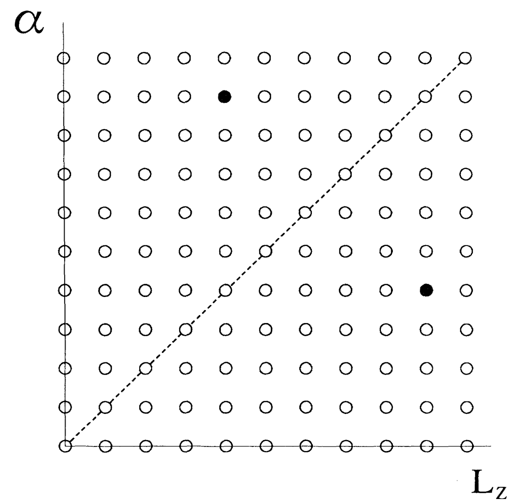

FIG. 1. Plot for $n = 11$ of the reduced electric-field (Ref. 7) values $\alpha = k$ vs the angular momentum $L_z = M$ for supersymmetric situations of the parallel-electric-and-magnetic-field energy diagram. This occurs only for integer values of α such that $0 \le k \le n-1$. Two conjugate situations (k,M) and (M,k) are shown (solid circles) for which the spectra are identical (to within a constant) and the wave functions are related by the $Q^{\dagger(k-M)}$ operator which raises L_z by $k - M$ units and lowers α by the same amount.

which can be demonstrated by considering the situation where $M = 0$. Hence,

$$W^k(\alpha = 0)Q^{\dagger k} = Q^{\dagger k}[W^0(\alpha = k) - 4k^2]\,, \tag{8}$$

which means that the parallel-field Hamiltonian for $\alpha = k$ and $M = 0$ is the supersymmetric partner of "atomic diamagnetism" (for zero electric field) for $L_z = k$. The latter situation is well known[10-13] and the spectrum displays a rovibrational organization with, at top, rotational states with almost perfect $\boldsymbol{\lambda}$ rotational symmetry and, at bottom, vibrational states with parabolic-type symmetry. These states (which only exist if $|M| < n/\sqrt{5}$) are almost degenerate in parity due to an exponentially-small-with-n tunneling through a barrier at the bottom of the band.[10] When adding a small electric field, this will result in quasilinear behavior of the energies of these quasidegenerate states as shown in Fig. 2, with small anticrossings at successive field values.

As remarked in Ref. 1, the amazing thing is that *all* the anticrossings take place, at the same successive field values, although the parameters of the states involved (electric dipole, zero-field level spacing, polarizabilities) do vary from one to another. The origin of this remarkable phenomenon lies in the parallel-field Hamiltonian being associated with a supersymmetric partner, namely, atomic diamagnetism. From the exponentially small parity degeneracy of the latter for $M = k$, the former should present the same character for $M = 0$ at a

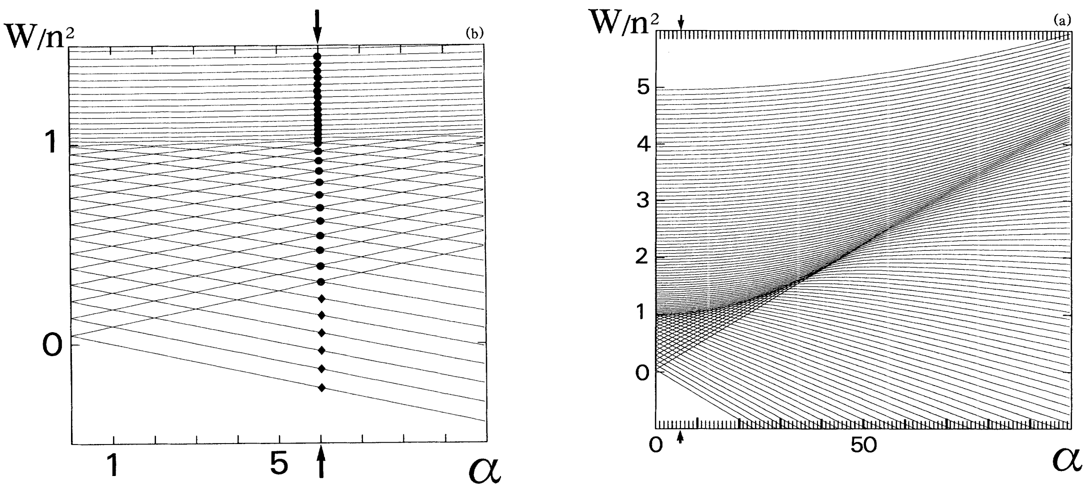

FIG. 2. (a) Energy diagram W/n^2 in parallel fields for $n=100$ and $L_z=0$ vs the reduced electric field α (Ref. 7). (b) Magnified view of anticrossing region. For the successive integer field values $\alpha=1,\ldots,k,\ldots n-1$, which are (exponentially) close to the anticrossing points when they exist, the spectrum is exactly the same as the one for atomic diamagnetism (to within a $4k^2$ shift) for the angular momentum $M=1,\ldots,k,\ldots n-1$, for the $n-k$ upper levels [shown as solid circles in (b) for $\alpha=k=6$]. The eigenfunctions are interconnected through the $Q^{\dagger k}$ operator. The k lowest levels [shown as rhombs in (b)] at the kth anticrossing act as a k-dimensional ground state with no supersymmetric pairing. Part of their properties can be deduced analytically.

specified $\alpha=k$ field value, with *exactly the same (exponentially small) spacings.* This implies that *all* the anticrossings take place "simultaneously" at the same field value $\alpha=k$, but to within exponentially small corrections.

Beyond these anticrossing aspects, the property is more generally valid for the rotational states and still holds true when $|M|>n/\sqrt{5}$. In Fig. 2, for $M=0$ the parallel-field spectrum at the kth "anticrossing" is exactly the same as the one for the diamagnetic interaction for $L_z=k$ (to within a constant shift) for the $n-k$ upper levels of the spectrum.

Finally this also leads to a relationship between the structure of the wave functions of the partner Hamiltonians,

$$|\Psi^k(\alpha=M)\rangle=Q^{\dagger(k-M)}|\Psi^M(\alpha=k)\rangle\,, \qquad (9)$$

which for $M=0$ implies that the whole set of eigenfunctions of atomic diamagnetism (whatever the $L_z=k$ value) is deduced by knowing the eigenfunctions in parallel fields for $M=0$ on a set of n integer values of the electric field. The levels at the bottom of the spectrum, which no longer experience an anticrossing, or more generally have no supersymmetric partner (see Fig. 2), have an eigenfunction which fulfulls

$$Q^{\dagger(k-M)}|\Psi^M(\alpha=k)\rangle=0\,. \qquad (10)$$

A limited exploration of the structure of these eigenfunctions can be done after rewriting the supercharge in a more convenient form (making use of, e.g., the Baker-Hausdorff formula):

$$Q=2e^{-\chi A_z}A_-e^{\chi A_z}\,, \qquad (11)$$

where $\chi=\ln[(1+\sqrt{5})/2]$ is the logarithm of the golden ratio. The Q and $Q^\dagger$ operators are thus related to the standard components (λ_+,λ_-) of the $\boldsymbol{\lambda}(A_x,A_y,L_z)$ angular momentum[14] operator through a nonunitary transformation. It follows from Eq. (10) that the $e^{-\chi A_z}|\Psi\rangle$ states are those which are annihilated by $k-M$ applications of the raising operator $\lambda_+=A_+=A_x+iA_y$ of the $\boldsymbol{\lambda}$ rotational basis.[14] Hence, the subspace of the $k-M$ eigensolutions $|\Psi^M(\alpha=k)\rangle$ is spanned by the nonorthonormal vectors $e^{\chi A_z}|n,\lambda,\lambda_z=M\rangle$ with $M\le\lambda\le k-1\le n-1$, which can be expanded on the parabolic basis[8] using appendix 1 of Ref. 14.

For $M=0$ and $k=1$ (the lowest level at the first anticrossing in Fig. 2), the (unnormalized) solution is oversimple in the parabolic basis:

$$|\Psi^0(\alpha=1)\rangle=\sum_{m=-j}^{m=j}\left(\frac{1+\sqrt{5}}{2}\right)^{2m}|jjm-m\rangle\,,$$

where the coefficients are powers of the golden ratio. Further use of Eq. (8) gives the energy $W^0(\alpha=1)=4$. More generally, if the dimension of the ground-state ensemble is 1 [hence $(k-M)=1$], its eigenfunction is $|\Psi^M(\alpha=M+1)\rangle=e^{\chi A_z}|n,\lambda=M,\lambda_z=M\rangle$ and the energy $W^M(\alpha=M+1)=4(2M+1)$.

To sum up, we have shown that the structure of Rydberg atoms in parallel electric and magnetic fields follows a somewhat unexpected rule very similar to supersymmetry. This allows the intertwining of the spectrum and eigenfunctions for situations in which the angular momentum L_z and the reduced electric field α are such that $(L_z=M, \alpha=k)$ and $(L_z=k, \alpha=M)$. Such a rule manifests itself in the characters of the experimental spectrum recorded on hydrogen and lithium and in numerical simulations.[1,2] It is also the origin of the early finding that the semiclassical integrals in the parallel-field problem are exactly the ones arising in the semiclassical theory of atomic diamagnetism.[1,15] Although the nature and implications of this property are still elusive, it raises new questions in the seemingly well understood situation of atomic diamagnetism at low field. For a given n, this problem is *separable* in momentum space, in the elliptic-cylindrical coordinates of $R(4)$:[10,16] How does this translate in the supersymmetric-conjugate parallel-field situation and is there any implications for the strong-field nonintegrability and chaotic behaviors in these systems?

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[8] The main advantage is that $\mathbf{j}_1$ and $\mathbf{j}_2$ commute with each other and fulfill the standard commutation relations of 3D angular momenta, while $(\mathbf{L},\mathbf{A})$ fulfill the one of SO(4). Another advantage is that the $|jjm_1m_2\rangle$ basis coincides with the parabolic basis, to within a phase factor.

[9] Actually, Q can be given the formal structure of a supercharge by adding a fictitious degree of freedom represented by the Pauli matrices. It then becomes $\hat{O}=Q\sigma^+$.

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