ATOMIC SUPERSYMMETRY

V. Alan Kostelecký

Physics Department, Indiana University
Bloomington, IN 47405, U.S.A.

Atomic supersymmetry is a quantum-mechanical supersymmetry connecting the properties of different atoms and ions. In this talk, I provide a short description of some established results in the subject and discuss a few recent developments, including the extension to parabolic coordinates and the calculation of Stark maps using supersymmetry-based models.

1. Introduction

It can often be impractical to find exact solutions to the equations determining the properties of a physical system. The identification and use of symmetries is one method that can be useful in the search for a mathematically simpler but physically sufficient description.

An example is provided by the behavior of the valence electron in alkali-metal atoms, which is governed in detail by the solution to an involved many-body problem. The essential physics of this situation can largely be contained in a single-electron model with an effective central potential [1]. This talk concerns symmetry issues involved in this approach, in particular, the role played by supersymmetry in a realistic central-potential approximation.

The first part of this talk (sections 2-5) provides some background and an overview of established results in atomic supersymmetry using spherical coordinates. The second part (sections 6-8) discusses recently developed extensions of these ideas to other coordinate systems and to the supersymmetry-based description of the Stark effect. More information on the approach used, its relation to other methods, and recent developments can be found in the references cited.

2. Supersymmetric Quantum Mechanics

A quantum-mechanical system is called supersymmetric [2] if its hamiltonian H commutes with N supersymmetry generators Q_j satisfying $\{Q_j, Q_k\} = \delta_{jk} H$. The superalgebra generated by H and Q_j is denoted sqm(N). Of interest here is the

special case sqm(2), for which it is convenient to consider the linear combination $Q = (Q_1 + iQ_2)/\sqrt{2}$ satisfying $H = \{Q, Q^\dagger\}$.

A simple representation of sqm(2) sets

$$Q = \begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix} \ , \qquad H = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix} \ , \tag{2.1}$$

where $A = -i\partial_x - iU'/2$ with $U' = dU/dx$ for some function $U = U(x)$. The components $H_\pm$ satisfy

$$H_\pm \Psi_{\pm n} \equiv \left[-\frac{d^2}{dx^2} + V_\pm(x) \right] \Psi_{\pm n} = \epsilon_n \Psi_{\pm n} \ , \tag{2.2}$$

where $V_\pm(x) = U'^2/4 \mp U''/2$.

If the supersymmetry is unbroken, the energy of the ground state is zero. The eigenspectra of $H_\pm$ are degenerate except for this state, which is associated with H_+. The spectra of H_+ and H_- are called, respectively, the bosonic and fermionic stacks. Degenerate states in the bosonic and fermionic stacks are mapped into one another by the supersymmetry generators $Q, Q^\dagger$.

3. Atomic Supersymmetry

The Schrödinger equation for the hydrogen atom separates in spherical polar coordinates. The radial piece can be written in atomic units as

$$\left[-\frac{d^2}{dy^2} - \frac{1}{y} + \frac{l(l+1)}{y^2} - \frac{1}{2}E_n \right] \chi_{nl}(y) = 0 \ , \tag{3.1}$$

where $y = 2r$, $E_n = -1/2n^2$, and $\chi_{nl}(2r) = rR_{nl}(r)$. The radial wave functions are

$$R_{nl}(r) = \frac{2}{n^2} \left[\frac{\Gamma(n-l)}{\Gamma(n+l+1)} \right]^{\frac{1}{2}} \left(\frac{2r}{n} \right)^l \exp\left(-\frac{r}{n} \right) L_{n-l-1}^{(2l+1)}\left(\frac{2r}{n} \right) \ , \tag{3.2}$$

where the Sonine-Laguerre polynomials are defined by

$$L_n^{(\alpha)}(x) = \sum_{p=0}^{n} (-x)^p \frac{\Gamma(n+\alpha+1)}{p!\,(n-p)!\,\Gamma(p+\alpha+1)} \ . \tag{3.3}$$

The idea is to identify the radial equation (3.1) for fixed l with the hamiltonian H_+ of a supersymmetric quantum mechanics, as in Eq. (2.2). One can then

construct the supersymmetry generator Q, determine H_-, and seek a physical interpretation [3].

The supersymmetry is determined by specifying the function U. For the Coulomb problem, it is $U(y) = y/(l+1) - 2(l+1)\ln y$. The partner hamiltonian H_- can be shown to have the same form as H_+ except that l is replaced with $(l+1)$ in the $1/y^2$ term. This means that the eigenfunctions of H_- at fixed l are $R_{n,l+1}$ with $n \geq 2$. These form a complete and orthonormal set.

To understand the physical interpretation, recall that H_- has the same spectrum as H_+, excluding the lowest state. This suggests H_- describes a physical system that looks hydrogenic except that the ground state is inaccessible. The idea is to attribute this to the Pauli principle. The partner system is then an atom with the lowest state filled with electrons, and H_- is an effective hamiltonian for the valence electron. For example, if $l = 0$ the spectrum of H_+ spans the s orbitals of hydrogen and the spectrum of H_- represents the s orbitals accessible to the valence electron in lithium. Evidently, the supersymmetry holds only if the non-hydrogenic electron interactions are disregarded. The incorporation of these symmetry-breaking effects is described in section 5.

In the exact-symmetry limit, the supersymmetry can be extended. For example, the s orbitals of lithium and sodium can also be viewed as supersymmetric partners. There are supersymmetric connections of this sort among atoms and ions across the periodic table, all physically incorporating the effects of the Pauli principle and mathematically implemented by integer shifts in the angular quantum number l.

Ref. [3] presents more details of the construction and discusses the experimental support for this atomic supersymmetry.

4. Oscillator Formulation

The oscillator formulation of atomic supersymmetry outlined in section 3 is closely related to harmonic oscillators. Indeed, connections exist in arbitrary dimensions among the radial equations for the Coulomb problem, the harmonic oscillator, and the two sqm(2) supersymmetric partners of these systems [4].

The radial equation for the d-dimensional Coulomb problem can be written in atomic units as

$$\left[-\frac{d^2}{dy^2} - \frac{1}{y} + \frac{(l+\gamma)(l+\gamma+1)}{y^2} - \frac{1}{2}E_{dn}\right]v_{dnl}(y) = 0 \ , \tag{4.1}$$

where $y = 2r$, $E_{dn} = -1/2(n+\gamma)^2$, $\gamma = (d-3)/2$, and the radial wave functions are

$$v_{dnl}(y) = c_{dnl}\, y^{l+\gamma+1} \exp\bigl(-y/2(n+\gamma)\bigr) L_{n-l-1}^{(2l+2\gamma+1)}\bigl(y/(n+\gamma)\bigr) \ , \tag{4.2}$$

with c_{dnl} a normalization constant. If the operator in Eq. (4.1) is interpreted as H_+ in an sqm(2) supersymmetry, the partner H_- can be shown to have the same form but with l replaced by $l + 1$.

The radial equation for the D-dimensional harmonic oscillator with unit angular frequency in atomic units is

$$\left[-\frac{d^2}{dY^2} - \frac{1}{Y} + \frac{(L+\Gamma)(L+\Gamma+1)}{Y^2} - E_{DN}\right]V_{DNL}(Y) = 0 \ , \qquad (4.3)$$

where Y is the radial variable, $E_{DN} = 2N + 2\Gamma + 3$, $\Gamma = (D-3)/2$, and the radial wave functions are

$$V_{DNL}(Y) = C_{DNL} \ Y^{L+\Gamma+1} \exp(-Y^2/2) L_{N/2-L/2}^{(L+\Gamma+1/2)}(Y^2) \ , \qquad (4.4)$$

where C_{DNL} is a normalization constant. The sqm(2) partner H_- to the operator H_+ in Eq. (4.3) again has the same form but with L replaced by $L + 1$.

A state in the d-dimensional Coulomb problem can be related by a one-parameter mapping to a state in a D-dimensional oscillator [4]. The eigenfunctions v_{dnl} and V_{DNL} are related by $v_{dnl}((n+\gamma)Y^2) \propto Y^{1/2}V_{DNL}(Y)$ with $N = 2n-2+\lambda$, $L = 2l+\lambda$, and even $D = 2d-2-2\lambda$. The parameter λ is an integer. Restrictions on the possible choices of the parameter, the dimensionality, and the quantum numbers can arise if several Coulomb-problem states from one system are required to be mapped to a specified harmonic oscillator. The map can be combined with the supersymmetric maps shifting the angular quantum numbers, resulting in a commutative diagram between states of the four systems. The reader is referred to [4] for further details.

5. Supersymmetry-Based Quantum-Defect Theory

The energy eigenvalues of the valence electron in an alkali-metal atom are shifted relative to the hydrogenic values by interactions with the core. The eigenvalues can be expressed as the Rydberg series [5] $E_{n^*} = -1/2n^{*2}$ with $n^* = n - \delta(n, l)$, where for given l the quantum defect $\delta(n, l)$ rapidly approaches an asymptotic value $\delta(l)$ as n increases. These shifts break the supersymmetries described in section 3.

Despite this, it is possible to develop a central-potential model incorporating supersymmetric features that has analytical wavefunctions as solutions and eigenenergies given by the Rydberg series [6]. The theory is defined by a radial equation obtained from Eq. (3.1) by replacing n, l, E_n with n^*, l^*, E_{n^*}. Here, l^* is a new angular quantum number given by $l^* = l - \delta(l) + I(l)$, where $I(l)$ is an integer shift characteristic of supersymmetry. The eigenfunctions are given by

the replacement of n and l in Eq. (3.2) with n^* and l^*. The Sonine-Laguerre polynomials still appear because $n^* - l^* - 1 = n - l - I(l) - 1$ remains an integer. For asymptotic quantum defects $\delta(l)$, these eigenfunctions form an orthonormal and complete set.

Ref. [6] contains more details about this model and demonstrates that the analytical eigenfunctions yield transition probabilities that are in agreement with experiment and with accepted values [7]. Related developments, other than those to be discussed in the remainder of this paper, include the following.

- The eigenfunctions of the model have been used as trial wavefunctions for detailed atomic calculations [8].

- The validity of the theory at short distances has been examined by investigating predictions for the fine structure of alkali-metal atoms [9]. Certain key features observed experimentally are reproduced and the Landé semiempirical formula naturally appears in the model.

- The model has been used to examine transition probabilities for other atoms, notably alkaline-earth ions [10].

- The mathematical structure of the model has been shown to be connected with parastatistics [11].

6. Separable-Coordinate Supersymmetries

The Schrödinger equation with a Coulomb potential $V(r) = -1/r$ separates directly (no modulation factor) in four different coordinate systems: spherical, conical, prolate-spheroidal, and parabolic. Each separation results in three ordinary differential equations, so *a priori* there are twelve candidate equations for the role of a supersymmetric partner hamiltonian in an sqm(2) realization. However, additional constraints arise from the structure of Eq. (2.2): to play the role of H_+, an equation must be expressed in the appropriate form and the eigenspectrum must involve a tower of states labeled by the appropriate eigenvalue. Some results of an examination of possible sqm(2) supersymmetries involving the twelve candidate equations are described in this section. More details are provided in ref. [12].

First, consider spherical coordinates. The eigenfunctions for the Coulomb problem separate into a product of radial wave functions given in Eq. (3.2) and the spherical harmonics, which in turn decompose into products of associated Legendre functions and exponentials. As discussed in section 3, the radial equation does admit a supersymmetric partner. The equation for the associated Legendre functions can be rewritten in the form of Eq. (2.2) by admitting a modulation factor, but the ensuing equation lacks an eigenvalue representing an infinite tower

447

of states. The remaining azimuthal equation is uninteresting because it has zero potential. Therefore, the only interesting sqm(2) supersymmetry in spherical coordinates appears in the radial equation.

In conical coordinates, the coordinate surfaces are spheres and cones of elliptic cross section along the z and x axes. One coordinate is just the radial variable, and the eigenfunctions for hydrogen are products of Lamé functions with the same radial wavefunctions as in spherical coordinates. The radial equation has the supersymmetry described in section 3 and the same physical interpretation applies, although the complete eigenfunctions for the supersymmetric partner states involve Lamé functions rather than the spherical harmonics. Each of the other two separated equations can be rewritten without a linear derivative term as in Eq. (2.2), but no interesting supersymmetry exists.

The Schrödinger equation for the Coulomb problem also separates in prolate-spheroidal coordinates. It can be shown that none of the three resulting equations admits an interesting sqm(2) structure.

Finally, consider parabolic coordinates. These are defined by $\rho = r + z$, $\sigma = r - z$, $\phi = \tan^{-1}(y/x)$, where r is the radial coordinate. The hydrogen eigenfunctions in parabolic coordinates can be written as the product $u(\rho)v(\sigma)\Phi(\phi)$. The equation determining $\Phi(\phi)$ is uninteresting in the present context. The equation for $u(\rho)$ can be expressed in the form of an H_+ by extracting a modulation factor $u(\rho) = \rho^{-1/2}\chi_1(\rho)$. The ensuing equation for χ_1 is

$$\left[\frac{d^2}{d\rho^2} + \frac{1-m^2}{4\rho^2} + \frac{Z_1}{\rho} + \frac{E}{2}\right]\chi_1(\rho) = 0, \tag{6.1}$$

where E is the energy and m is the magnetic quantum number. A similar analysis can be carried out for $v(\sigma)$, resulting in an identical equation but with χ_1, ρ, and Z_1 replaced by χ_2, σ, and Z_2. The separation constants Z_1 and Z_2 are required to satisfy $Z_1 + Z_2 = 1$. The eigensolutions have the form

$$u_{n_1 n_2 m}(\rho) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}}\varepsilon^{\frac{m}{2}+1}\left[\frac{\Gamma(n_1+1)}{\Gamma(n_1+m+1)}\right]^{\frac{1}{2}}e^{-\frac{\varepsilon}{2}\rho}\rho^{\frac{1}{2}m}L_{n_1}^{(m)}(\varepsilon\rho), \tag{6.2}$$

with a similar expression for $v_{n_1 n_2 m}(\sigma)$. Here, $n_1 = Z_1/\varepsilon - (m+1)/2$, $n_2 = Z_2/\varepsilon - (m+1)/2$ are nonnegative integers, and $\varepsilon = \sqrt{-2E}$ for $E_n = -1/2n^2$ with $n = n_1 + n_2 + m + 1$.

The equations for χ_1, χ_2 admit supersymmetric partners. The functions $U(\rho)$, $U(\sigma)$ determining the supersymmetry are $U(\rho) = 2Z_1\rho/(m+1) - (m+1)\ln\rho$ and $U(\sigma) = 2Z_2\sigma/(m+1) - (m+1)\ln\sigma$. Ref. [12] shows that the superpartner equations and eigensolutions have the same form as Eqs. (6.1), (6.2) and their analogues for the σ coordinate, but with the replacements $n_1 \to n_1 - 1$, $n_2 \to$

$n_2 - 1$, $m \to m + 2$. The supersymmetry leaves invariant the principal quantum number n, as needed for a mapping between degenerate states.

The basic approach to a physical interpretation is analogous to the spherical-coordinate case but the existence of two supersymmetries permits more possibilities. Only two (natural) cases are mentioned here; see ref. [12] for more details.

The valence-electron states for light alkali-metal atoms can be labeled using a spectroscopic notation based on the parabolic quantum numbers n_1, n_2, m. For convenience, the lowest- and highest-energy sublevels in a manifold of states with fixed $m \geq 0$ are called the red and blue levels, respectively. It turns out that a natural choice for the bosonic stack is the set of all blue states of hydrogen. Interpreting the absence of a fermionic-stack partner for the ground state as a consequence of the Pauli principle and treating electron-electron interactions as supersymmetry-breaking effects, the blue lines of hydrogen can be shown to be partnered by the blue lines of lithium. A similar construction can be made for the red lines of hydrogen and lithium. These supersymmetries extend to other alkali-metal atoms in a manner analogous to the spherical-coordinate case.

7. Quantum-Defect Theory in Parabolic Coordinates

The interactions breaking the supersymmetries in parabolic coordinates can be incorporated using notions from quantum-defect theory. For this case, the asymptotic quantum defects δ entering the Rydberg expression for the eigenenergies depend on the two parabolic quantum numbers n_1 and m. It can be shown that an effective potential exists for the two-dimensional separated equation in ρ and σ that has analytical eigenfunctions of the same form as in section 6 with the Rydberg series as eigenvalues, while incorporating the integer shifts characteristic of supersymmetry [12].

In separated form, the model is specified by

$$\left[\frac{d^2}{d\rho^2} + \frac{1 - m_1^{*2}}{4\rho^2} + \frac{Z_1^*}{\rho} + \frac{E^*}{2}\right]\chi_1^*(\rho) = 0 \tag{7.1}$$

and a similar expression for the equation in σ with subscripts 1 replaced by subscripts 2. The functions $\chi_1^*(\rho)$ play a role analogous to $\chi_1(\rho)$ in section 6, and the separation constants Z_1^* and Z_2^* satisfy $Z_1^* + Z_2^* = 1$.

Solutions to these equations exist only if $n_1^* = Z_1^*/\sqrt{-2E^*} - (m_1^* + 1)/2$ and $n_2^* = Z_2^*/\sqrt{-2E^*} - (m_2^* + 1)/2$ are nonnegative integers. Note that $n^* \equiv n - \delta = n_1^* + n_2^* + (m_1^* + m_2^*)/2 + 1$. The wavefunctions are

$$u_{n_1^* n_2^* m_1^* m_2^*}(\rho) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}}(n^*)^{-(\frac{m_1^*}{2}+1)}\left[\frac{\Gamma(n_1^* + 1)}{\Gamma(n_1^* + m_1^* + 1)}\right]^{\frac{1}{2}}e^{-\frac{\rho}{2n^*}}\rho^{\frac{1}{2}m_1^*}L_{n_1^*}^{(m_1^*)}\left(\frac{\rho}{n^*}\right),$$
$$\tag{7.2}$$

with an analogous result for the σ-dependent equation. It can be shown that these model wavefunctions are not fully orthogonal for physical values of the asymptotic quantum defect, although the off-diagonal matrix elements are numerically small.

The four quantum numbers that appear depend on the parabolic quantum numbers, the quantum defect, and the supersymmetry integers. Define $n_1^* = n_1 - I_1$, $n_2^* = n_2 - I_2$, where I_1 and I_2 are integers, and $m_1^* = m + \alpha_1$, $m_2^* = m + \alpha_2$, with the constraint $\alpha_1 + \alpha_2 = 2I_1 + 2I_2 - 2\delta$. If δ is set to zero, the constraint reduces the four variables I_1, I_2, α_1, α_2 to three and the exact supersymmetry limit of section 6 can be recovered.

8. The Stark Effect

In an external electric field of strength F, the energy levels of the valence electron in an alkali-metal atom are shifted by amounts depending on F. A plot of the eigenenergies as a function of F is called a Stark map. An exact theoretical treatment for Stark maps of alkali-metal atoms is impractical. However, numerical approximation methods yield Stark maps in good agreement with experiment [13].

The analytical eigenfunctions obtained from supersymmetry-based quantum-defect theories in parabolic and spherical coordinates provide another approach to obtaining Stark maps [12]. In parabolic coordinates, the nonorthogonality of the eigenfunctions is a barrier to exact analysis. One possible approximation is to neglect the small off-diagonal components of the zero-field energies. This calculation yields Stark maps with curves that are largely linear, in disagreement with experimental results.

This difficulty is absent in spherical coordinates. The zero-field wavefunctions of the model described in section 5 can be used to calculate Stark matrix elements, and the ensuing energy matrix can be diagonalized for a subset of the perturbation basis. Ref. [12] contains detailed results for the $n = 15$ Stark states of lithium and sodium for $m = 0$ and $m = 1$, evaluated over the ranges used in ref. [13] for the energies and electric field strengths. The non-hydrogenic structure is clearly reproduced, demonstrating the expected sizable anticrossings and small-field quadratic Stark effects for the s and p levels. All the Stark maps generated for the $n = 15$ lines of lithium and sodium by the supersymmetry-based theory are indistinguishable from the numerical and experimental results of ref. [13].

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