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Supersymmetry in atomic physics and the radial problem

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Abstract. A correct procedure for constructing supersymmetry in three dimensions is presented. The degeneracies are found between states of the same l but different n and Z and the previous results on the Coulomb and the three-dimensional isotropic oscillator problems are reestablished. We also consider the hydrogen-helium problem and find supersymmetry to hold to a good approximation.

1. Introduction

The study of supersymmetric quantum mechanics has evinced [1-5] a lot of interest of late. As is well known [6], the theory of supersymmetry (SUSY) relates integral spins to half-integral spins and all the essential features of it are contained in field theories of $(1+0)$ dimensions, i.e. supersymmetric quantum mechanics. In fact, SUSY has been found to give encouraging results towards understanding degeneracies in atoms and establishing interesting atomic connections.

Mathematically, a one-dimensional Hamiltonian

$$H = \begin{pmatrix} H_- & 0 \\ 0 & H_+ \end{pmatrix} \tag{1}$$

is supersymmetric if the corresponding potentials satisfy

$$V_\pm = \tfrac{1}{8}U'^2 \mp \tfrac{1}{4}U'' \tag{2}$$

where the primes denote derivatives with respect to the variable x and $U(x)$ is related to the ground-state wavefunction $\psi_0(x)$ as

$$U = -2 \log \psi_0(x). \tag{3}$$

The above relation implies that no nodes are associated [3] with the ground-state wavefunction, $U(x)$ being a real function of x.

It is easy to establish (2) if we note that ψ_0 satisfies

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right)\psi_0 = E_0\psi_0 \tag{4}$$

where $V(x)$ is the potential associated with the Hamiltonian H. We thus have

$$V - E_0 = \tfrac{1}{8}U'^2 - \tfrac{1}{4}U'' \tag{5a}$$

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and as a result

$$V_+ = V - E_0 \qquad V_- = V - E_0 + \tfrac{1}{2}U''. \tag{5b}$$

These are same as (2). Thus the lowest state of V_+ lies at zero energy, the negative sign in (3) ensuring that U'' remains positive.

Given a connecting potential U, a supersymmetric Hamiltonian H may be set up as follows:

$$H = \tfrac{1}{2}(Q\bar{Q} + \bar{Q}Q) = \tfrac{1}{2}(p^2 + \tfrac{1}{4}U'^2)I + \tfrac{1}{4}U''\sigma_Z \tag{6a}$$

where Q and $\bar{Q}$ are defined as

$$Q \equiv (p - \mathrm{i}\tfrac{1}{2}U')\sigma^+ \qquad \bar{Q} \equiv (p + \mathrm{i}\tfrac{1}{2}U')\sigma^- \tag{6b}$$

with $\{\sigma^-, \sigma^+\} = 1$, $[\sigma^+, \sigma^-] = \sigma_Z$. The supersymmetric generators $(Q, \bar{Q})$ obey the algebra

$$\begin{aligned} &[Q, H] = [\bar{Q}, H] = 0 \\ &\{\bar{Q}, \bar{Q}\} = \{Q, Q\} = 0 \\ &\{\bar{Q}, Q\} = 2H. \end{aligned} \tag{7}$$

Explicitly, one may construct $(Q, \bar{Q})$ on the 2×2 matrix space of $H_+ = \frac{1}{2}\bar{Q}Q$ and $H_- = \frac{1}{2}Q\bar{Q}$ and it may be easily seen that, except for the lowest eigenvalue of H_+, those of H_+ and H_- coincide, thereby constituting a supersymmetric spectrum. Furthermore, if one expresses H_+ and H_- in terms of the creation and annihilation operators, the bosons and fermions correspond to H_+ and H_-, respectively.

The above gives very briefly the basic steps in constructing a supersymmetric Hamiltonian for any one-dimensional quantum mechanical system whose ground-state energy and wavefunction are known. As an example, one may consider [1] the case of the one-dimensional harmonic oscillator.

To formulate SUSY in three dimensions, one may subject the radial part of the Schrödinger equation to a one-dimensional construction of SUSY. In fact, this is how Kostelecky and Nieto (KN) [2, 4] have proposed a supersymmetric construction of the hydrogen atom. They have found the spectrum of V_+ and V_- to describe the hydrogenic ns–np degeneracy and have thus interpreted their results as giving a supersymmetric connection between various atoms.

However, a non-trivial aspect of the interpretation of SUSY for the radial problem has recently been pointed [3] out by Haymaker and Rau (HR). They have argued that the radial equation being defined in the region $0 < r < \infty$ is not a truly one-dimensional problem. As such, the SUSY construction developed for the one-dimensional problem is not formally applicable to such radial problems. As a counter-example, they have pointed out the isotropic oscillator problem whose energy eigenvalues are separated by jumps of two units of 1. The standard one-dimensional approach would only establish degeneracies between partner states with l and $l+1$, respectively.

HR have advocated a transformation of the half-line problem to a full-line $(-\infty, \infty)$ one through a transformation of the type $x = \ln y$ thereby passing from the radial to the Morse problem. In this paper we would like to take up the three-dimensional problem and establish a procedure for constructing the relevant SUSY transformations. In fact, the approach of HR is beset with some difficulties, the chief being that the connecting potential turns out to be n dependent.

2. Supersymmetry in three dimensions

2.1. The model of KN

It is well known [7] that for a spherically symmetric potential, the Schrödinger equation in three dimensions separates into an angular and a radial part. The solution of the former is in the standard form of spherical harmonics and does not play any significant role in our discussion. The radial equation, being a single-variable equation, may be subjected to a one-dimensional construction of SUSY.

To this end, let us examine the standard one-dimensional approach by setting up a supersymmetric scheme of the Coulomb problem. We follow the approach [2] of KN as analysed [3] by HR.

The radial equation of the Coulomb problem is

$$\left(-\frac{1}{2}\frac{d^2}{dy^2}-E_n-\frac{1}{y}+\frac{l(l+1)}{2y^2}\right)\chi_{nl}(y)=0 \tag{8}$$

where $n \geqslant l+1$ and $\chi_{nl}(0)=0$, $E_n=-1/2n^2$, $y=\frac{1}{2}mZe^2$.

To find the connecting potential $U(y)$, we then solve (2) for a fixed value of l. Thus

$$\tfrac{1}{8}U'^2-\tfrac{1}{4}U''=-E_0-\frac{1}{y}+\frac{l(l+1)}{2y^2} \tag{9}$$

where the primes now denote derivatives with respect to the variable y. By inspection, the solution of this equation can be found to be

$$U(y)=\frac{2y}{l+1}-2(l+1)\ln y. \tag{10}$$

It may be remarked that $U(y)$ is independent of n which is as it should be. Relation (10) gives V_+ as

$$V_+=-\frac{1}{y}+\frac{1}{2(l+1)^2}+\frac{l(l+1)}{2y^2} \tag{11a}$$

which defines a series of Bohr levels with n starting from $l+1$, i.e. $n \geqslant l+1$ and energies $\frac{1}{2}[(l+1)^{-2}-n^{-2}]$.

Given V_+, its SUSY partner V_- can be constructed using (5b). V_- is found to be

$$V_-=-\frac{1}{y}+\frac{1}{2(l+1)^2}+\frac{(l+1)(l+2)}{2y^2}. \tag{11b}$$

However, for V_- the lowest state of Bohr levels begins from $n=l+2$, i.e. $n \geqslant l+2$.

Thus the spectrum of V_+ and V_- can be used to give a supersymmetric interpretation of the well known hydrogenic ns–np degeneracy. To see this point more clearly, we may set $l=0$. Then V_+ describes the ns states with $n \geqslant 1$ while V_- corresponds to np levels with $n \geqslant 2$.

In this way, KN were led to formulate a supersymmetric connection between atoms in three dimensions. It is not out of place to mention that this formalism establishes degeneracies between states of same n but different l.

As is obvious from (2), in order to obtain the connecting potential $U(y)$, one is required [8] to solve a second-order differential equation which is of Riccati form. As such, (2) is solvable only for some particular forms of the potential. Besides the

Coulomb potential, the radial equation also turns out to be solvable for the isotropic oscillator case. In the following we apply the approach of KN to this problem.

The radial equation for the isotropic oscillator is

$$\left(-\frac{1}{2}\frac{d^2}{dy^2}+\tfrac{1}{2}y^2+\frac{l(l+1)}{2y^2}-E_n\right)\chi_n(y)=0 \tag{12}$$

where $n=l, l+2, l+4, \ldots$, and $E_n=n+\frac{3}{2}$, $y=(m\omega/\hbar)^{1/2}r$.

Proceeding as before, the connecting potential $U(y)$ may be found easily. $U(y)$ turns out to be

$$U(y)=y^2-2(l+1)\ln y \tag{13}$$

and the corresponding supersymmetric partner potentials $V_\pm$ are

$$V_+=\tfrac{1}{2}y^2+\frac{l(l+1)}{2y^2}-(l+\tfrac{3}{2}) \tag{14a}$$

$$V_-=\tfrac{1}{2}y^2+\frac{(l+1)(l+2)}{2y^2}-(l+\tfrac{1}{2}). \tag{14b}$$

As in the Coulomb case, here we find a degeneracy of partner states with l and $l+1$. However, in contrast to the Coulomb problem, the energy levels of the isotropic oscillator are separated by two units.

Thus the isotropic oscillator problem serves as a good counter-example to show that a straightforward one-dimensional approach does not always work towards establishing the correct supersymmetric connection between energy levels.

In the next subsection we go on to describe the scheme of HR which does seem to avoid the difficulties of the naive one-dimensional approach. As we shall see, a connection between isoelectronic ions emerges quite naturally, in contrast to those between states of different atoms.

2.2. The model of HR

The model [3] of HR rests on a very pertinent observation that a radial equation being defined only on a half line $(0,\infty)$ is not a true one-dimensional problem. To apply the supersymmetric construction procedure developed for the one-dimensional problems, the prescription of these authors is to go the full line $(-\infty,\infty)$ through a transformation of the type $x=\ln y$. From the transformed equation one could construct the V_-. The equation for V_-, when transformed back to the half line, ought to give the correct supersymmetric partner equation to (8) or (12).

Consider the Coulomb case. Using $x=\ln y$, the radial equation (8) for the Coulomb problem takes the form

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}-E_n\,e^{2x}-e^x+\tfrac{1}{2}(l+\tfrac{1}{2})^2\right)\phi(x)=0. \tag{15}$$

One can again solve for $U(x)$ to obtain

$$U(x)=2e^x/n+(1-2n)x. \tag{16}$$

Note that in this approach $U(x)$ becomes n dependent. From (16), the supersymmetric partner potentials can be found easily. These are

$$V_+=e^{2x}/2n^2-e^x+\tfrac{1}{2}(\tfrac{1}{2}-n)^2 \tag{17a}$$

$$V_-=e^{2x}/2n^2-(1-1/n)\,e^x+\tfrac{1}{2}(\tfrac{1}{2}-n)^2. \tag{17b}$$

After such a construction with the true one-dimensional variable x, one should not transform (17*b*) back to the original variable y to get the correct supersymmetric partner equation to (8). In terms of y, we obtain

$$\left[-\frac{1}{2}\frac{d^2}{dy^2}+\frac{1}{2n^2}-\left(1-\frac{1}{n}\right)\frac{1}{y}+\frac{l(l+1)}{2y^2}\right]\chi_{nl}(y)=0. \tag{18}$$

This equation is identical to (8) except for the coefficient of the $1/y$ term. However, if we divide (18) by $(1-1/n)^2$, then redefine $(1-1/n)y$ as the running variable y and absorb the $(1-1/n)$ factor into the definition of the nuclear charge Z, we find that (18) describes states with quantum numbers l and $n-1$ and charge $Z(1-1/n)$. Thus comparing (18) with (8) we find that the degeneracy arises (note that both (8) and (18) have the same eigenenergy) between states of the same l but different n and Z.

Thus the procedures of KN and HR lead to two different types of degeneracies for the Coulomb problem. However, as we shall presently see, the method of HR does enable one to explain the degeneracy of the isotropic oscillator if properly applied.

Let us transform (12) to the full line through a transformation $x=2\ln y$. We obtain

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\tfrac{1}{8}e^{2x}-\tfrac{1}{4}E_n\,e^{x}+\tfrac{1}{8}(l+\tfrac{1}{2})^2\right)\phi(x)=0. \tag{19}$$

This gives a connecting potential $U(x)$ as

$$U(x)=e^{x}-(n+\tfrac{1}{2})x \tag{20}$$

and the corresponding supersymmetric partner potentials $V_{\pm}$ turn out to be

$$V_{+}=\tfrac{1}{8}e^{2x}-\tfrac{1}{4}(n+\tfrac{3}{2})\,e^{x}+\tfrac{1}{8}(n+\tfrac{1}{2})^2 \tag{21}$$

$$V_{-}=\tfrac{1}{8}\,e^{2x}-\tfrac{1}{4}(n-\tfrac{1}{2})\,e^{x}+\tfrac{1}{8}(n+\tfrac{1}{2})^2. \tag{22}$$

Transforming V_{-} back to half line, the partner equation to (12) may be readily obtained:

$$\left(-\frac{1}{2}\frac{d^2}{dy^2}+\tfrac{1}{2}y^2+\frac{l(l+1)}{2y^2}+2-E_n\right)\chi_{nl}=0. \tag{23}$$

One can at once see that (23) correctly describes the degeneracies of the isotropic oscillator problem, the energy difference between (12) and (23) yielding the correct factor of two units. It may be noted that the l value in (23) remains the same as in (12).

Although this approach does explain the shift of the energy eigenvalues of the isotropic oscillator, it is not free from difficulties. For one thing, the connecting potential U in (16) as well as in (20) turns out to be n dependent whereas, by definition, (3) is related to the ground-state wavefunction only.

In the next section we take up this problem and establish a procedure for constructing the relevant supersymmetric transformations. Throughout, we shall focus our attention on the three-dimensional isotropic oscillator case. For the Coulomb problem, the approach is analogous and shall not be considered in detail.

3. A modified approach

A crucial point not noted [3] by HR (or at least one which does not come out clearly from their work) is that to each value of E_n in (12), the transformed expression for V_{+} in the full line can have an arbitrary number (say m) of energy eigenvalues. In

other words, on transforming to the full line, there can be n Hamiltonians (H_+) each having a set of m eigenvalues. These $(n \times m)$ possible levels of eigenvalues can be arranged in the form of a matrix. Thus, while the energy matrix E corresponding to (12) is only diagonal (the diagonal members being $E_1, E_2, \ldots$), the transformed matrix E' contains off-diagonal entries as well. In this way we have one set of E' for V_+ and another for V_-. However, when we transform V_- back to the half line, the resulting diagonal matrix may be considered as a supersymmetric partner to (12).

With these remarks, we proceed to the full-line construction of the isotropic oscillator equation (12). Employing as usual the following transformations:

$$x = 2 \ln y \qquad \chi = \phi(x) \exp(\tfrac{1}{4}x) \tag{24}$$

one finds

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \tfrac{1}{8}e^{2x} - \tfrac{1}{4}E_n e^x + \tfrac{1}{8}(l+\tfrac{1}{2})^2\right)\phi(x) = 0 \tag{25}$$

which represents the equation of a one-dimensional Morse potential $\frac{1}{8}e^{2x} - \frac{1}{4}E_n e^x$ with eigenvalues $-\frac{1}{8}(l+\frac{1}{2})^2$. However, the Morse potential depends on n. As such, for each value of n in (25) one can define a V_+, each having a spectrum of m eigenvalues.

Consider $n = 1$. The corresponding V_+ is

$$V_+ = \tfrac{1}{8}e^{2x} - \tfrac{1}{4}(\tfrac{5}{2})e^x + \tfrac{1}{8}(m+\tfrac{1}{2})^2 \tag{26}$$

having as energy eigenvalues $\frac{1}{8}(m-l)(m+l+1)$. Note that l has been kept fixed. Since we are interested in the diagonal terms only (for only these will be relevant when we transform back to the half line), we set $m = 1$ in (26) and solve for U and V_- from (2). We find

$$U = e^x - \tfrac{5}{2}x \tag{27a}$$

$$V_- = \tfrac{1}{8}e^{2x} - \tfrac{1}{4}(\tfrac{1}{2})e^x + \tfrac{1}{8}(\tfrac{3}{2})^2. \tag{27b}$$

In a similar way, the potentials V_- corresponding to $n = m = 2$, $n = m = 3, \ldots$, can be found. These are

$$V_- = \tfrac{1}{8}e^{2x} - \tfrac{1}{4}(\tfrac{3}{2})e^x + \tfrac{1}{8}(\tfrac{5}{2})^2 \tag{27c}$$

$$V_- = \tfrac{1}{8}e^{2x} - \tfrac{1}{4}(\tfrac{5}{2})e^x + \tfrac{1}{8}(\tfrac{7}{2})^2. \tag{27d}$$

and so on.

It may be noted that the energy eigenvalues corresponding to (27*b*), (27*c*), (27*d*), ..., form the diagonal members of a general $(n \times m)$ matrix E_{mn}.

We are now left with the task of transforming back to the half line. Using (24) again, we transform (27*b*), (27*c*), (27*d*) and similar expressions for $m = 4, 5, \ldots$, to the half line to obtain

$$\left(-\frac{1}{2}\frac{d^2}{dy^2} + \tfrac{1}{2}y^2 + \frac{1}{2}\frac{l(l+1)}{y^2} + 2 - E_m\right)\chi_m(y) = 0 \tag{28}$$

as the partner equation to (12) for $n = m$. As expected, the energy eigenvalues in (28) are shifted by two units, thus exhibiting the spectra of the isotropic oscillator.

The whole purpose of presenting this exercise is to point out that the indices n and m in (25) and (26) are arbitrary indices (for a fixed value of l) and one can choose any value of one quite independent of the other. This idea is not brought out clearly

in the approach of HR. In fact, with $U(y)$ defined by (16) or (20), this freedom does appear to be lost. The fact that the end results are the same is not a surprise since the diagonal values of E_{nm} are only meaningful in the half line.

In the present formalism, the U have been considered individually in the full line. As a result, when we transform back to the half line, we obtain a series of possible V_- each having the energy value separated from the corresponding V_+ by two units. In this way, the approach of HR has been put on a sounder logical basis.

We do not consider the Coulomb problem because the approach is quite analogous and the results of HR may be reestablished as in this case.

4. Concluding remarks

We conclude with some remarks on the evidence for SUSY in the hydrogen-helium problem. We recall the result of HR obtained in § 2 that SUSY links states of isoelectronic ions under the simultaneous change $n \to (n-1)$ and $Z \to Z(1-1/n)$, where n and Z stand for the principal quantum number and the nuclear charge, respectively.

Consider the case of the helium atom. If the orbits of the two electrons are separated far apart then, on the average, the Schrödinger equation for the He atom (with nuclear charge Z) separates into two equations [9]

$$-\left(\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r_1^2}+\frac{Z}{r_1}\right)u(r_1) = E_1 u(r_1) \tag{29a}$$

$$-\left(\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r_2^2}+\frac{Z}{r_2}\right)v(r_2) = E_2 v(r_2) \tag{29b}$$

each of which is the same as the Schrödinger equation for the hydrogen atom. Note that $E_1 = -Z^2/2n_1^2$ and $E_2 = -Z^2/2n_2^2$.

To apply the considerations of SUSY, one should first transform (29) to the full line. Then a double degeneracy of the excited states will be found to be between states of different n (but same l) and simultaneously different Z. For instance, let us assume that the outer electron of the He atom (namely the one described by (29b)) is at the $n = 2$s state. Then if SUSY is exact, a double degeneracy is expected (although approximately!) between this state and the one with the same l (here $l = 0$) but with n decreased by unity and Z changed to $Z(1-\frac{1}{2})$. Naively, the latter would correspond to the 1s state of the H atom since for helium $Z = 2$. However, keeping in mind the so-called charge shielding of the nucleus by the inner electron of the helium atom, one should ascribe $Z = 1$ to the outer electron as the effective charge that it sees†. (Certainly, the inner electron would have $Z = 2$.) The energy necessary to liberate this electron is 13.6 $(1^2)/(2^2) = 3.4$ eV. The supersymmetric transformations establish a double degeneracy between this electron and the one in the 1s state of the hydrogen atom but with charge $Z = \frac{1}{2}$. The ionisation energy in this case also turns out to be 13.6 $(\frac{1}{2})^2/1^2 = 3.4$ eV. Since the energy liberated when one electron of the helium atom is removed from the 2s state is of the order [10] of 4–5 eV, SUSY is seen to hold to a reasonable degree of approximation.

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