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N-dimensional hydrogen atom in an external spherically symmetric field*

Symbolic computation and explicit expressions derived from Rayleigh–Schrödinger-type perturbation theory

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The N-dimensional hydrogen atom in external fields of the type λr and λr^2 is studied. We describe how Lie algebras are used to obtain RS-type perturbation expansions. We present expressions for the perturbation energy up to 4th order for arbitrary dimension and arbitrary state of the hydrogen atom. With symbolic computation, results are obtained in compact and transparent form.

Key words: Lie algebras — Perturbation theory — Symbolic computation — Perturbed hydrogen atom

Introduction

The hydrogen atom in an external spherically symmetric field is a very interesting system from many different points of view. Let us mention as examples the study of screened Coulomb potential which is very important in solid state physics [1-3] and the external potentials of the type r^a, $a = 1, 2, 3, \ldots$, which is relevant to the confinement of quarks. The latter problem has been studied in a number of recent papers [4-8]. The problem most relevant to quantum chemistry consists in the case of the two-dimensional hydrogen atom in a strong magnetic field. In

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* Dedicated to Professor J. Koutecký on the occasion of his 65th birthday

addition to the description of the physics of this problem, the comprehensive paper by MacDonald and Ritchie [9] also includes the perturbation series expansions for the cases of weak and strong magnetic fields. Moreover, they show that two-point Padé approximants provide a reliable interpolation between these two limiting situations. Although their study constitutes an admirable work in dealing with the very difficult case of strong coupling, they were able to obtain only a first order low-field correction, which is quadratic in the intensity of the effective magnetic field. The major difficulty resides in the fact that the hydrogen atom has both a discrete and a continuum spectrum. We have shown in a series of papers [10–22] and also in a review article [23] that this difficulty can easily be overcome by using algebraic methods, see also [24–27]. For perturbations of the type λr^a, states with principal quantum numbers n and n' are coupled only if $|n-n'| \leq a+1$. Moreover, the application of a modified Rayleigh–Schrödinger perturbation is very straightforward. There is thus no special need to avoid the wavefunction in the calculations.[1]

In the above-mentioned papers, almost all results were formulated in three space dimensions. It turns out that relatively small modifications permit us to calculate perturbation coefficients for arbitrary dimension and arbitrary hydrogen quantum numbers. In this paper, we present the use of the $so(2,1)$ algebra to study the N-dimensional hydrogenic perturbation problem ($a=1$, for "charmonium" and $a=2$, for "harmonium"). There are enough indications that with the $so(4,2)$ algebra, general anisotropic perturbations could also be considered in a similar way. Thus, this paper is, in a sense, a starting point for more complicated problems.

The use of symbolic computation opened a new vista in this work. The calculations were done in the language MAPLE which is being developed at Waterloo [31]. After some careful manipulations, we were able to obtain all expressions symbolically. After the application of a modified perturbation theory which produced an algebraic expression for the Taylor expansion of the wavefunction, a simple MAPLE command provided us with the contributions for the perturbation energy.

In order to keep the size of this communication reasonable, we indicate only the basic ideas and describe final results. A detailed description of our technique will be published later. We also limited ourselves to the evaluation of perturbation coefficients. It will be shown by Adams [32] in a paper published in this issue, how these results can be used for the construction of Padé approximants.

Finally, while we are only concerned in getting the perturbation energy in this paper, we are currently pursuing the study of upper and lower bounds for the energy using two other methods, namely: renormalized inner projection [33–40] and a method of moments [41–43]. The final results are very encouraging and will be published later.

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[1] There are two other alternative formulations of this problem: explicit calculation of the wavefunction is avoided by Killingbeck [28] whereas logarithmic perturbation expansion is used by Privman [29], both treating spherically symmetric problems only. The Stark effect has been studied by Austin [30] using Killingbeck procedure. A comparison of these methods with the present work is in preparation

Algebraic formulation of the problem

Let us consider the N-dimensional hydrogen atom in radial external field of the type $V(r)=\lambda r^a$, where $a=1$ corresponds to "charmonium" while $a=2$ corresponds to "harmonium". The Schrödinger equation for this system can be written in the form:

$$\left[-\tfrac{1}{2}\nabla^2-\frac{1}{r}+\lambda r^a\right]\Psi=E\Psi. \tag{1}$$

The radial hydrogenic equation for each perturbed states is easily obtained by separation of variables and regrouping of terms:

$$\left[\tfrac{1}{2}\hat{p}_r^2+\frac{\xi}{2r^2}+\lambda r^a\right]\Psi=[E_n+\Delta E]\Psi, \tag{2}$$

where

$$\hat{p}_r=-i\left[\frac{\partial}{\partial r}+\frac{1}{2}\frac{(N-1)}{r}\right],$$

$$\xi=k(k+1)=\frac{(N-1)(N-3)}{4}+l(l+N-2),$$

$$k=l+\frac{N}{2}-\frac{3}{2},$$

$$E_n=-\frac{1}{2n^2},$$

$$n=k+1+n_r=l+\frac{N}{2}-\frac{1}{2}+n_r.$$

In this equation, n is a principal quantum number and the label of the state considered, l an angular momentum quantum number and n_r is a radial quantum number.

In order to express the hydrogenic eigenvalue problem in terms of the $so(2,1)$ algebra generators, we first need to introduce the scaling transformation [11]:

$$R=\frac{r}{n} \quad \text{and thus } \hat{P}_r=n\hat{p}_r.$$

After multiplication by the model space variable R, eq. (2) becomes

$$\left[\tfrac{1}{2}R\hat{P}_R^2+\frac{\xi}{2R}+\tfrac{1}{2}R-n+\lambda n^{a+2}R^{a+1}\right]\Psi=n^2\,\Delta E\,R\Psi. \tag{3}$$

Let us use the realization of the $so(2,1)$ algebra in the scaled coordinate system and introduce the following generators [25]:

$$\hat{T}_1=\tfrac{1}{2}[\hat{R}\hat{P}_R^2+\xi\hat{R}^{-1}-\hat{R}],$$

$$\hat{T}_2=\hat{R}\hat{P}_R,$$

$$\hat{T}_3=\tfrac{1}{2}[\hat{R}\hat{P}_R^2+\xi\hat{R}^{-1}+\hat{R}],$$

and the Casimir operator

$$\hat{T}^2 = \hat{T}_3^2 - \hat{T}_1^2 - \hat{T}_2^2.$$

The perturbed hydrogenic eigenvalue problem can now be reformulated in terms of these generators as

$$[(\hat{T}_3 - n) + \lambda n^{a+2}(\hat{T}_3 - \hat{T}_1)^{a+1} - n^2 \Delta E\ (\hat{T}_3 - \hat{T}_1)]\Psi = 0,$$

or equivalently in a more compact form

$$[\hat{K} + \lambda \hat{W} - \Delta E\, \hat{S}]\Psi = 0, \tag{4}$$

where

$$\hat{K} = \hat{T}_3 - n,$$
$$\hat{R} = \hat{T}_3 - \hat{T}_1,$$
$$\hat{W} = n^{a+2}\hat{R}^{a+1},$$
$$\hat{S} = n^2\hat{R}.$$

Since $\hat{T}^2$ and $\hat{T}_3$ commute, they can be simultaneously diagonalized. We denote their common normalized eigenvectors by $|kq\rangle$ and write

$$\hat{T}^2|kq\rangle = k(k+1)|kq\rangle,$$
$$\hat{T}_3|kq\rangle = q|kq\rangle,$$

where $q = k + 1 + q_{\hat{R}}$, for $q_{\hat{R}}$ any non-negative integer.[2]

The matrix elements of $\hat{R} = \hat{T}_3 - \hat{T}_1$ can be then easily obtained by the relation

$$\hat{R}|kq\rangle = q|kq\rangle - \tfrac{1}{2}[[(q-k)(q+k+1)]^{1/2}|k, q+1\rangle + [(q+k)(q-k-1)]^{1/2}|k, q-1\rangle]. \tag{5}$$

All other matrix elements can be obtained using Eq. (5) and matrix operations.

Modified perturbation theory

We are now ready to apply perturbation theory. As mentioned previously, the explicit form for the eigenfunctions presents no particular difficulties. However, since our problem is essentially "non-orthogonal" due to the presence of the operator $\hat{S}$ [10], we need to consider a "modified" perturbation theory. Let us normalize the vectors $|\Psi\rangle$ in such a way that $\langle kn|\Psi\rangle = 1$ and define the resolvent operator associated with Eq. (4),

$$\hat{Q} = \sum_{q \neq n} \frac{|kq\rangle\langle kq|}{n - q},$$

---

[2] Note the difference between the label n of the energy level of concern and q, the general eigenvalue of the generator $\hat{T}_3$

and the "perturbation" operator $\hat{X}$,

$$\hat{X} = \hat{W} - \omega \hat{S}.$$

In order to write the wavefunction in a most compact form, we have introduced the new constant ω such that $\lambda\omega = \Delta E$.

If we denote $|kn\rangle$ by $|\Phi\rangle$, the expression for the wavefunction becomes

$$|\Psi\rangle = |\Phi\rangle + \lambda \hat{Q}\hat{X}|\Psi\rangle,$$

or

$$|\Psi\rangle = |\Phi\rangle + \lambda \hat{Q}\hat{X}|\Phi\rangle + \lambda^2 \hat{Q}\hat{X}\hat{Q}\hat{X}|\Phi\rangle + \cdots. \tag{6}$$

From Eq. (4), we obtain the following relation,

$$\langle\Phi|\hat{X}|\Psi\rangle = 0. \tag{7}$$

Substituting Eq. (6) in Eq. (7) yields the following expression for the calculation of the energy up to 4th order:

$$\begin{aligned}0 = {} & \lambda\langle\Phi|\hat{X}|\Phi\rangle + \lambda^2\langle\Phi|\hat{X}\hat{Q}\hat{X}|\Phi\rangle + \lambda^3\langle\Phi|\hat{X}\hat{Q}\hat{X}\hat{Q}\hat{X}|\Phi\rangle \\ & + \lambda^4\langle\Phi|\hat{X}\hat{Q}\hat{X}\hat{Q}\hat{X}\hat{Q}\hat{X}|\Phi\rangle + O(\lambda^5),\end{aligned} \tag{8}$$

or more explicitly

$$\Delta E\ \langle\Phi|\hat{S}|\Phi\rangle = \lambda\langle\Phi|\,\hat{W}|\Phi\rangle + \lambda^2\langle\Phi|\hat{X}\hat{Q}\hat{X}|\Phi\rangle + \lambda^3\langle\Phi|\hat{X}\hat{Q}\hat{X}\hat{Q}\hat{X}|\Phi\rangle + \cdots. \tag{9}$$

Symmetric perturbation theory is then applied to get expressions for the terms in Eq. (8) or Eq. (9). Namely, we use the "bra and ket symmetry" of the expressions involved.

If we were to use the analogy with the usual Rayleigh-Schrödinger perturbation theory, we would expand both the wavefunction and the energy as Taylor series in λ. Alternating substitution into Eq. (7) and Eq. (8) would then give an expression for the nth order of the perturbation energy.

Another way to obtain the same result would be to write explicitly the Taylor coefficients of the energy. This can be done by the bracketing technique or by Lagrange method. These two methods were formulated in a most transparent way by Silverstone [43-46].

However, in both of the above methods, a full expansion is needed before the actual numerical calculation. In our case, we have found it very convenient to first express Eq. (8) in terms of the parameters n, ξ and ω. As we are looking for the perturbation energy up to 4th order, we substitute into the first term of Eq. (8), i.e. $\langle\Phi|\hat{X}|\Phi\rangle$, the following expression for ω,

$$\omega = \Delta E_1 + \Delta E_2\lambda + \Delta E_3\lambda^2 + \Delta E_4\lambda^3. \tag{10}$$

But only the expansion up to the second power of λ is substituted for ω in the second term of Eq. (8), and similarly, decreasing powers of λ are needed in the expansion of ω to be then substituted in the next terms of Eq. (8), i.e. we let[3]:

$$\omega = \Delta E_1 + \Delta E_2 \lambda + \Delta E_3 \lambda^2 \quad \text{in the second term,}$$

$$\omega = \Delta E_1 + \Delta E_2 \lambda \quad \text{in the third term,}$$

$$\omega = \Delta E_1 \quad \text{in the fourth term.}$$

The coefficients of each power of the coupling constant are then collected. Although these manipulations can even be performed by hand, they were greatly facilitated by the use of the symbolic computation language MAPLE, which possesses a simple command "coeff" that automatically executes this regrouping of terms. We can then write the following relations for the coefficients in the expansion of the perturbation energy[4]:

$$\Delta E_1 = f_1(n, \xi),$$

$$\Delta E_2 = f_2(n, \xi, \Delta E_1),$$

$$\Delta E_3 = f_3(n, \xi, \Delta E_1, \Delta E_2),$$

$$\Delta E_4 = f_4(n, \xi, \Delta E_1, \Delta E_2, \Delta E_3).$$

Final results

By successive substitutions, we obtain the following expressions for the coefficients of the perturbation energy.

For charmonium, we have:

$$\Delta E_1 = \tfrac{3}{2} n^2 - \tfrac{1}{2} \xi,$$

$$\Delta E_2 = -\tfrac{1}{8} n^2 (7n^4 + 5n^2 - 3\xi^2),$$

$$\Delta E_3 = \tfrac{1}{16} n^4 (33n^6 + 75n^4 - 7n^2\xi^2 - 10\xi^3),$$

$$\Delta E_4 = -\tfrac{1}{64} n^6 (465n^8 + 2275n^6 + 440n^4 - 99n^4\xi^2 - 90n^2\xi^3 - 180n^2\xi^2 - 84\xi^4).$$

And for harmonium, we have:

$$\Delta E_1 = \tfrac{1}{2} n^2 (5n^2 + 1 - 3\xi),$$

$$\Delta E_2 = -\tfrac{1}{16} n^6 (143n^4 + 345n^2 + 28 - 90n^2\xi - 21\xi^2 - 126\xi),$$

$$\Delta E_3 = \tfrac{1}{16} n^{10} (1530n^6 + 11145n^4 + 8645n^2 + 484 - 1305n^4\xi - 6825n^2\xi - 33\xi^3 + 33\xi^2 - 2706\xi),$$

---

[3] We could substitute Eq. (10) in all terms of Eq. (8) but then larger expressions having a greater number of unnecessary terms for the calculation of the perturbation energy up to 4th order would be produced: of course, in this case the computer time required would be negligible. However, in order to keep demands on the computer memory minimal as well as to illustrate a pattern for the nth order perturbation energy, we introduce the following substitutions for ω

[4] Intermediary steps illustrating the substitutions and regrouping of terms are shown in the Appendix

$$
\begin{aligned}
\Delta E_4 = -\tfrac{1}{1024}n^{14}(&1\,502\,291n^8 + 22\,937\,530n^6 + 54\,811\,295n^4 \\
&+ 25\,371\,140n^2 + 1\,137\,344 - 1\,640\,100n^6\xi + 251\,370n^4\xi^2 \\
&- 19\,742\,520n^4\xi - 3060n^2\xi^3 + 2\,184\,330n^2\xi^2 - 31\,859\,700n^2\xi \\
&- 4005\xi^4 - 7260\xi^3 + 1\,425\,540\xi^2 - 7\,286\,640\xi).
\end{aligned}
$$

Reformulation of the problem in rational arithmetic

Although this whole procedure can be performed with normalized basis vectors $|kq\rangle$, it would take considerable additional computer time to eliminate the irrational factors. For this reason, we introduce, in a similar fashion as Silverstone did in [47], the following unnormalized vectors:

$$|kq\rangle^{\#} = \left[\frac{(k+q)!}{(q-k-1)!}\right]^{1/2} |kq\rangle,$$

and

$$|kq\rangle^{\#\#} = \left[\frac{(q-k-1)!}{(k+q)!}\right]^{1/2} |kq\rangle.$$

We then have the following relations between these two vectors

$$|kq\rangle^{\#\#} = |-k-1, q\rangle^{\#},$$

and for arbitrary vectors v_1 and v_2

$$^{\#\#}\langle v_1 | v_2\rangle^{\#} = \langle v_1 | v_2\rangle.$$

In terms of the new basis vectors, Eq. (5) now becomes:

$$\hat{R}|kq\rangle^{\#} = q|kq\rangle^{\#} - \tfrac{1}{2}[(q-k)|k, q+1\rangle^{\#} + (q+k)|k, q-1\rangle^{\#}].$$

We also have the following expressions for $\hat{R}^2$ and $\hat{R}^3$:

$$
\begin{aligned}
\hat{R}^2|kq\rangle^{\#} = {}& \tfrac{1}{2}[3q^2 - k(k+1)]|kq\rangle^{\#} - \tfrac{1}{2}[(2q+1)(q-k)|k, q+1\rangle^{\#} + (2q-1) \\
& \times (q+k)|k, q-1\rangle^{\#}] \\
& + \tfrac{1}{4}[(q-k+1)(q-k)|k, q+2\rangle^{\#} + (q+k-1)(q+k)|k, q-2\rangle^{\#}] \\
\hat{R}^3|kq\rangle^{\#} = {}& \tfrac{1}{2}q[1 + 5q^2 - 3k(k+1)]|kq\rangle^{\#} \\
& - \tfrac{3}{8}[(5q^2 + 5q + 2k(k+1))(q-k)|k, q+1))^{\#} + (5q^2 - 5q \\
& + 2k(k+1))(q+k)|k, q-1\rangle^{\#}] \\
& + \tfrac{3}{4}[(q+1)(q-k+1)(q-k)|k, q+2\rangle^{\#} \\
& + (q-1)(q+k-1)(q+k)|k, q-2\rangle^{\#}] \\
& - \tfrac{1}{8}[(q-k+2)(q-k+1)(q-k)|k, q+3\rangle^{\#} \\
& + (q+k-2)(q+k-1)(q+k)|k, q-3\rangle^{\#}].
\end{aligned}
$$

All matrix elements are in rational form, so the final expressions are in rational form. Moreover, in all expressions, we use the property that coefficients of $|k, q-\Delta q\rangle^{\#}$ can be obtained from the coefficients of $|k, q+\Delta q\rangle^{\#}$ by substituting q by $-q$ and then multiplying by $(-1)^b$ in matrix elements related to $\hat{R}^b$. Finally, let us mention that in order to keep the simplicity of the normalizing factors, we have defined all basis vectors in terms of k and q, and later in intermediate steps, simplified the expressions by replacing the factor $k(k+1)$ by its value ξ.

Conclusions

In this paper, we have obtained the perturbation energy up to the 4th order. The use of symbolic computation language was invaluable in efficiently producing simple expressions in terms of all parameters. Our results were then numerically checked with [19] and [28, 29] for "charmonium" and with [29] for "harmonium", by suitably replacing values for k and n. Although we only presented the perturbation energy up to the 4th order, it seems to be relatively easy to get a similar general expression for the nth order.

Further, let us stress that we can easily obtain an expression for the wavefunction by simply substituting our results for the perturbation energy ΔE in the operator $\hat{X}$, and then use the MAPLE command "coeff" to get the desired Taylor wavefunction expression in λ. In such a way, we are able to calculate additional mean values of observables other than the energy.

Finally let us mention that our results for $N=2$, $n=0$, $\xi=0$ were successfully used for the construction of Padé approximants for the energy for the physically important system of the two-dimensional hydrogen atom in a strong magnetic field [32].

Appendix

Here, we show the intermediate steps involved in getting the final formula for ΔE_2 as well as the contributions for ΔE_3 and ΔE_4, originating from the expression for the second term of Eq. (8), i.e. $\langle\Phi|\hat{X}\hat{Q}\hat{X}|\Phi\rangle$.

From Eq. (9), we then have:

$$\frac{\lambda^2\langle\Phi|\hat{X}\hat{Q}\hat{X}|\Phi\rangle}{\langle\Phi|\hat{S}|\Phi\rangle} = -\tfrac{1}{8}n^2(34n^4+5n^2-24\omega n^2-18\xi n^2+8\omega\xi+4\omega^2)\lambda^2.$$

After substituting ω by $\Delta E_1+\Delta E_2\lambda+\Delta E_3\lambda^2$, this last expression reads

$$\begin{aligned}&-\tfrac{1}{8}n^2[34n^4+5n^2-18n^2\xi-24\Delta E_1 n^2+8\Delta E_1\xi+4\Delta E_1^2\\&\quad-(24\Delta E_2 n^2-8\Delta E_2\xi-8\Delta E_1\Delta E_2)\lambda\\&\quad+(8\Delta E_3\xi+8\Delta E_1\Delta E_3+4\Delta E_2^2-24\Delta E_3 n^2)\lambda^2+8\Delta E_2\Delta E_3\lambda^3+4\Delta E_3^2\lambda^4]\lambda^2.\end{aligned} \tag{12}$$

Using the MAPLE command "coeff", the coefficient in λ^2 in Eq. (12) is found to be

$$-\tfrac{1}{8}n^2(34n^4+5n^2-18n^2\xi-24\Delta E_1 n^2+8\xi\Delta E_1+4\Delta E_1^2).$$

Replacing the value of ΔE_1, one obtains the following expression for the second order perturbation energy:

$$\Delta E_2=-\tfrac{1}{8}n^2(7n^4+5n^2-3\xi^2).$$

Let us notice the simplicity of this final result which is due to the cancellation and regrouping of terms after the substitution of ΔE_1.

The coefficient A of λ^3 in Eq. (12) is a contribution to the calculation of ΔE_3:

$$A=n^2\Delta E_2(3n^2-\xi-\Delta E_1).$$

Similarly, the coefficient B of λ^4 in Eq. (12) will have to be accounted for in the calculation of ΔE_4.

$$B=\tfrac{1}{2}n^2(6\Delta E_3 n^2-2\xi\Delta E_3-2\Delta E_1\Delta E_3-\Delta E_2^2).$$

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