

On the theory of the Stark effect: the influence of dimensionality

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A theory of the Stark effect in the D -dimensional “hydrogen atom” is developed. Recursion relations determining the higher-order perturbation terms E_k for the ground state are obtained, and the behavior of the coefficients E_k as k is increased, as well as their asymptote as $k \rightarrow \infty$, are investigated. Analogous problems for the D -dimensional funnel potential are also considered.

INTRODUCTION

In a prediction dating back to Ehrenfest¹ the generalization of a physical theory to a space of an arbitrary dimensionality D often leads to a new and unexpected perspective of the problem at hand. Over the last years, this approach has been widely used in theoretical physics. It provides a basis for the $1/D$ -expansion, or dimensional-scaling, approach^{2–9}—a novel quantum-mechanical computational method which has been applied, in particular, to the study of the properties of atoms in strong external fields,^{5–9} to the two-center problem,¹⁰ and to many other problems (the state-of-the-art of the method and its applications to quantum mechanics, atomic and molecular theory, quantum chemistry etc., are reviewed in the articles collected in Ref. 4).

The problem of a “hydrogen atom” in a D -dimensional Euclidean space was first treated by one of the authors,¹¹ who showed (following the classical work of Fock¹²) that the “latent” symmetry group for the discrete spectrum case is $SO(D+1)$ (this fact can also be established by a purely algebraic method¹³ similar to the Bargmann approach¹⁴). The “latent” symmetry of the Coulomb problem for a continuous spectrum and zero-energy states has been considered in Refs. 15 and 16; the use of the symmetry considerably simplifies the calculation of the Coulomb Green’s function.^{15,17} Applications to some atomic physics problems, including the evaluation of matrix elements and radiation transition probabilities, are contained in Refs. 18–20. Further references and a summary of available results may be found in Refs. 16 and 21.

In the present paper we consider the problem of a D -dimensional hydrogen atom in a uniform electric field, evaluate higher-order perturbation-theory terms, and investigate the structure of perturbation-theory series as functions of D . While one- and two-dimensional generalizations of the standard ($D=3$) perturbation theory of the Stark effect have been carried out by many authors,¹ in $D=2$ there are at present only the first three perturbation terms available for the case of the ground state.²⁶ We will show that the application of logarithmic perturbation theory^{27–30} to the present problem simplifies calculations

radically and makes it possible to compute the perturbation theory coefficients E rapidly up to $k=50$.²⁾

HIGHER-ORDER PERTURBATION THEORY

The Schrödinger equation for a D -dimensional “hydrogen atom” in a uniform electric field ε has the form ($\hbar=m=e=1$):

$$\Delta\psi + 2(E+r^{-1})\psi - \varepsilon(\xi - \eta)\psi = 0. \quad (1)$$

By separating variables we are led to the equation

$$\xi \frac{d^2 f_1}{d\xi^2} + \frac{D-1}{2} \frac{df_1}{d\xi} + \left(\frac{1}{2} E\xi + \beta_1 - \frac{1}{4} \varepsilon\xi^2 \right) f_1 = 0, \quad (2)$$

where β_1 is the separation constant, E is the energy, and ξ and η are parabolic coordinates [see formulas (A4) and (A5) in Appendix A]. The equation for the function $f_2(\eta)$ differs from (2) only through the replacements $\beta_1 \rightarrow \beta_2$ and $\varepsilon \rightarrow -\varepsilon(\beta_1 + \beta_2 = 1)$. Following logarithmic perturbation theory,^{27–29,32} we look for f_1 of the form

$$f_1(\xi) = \exp \left\{ -\frac{1}{2} \int_0^\xi x(t) dt \right\} \quad (3)$$

and obtain for the function $x(\xi)$ the (Riccati) equation

$$\xi \frac{dx}{d\xi} + \frac{D-1}{2} x - \frac{1}{2} \xi x^2 - 2\beta_1 - E\xi + \frac{1}{2} \varepsilon\xi^2 = 0, \quad (3')$$

for which we seek a solution of the form

$$x(\xi) = \sum_{k=0}^{\infty} x_k(\xi) \varepsilon^k, \quad x_k(\xi) = \sum_{j=0}^k a_j^{(k)} \xi^j, \quad (4)$$

$$E(\varepsilon) = \sum_{k=0}^{\infty} E_k \varepsilon^k, \quad E_0 = -2(D-1)^{-2}. \quad (5)$$

Substituting these expansions in (3) we arrive at recursion relations for the coefficients $a_j^{(k)}$:

$$a_0^{(0)} = \frac{2}{D-1}, \quad a_1^{(1)} = \frac{D-1}{4}, \quad a_0^{(1)} = \frac{(D-1)^2(D+1)}{16},$$

$$a_k^{(k)} = -\frac{D-1}{4} \sum_{l=1}^{k-1} a_l^{(l)} a_{k-l}^{(k-l)},$$

$$a_j^{(k)} = \frac{D-1}{2} \left\{ \left(j+1 + \frac{D-1}{2} \right) a_{j+1}^{(k)} - \frac{1}{2} \sum_{l=1}^{k-1} \sum_{p+q=j} a_p^{(l)} a_q^{(k-l)} \right\}, \quad j=k-1, \dots, 1, \quad (6)$$

$$a_0^{(k)} = \begin{cases} 0, & k \text{ - even} \\ \frac{D-1}{2} \left\{ \left(1 + \frac{D-1}{2} \right) a_1^{(k)} - \frac{1}{2} \sum_{l=1}^{k-1} a_0^{(l)} a_0^{(k-l)} \right\}, & k \text{ - odd.} \end{cases} \quad (6')$$

The k -order perturbation of the ground-state energy is

$$E_k = \begin{cases} 0, & k \text{ - odd,} \\ \left(1 + \frac{D-1}{2} \right) a_1^{(k)} - \frac{1}{2} \sum_{l=1}^{k-1} a_0^{(l)} a_0^{(k-l)}, & k \text{ - even.} \end{cases} \quad (7)$$

Comparing the recursion relations (6) and (7)³⁾ with analogous relations for states with parabolic quantum numbers (0, 0, $n-1$) in three dimensions,^{29,30} they are readily seen to be identical if we set

$$n = \frac{D-1}{2}. \quad (8)$$

Thus, for odd dimensionalities $D=3, 5, \dots$ the coefficients E may be taken from previous work,²⁹⁻³¹ whereas for $D=2, 4, \dots$ they correspond to half-integer values of the principal quantum number n , which are not realizable in the three-dimensional problem.

In Eqs. (6) one can dispose of the fractions by going over to integer *number* recursion relations (see Appendix B), which makes it possible to calculate the perturbation coefficients exactly. It can be shown that

$$E_k = -\frac{(D-1)^{3k-2}}{2^{5k-3}} \cdot p_k \left(\frac{D+1}{2} \right), \quad (9)$$

where the p_k are polynomials of degree k :

$$\begin{aligned} p_2(z) &= 4z^2 + z, & p_4(z) &= 192z^4 + 357z^3 + 260z^2 + 71z, \\ p_6(z) &= 2(11\,776z^6 + 50\,133z^5 + 97\,230z^4 + 104\,680z^3 \\ &\quad + 61\,078z^2 + 15\,103z), \\ p_8(z) &= 4\,063\,232z^8 + 29\,383\,661z^7 + 102\,352\,108z^6 \\ &\quad + 218\,773\,427z^5 + 304\,535\,390z^4 \\ &\quad + 271\,420\,021z^3 + 141\,052\,150z^2 \\ &\quad + 32\,420\,011z, \dots \end{aligned} \quad (9')$$

Note that $p_k(0)=0$ (for the ground state, the perturbation coefficients E_k are different from zero only for even k).

The computed coefficients E_k are presented in Fig. 1, in which one sees a rapid growth of the higher order perturbation-theory coefficients. It is interesting to note that for $D \geq 3$ this growth starts immediately at $k=2$, whereas in the two-dimensional hydrogen atom the $|E_k|$ first decrease and their growth starts at $k \geq 10$. Using (8)

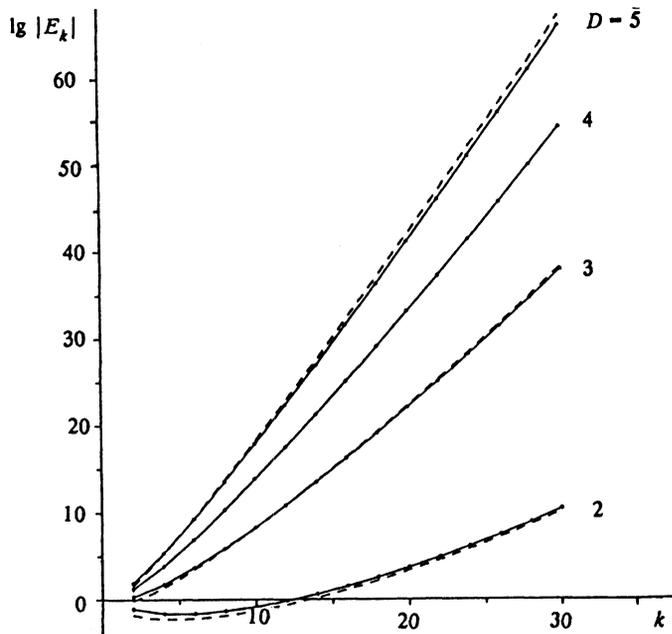


FIG. 1. Higher order perturbation-theory coefficients. Solid curves: Stark effect; dashed curves: funnel potential (the ground state; k is the order of the perturbation theory). The curves are labeled by the space dimensionality D .

together with formulas (4.4) of Ref. 30 we find the asymptotes of the coefficients E_k in the D -dimensional case:

$$\begin{aligned} E_k &\approx \Gamma \left(k + \frac{D-1}{2} \right) - a^k \left(c_0 + \frac{c_1}{k} + \dots \right), \quad k \rightarrow \infty, \\ a &= \frac{3}{16} (D-1)^3, \quad c_0 = -\frac{2^{D+1/2} 3^{D-1/2}}{\pi (D-1)^2 \Gamma \left(\frac{D+1}{2} \right)}. \end{aligned} \quad (10)$$

From this it follows that the quantities $|E_k|$ have a minimum at $k \sim k_0$,

$$k_0 = a^{-1} = \frac{2}{3} \left(\frac{D-1}{2} \right)^{-3}. \quad (11)$$

In particular, $k_0 \sim 5$ for $D=2$, and for $D \geq 3$ we have $k_0 < 1$. This accounts for the difference between the corresponding curves in Fig. 1.

Thus the second-order perturbation coefficients increase factorially as $k \rightarrow \infty$, which makes the perturbation series (5) divergent for an arbitrarily small electric field $\varepsilon \neq 0$. At the present time the technique of summing such series is fairly well advanced in quantum mechanics; the Borel transformation³³ and Padé-Hermite approximants^{7,9,10} may be used to this end.

FUNNEL POTENTIAL

Let us discuss briefly the funnel potential

$$V(r) = -r^{-1} + gr, \quad (12)$$

which for $g > 0$ possesses only a discrete spectrum and for $g < 0$ represents a spherical model of the Stark effect in the hydrogen atom.

Recursion relations for this problem are given in Ref. 34, Eq. (16). Setting $n = (D-1)/2$ in them we obtain the corresponding equations for the D -dimensional potential (12).

The perturbation series for the ground state energy is here of the form

$$E(g) = \sum_{k=0}^{\infty} \bar{E}_k g^k, \quad (13)$$

$$\bar{E}_k = \frac{(-1)^{k+1}}{2^{5k-3}} \cdot D(D+1)(D-1)^{3k-2} \bar{p}_k \left(\frac{D+1}{2} \right), \quad k \geq 2, \quad (14)$$

where

$$\bar{E}_1 = \frac{1}{4} D(D-1),$$

$$\bar{p}_2(z) = 1,$$

$$\bar{p}_3(z) = 2(4z+1), \quad \bar{p}_4(z) = 2(48z^2+33z+7),$$

$$\bar{p}_5(z) = 8(176z^3+225z^2+116z+22),$$

$$\bar{p}_6(z) = 16(1456z^4+2913z^3+2609z^2+1157z+202),$$

$$\bar{p}_7(z) = 16(26\,112z^5+74\,124z^4+99\,496z^3+74\,706z^2+29\,927z+4\,899), \dots \quad (14')$$

Unlike the previous case, the perturbation series for $g > 0$ is of alternating sign. However, on changing the sign of g (corresponding to changing from the funnel case to the Stark effect) the coefficients in the series all have the same sign.

A calculation using the formulas above gives the dashed curves of Fig. 1, which for $k \gg 1$ are close to the corresponding Stark-effect curves (for the same dimensionality D). It can be shown that, asymptotically,

$$\rho_k = |\bar{E}_k/E_k| = \beta k + O(1), \quad (15)$$

where β is a constant dependent on D . From Fig. 2 it is seen that for $k \geq 10$ the linear dependence (15) does indeed hold.

In Tables I and II are listed the perturbation-theory coefficients E_k and \bar{E}_k as calculated (exactly) by the recursion relations given in Appendix B. Note that in the case $D=3$ the coefficients E_k were known before,^{29-31,35} whereas the coefficients E_2 , E_4 , and E_6 for the two-dimensional hydrogen atom have been calculated (by a different method) in a more recent paper.²⁶ The perturbation coefficients for the funnel potential have been calculated for $D=3$ in Ref. 36. In Table II we have corrected a misprint overlooked in Ref. 36, which gives (at p. 1575) an incorrect value for the coefficient E_5 for the three-dimensional funnel potential.

TABLE I. Higher orders of perturbation theory for the Stark effect (exact values).

k	D	Q_k	q_k
2	2	21	8
	3	9	2
	4	4 455	8
4	5	78	0
	2	22 947	20
	3	3 555	6
6	4	7 029 488 205	20
	5	221 952	0
	2	48 653 931	31
8	3	2 512 779	9
	4	18 766 948 307 571 765	31
	5	2 052 097 536	0
10	2	800 908 686 795	44
	3	13 012 777 803	14
	4	351 816 286 619 053 151 834 805	44
12	5	32 263 679 717 376	0
	2	5 223 462 120 917 049	55
	3	25 497 693 122 265	17
12	4	2,4071 · 10 ³⁰	55
	5	720 020 129 415 168 000	0
	2	98 276 453 573 919 203 439	67
12	3	138 963 659 571 727 791	21
	4	4,4418 · 10 ³⁷	67
	5	21 126 901 587 942 217 089 024	0

Note: perturbation coefficients E_k are written in the form of (B4); k is the order of the perturbation theory, D the spatial dimensionality.

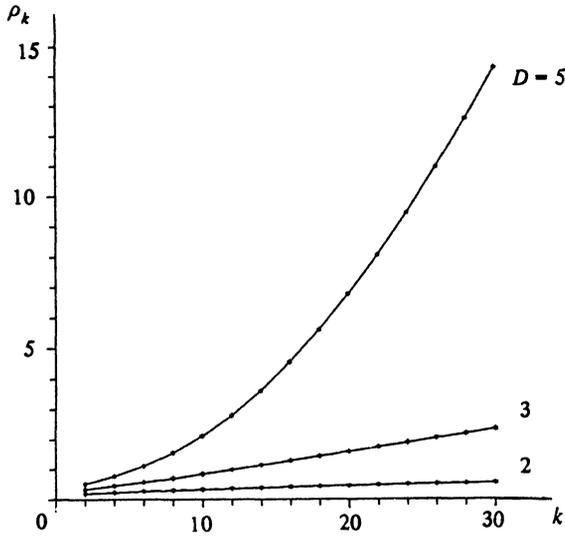


FIG. 2. The ratio ρ_k , Eq. (15), for a number of dimensionality D .

CONCLUSION

The above results quite clearly demonstrate both the efficiency of logarithmic perturbation theory and its advantages over conventional one, in which higher-order E_k 's require complex multiple summations over the states of the discrete and continuous spectra.

We have restricted ourselves to the ground state calculation (which suffices to analyze the question of the divergence of the perturbation series), and the logarithmic-perturbation-theory approach is simplest in this case. A generalization to excited states with node-containing wave functions has been carried out in Refs. 27, 30, and 32.

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APPENDIX A

It is not difficult to verify directly that the radial Schrödinger equation

$$R'' + \frac{D-1}{r} R' + 2(E+r^{-1})R=0, \quad r = \left(\sum_{i=1}^D x_i^2 \right)^{1/2}, \quad (\text{A1})$$

has the following ground-state solution:

$$E_0 = -2(D-1)^{-2}, \quad (\text{A2})$$

$$R_0(r) = \{2^D / (D-1)^D \Gamma(D)\}^{1/2} \exp\left(-\frac{2r}{D-1}\right). \quad (\text{A3})$$

In terms of parabolic coordinates ξ, η

$$\xi = r + x_D = r(1 + \cos \theta_{D-1}), \quad \eta = r - x_D = r(1 - \cos \theta_{D-1}) \quad (\text{A4})$$

the D -dimensional Laplacian takes the form

$$\Delta \Psi = \frac{4}{\xi + \eta} \left\{ \xi \frac{\partial^2 \Psi}{\partial \xi^2} + \eta \frac{\partial^2 \Psi}{\partial \eta^2} + \frac{D-1}{2} \left(\frac{\partial \Psi}{\partial \xi} + \frac{\partial \Psi}{\partial \eta} \right) \right\} + \frac{1}{\xi \eta} \Delta^{(\text{ang})} \Psi, \quad (\text{A5})$$

where $\Delta^{(\text{ang})}$ is the angular part of the Laplace operator, dependent on the angles $\theta_1, \dots, \theta_{D-2}$. Using (A5), the variables in the Schrödinger equation (1) are separable into $\Psi(x_1, \dots, x_D) = f_1(\xi) f_2(\eta) \Phi(\theta_1, \dots, \theta_{D-2})$ and for $\Phi = \text{const.}$ we arrive at Eq. (2).

APPENDIX B

The coefficients E_k (i.e., higher-order terms in perturbation theory) are determined by Eqs. (6) and (7). One further simplification occurs when one makes the substitution

$$a_j^{(k)} = (-1)^{k+1} 2^{j-5k+2} (D-1)^{3k-j-1} A_j^{(k)}, \quad (\text{B1})$$

TABLE II. Perturbation-theory coefficients for the D -dimensional funnel potential (ground state).

k	D	S_k	q_k	k	D	S_k	q_k
1	2	1	1	6	2	600 243	25
	3	3	1		3	5 583	0
	5	5	0		5	3 436 661 760	0
2	2	3	6	7	2	13 526 613	29
	3	3	1		3	9 543 339	7
	5	60	0		5	485 458 513 920	0
3	2	21	10	8	2	2 770 115 403	36
	3	27	2		3	1 141 062 999	10
	5	3 120	0		5	75 431 036 682 240	0
4	2	987	16	9	2	79 111 307 439	40
	3	795	4		3	18 769 071 555	10
	5	258 240	0		5	1,2689 · 10 ¹⁶	0
5	2	15 555	20	10	2	4 978 189 192 881	45
	3	3 843	3		3	1 343 699 301 873	14
	5	27 444 480	0		5	2,2865 · 10 ¹⁸	0

Note: the coefficients $\overline{E_k}$ are written in the form of (B7).

which gives for $A_j^{(k)}$ the recursion relations ($k \geq j \geq 1$):

$$A_k^{(k)} = (2k-2)!/k!(k-1)! = C_k$$

$$A_j^{(k)} = \left(j + \frac{D+1}{2}\right) A_{j+1}^{(k)} + \sum_{l=1}^{k-1} \sum_{p+q=j} A_p^{(l)} A_q^{(k-l)}, \quad (B2)$$

where C_k are the Catalan numbers familiar from combinatorial analysis³⁷ and $A_0^{(k)} = \frac{1}{2}(D+1)A_1^{(k)}$ for odd k ; for even k we must set $A_0^{(k)} = 0$ in (B2). The k -order energy correction is

$$E_k = -2^{-2k}(D+1) \left(\frac{D-1}{2}\right)^{3k-2} \times \left\{ A_1^{(k)} + \frac{D+1}{2} \sum_{l=1}^{k-1} A_1^{(l)} A_1^{(k-l)} \right\}, \quad (B3)$$

where $k \geq 2$ is even and the index l assumes only odd values. It follows that the $A_j^{(k)}$ are positive rational (and for $D=3,5,\dots$, integer) numbers for all j and k , which makes it possible to calculate them on a computer with no loss of accuracy. The results of computations are listed in Table I, in which we have set

$$E_k = -Q_k 2^{-q_k}, \quad (B4)$$

where Q_k and $q_k \geq 0$ are integers. We should remark that Q_k and S_k (unlike the perturbation coefficients E_k) increase dramatically note that for $D=4$

$$Q_{10} = 2 \ 407 \ 113 \ 396 \ 813 \ 994 \ 071 \ 351 \ 833 \ 119 \ 815,$$

for example, and therefore Tables I and II give their approximate values in several cases.

From Table I it is seen that in a five-dimensional space all $q_k = 0$, that is, the perturbation coefficients are integers.⁴⁾ This is easily explained with the aid of formula (B3) which becomes ($D=5$)

$$E_k = -3 \cdot 2^{k-1} \left\{ A_1^{(k)} + 3 \sum_{l=1}^{k-1} A_1^{(l)} A_1^{(k-l)} \right\}. \quad (B5)$$

Note that $A_j^{(k)}$ is a polynomial of degree $(k-j)$ in $z = (D+1)/2$. We present explicitly the first few of the polynomials:

$$A_1^{(1)} = 1, \quad A_0^{(1)} = z, \quad A_2^{(2)} = 1, \quad A_1^{(2)} = 3z+1, \quad A_0^{(2)} = 0,$$

$$A_3^{(3)} = 2, \quad A_2^{(3)} = 10z+6, \quad A_1^{(3)} = 16z^2+18z+6,$$

$$A_0^{(3)} = z \quad A_1^{(3)}, \quad A_4^{(4)} = 5, \dots \quad (B6)$$

(and, in general, $A_0^{(k)} = z A_1^{(k)}$ for odd k).

Similar calculations have been performed for the funnel potential. In this case in Eq. (13)

$$\bar{E}_k = (-1)^{k+1} S_k \cdot 2^{-q_k}, \quad (B7)$$

and the numbers S_k and q_k are listed in Table II.

¹⁾See Refs. 22–26 and additional bibliography in Refs. 25 and 26.

²⁾This restriction depends on the power of the computer used.

³⁾Note that in the derivation of relations (6) and (7) it is essential that the unperturbed wave function have the form of the simple exponential of Eq. (A3).

⁴⁾The same is true for all dimensionalities $D=4m+1$.

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