

High-Order Perturbation Theory and Padé Approximants for a One-Electron Ion in a Generalized Central-Field Potential

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(Received 19 January 1970)

The solution to the nonrelativistic Schrödinger equation for a one-electron ion in a generalized central-field potential is investigated using high-order perturbation theory. It is shown that by utilizing a *finite* expansion of the perturbation-theory wave function in terms of associated Laguerre polynomials, perturbation-theory results can be obtained for any n, l state to arbitrarily high order. Results for the wave function and energy are explicitly given to third and fourth order, respectively. It is also shown that by reexpressing the high-order perturbation-theory energy expansion as a series of rational fractions (Padé approximants), accurate eigenvalues are obtained, even for large values of the expansion parameter.

I. INTRODUCTION

In this work we consider a one-electron ion in a generalized central-field potential of the form

$$V(r) = -(Z/r)B(\lambda r), \tag{1}$$

with

$$B(\lambda r) = \sum_{j=0}^{\infty} B_j(\lambda r)^j \tag{2}$$

and $B_0 = 1$. Therefore, we are considering a class of problems including the screened Coulomb potential, a potential of the form $-Z(e^{-\lambda r} \cos \lambda r)/r$, etc. The method we utilize is an expansion of the perturbation wave function in each order in terms of associated Laguerre polynomials. The advantage of the present work over the author's previous work on the screened Coulomb potential¹ is that the wave function and energy in each order can be written down explicitly for any arbitrary n, l state in one calculation. We are also considering here a wider class of potentials whose physical importance has been widely reviewed in the literature.¹⁻³

We obtain explicit results for the fourth-order energy in terms of the B_j 's. We also show that by resuming the high-order perturbation theory as Padé approximants, rapid convergence is obtained to accurate numerically integrated eigenvalue results.

II. HIGH-ORDER PERTURBATION THEORY

The radial Schrödinger equation for an electron in a generalized potential of form Eq. (1) is

$$-\frac{1}{2} \frac{d^2 \psi(r)}{dr^2} - \frac{1}{r} \frac{d\psi(r)}{dr} - \frac{Z}{r} B(\lambda r) \psi(r) + \frac{1}{2} \frac{l(l+1)}{r^2} \psi(r)$$

$$= E\psi(r). \tag{3}$$

Letting $\xi = Zr$ and expanding the $B(\lambda r)$ term, Eq. (3) becomes

$$-\frac{1}{2} \frac{d^2 \Psi(\xi)}{d\xi^2} - \frac{1}{\xi} \frac{d\Psi(\xi)}{d\xi} - \frac{1}{\xi} \Psi(\xi) + \sum_{t=1}^{\infty} B_t \epsilon^t \xi^{t-1} \Psi(\xi) + \frac{1}{2} \frac{l(l+1)}{\xi^2} \Psi(\xi) = \frac{E}{Z^2} \Psi(\xi), \tag{4}$$

where $\epsilon = \lambda/Z$. We now expand Ψ and E in perturbation-theory form:

$$\Psi(\xi) = \sum_{j=0}^{\infty} \Psi_j(\xi) \epsilon^j, \tag{5}$$

$$\frac{E}{Z^2} = \sum_{i=0}^{\infty} E_i \epsilon^i, \tag{6}$$

with

$$E_0 = -1/2n^2. \tag{7}$$

Substituting Eqs. (5) and (6) into Eq. (4) and setting the coefficient of ϵ^k equal to zero we obtain

$$-\frac{1}{2} \Psi_k'' - \frac{1}{\xi} \Psi_k' - \frac{1}{\xi} \Psi_k + \frac{1}{2} \frac{l(l+1)}{\xi^2} \Psi_k - E_0 \Psi_k = \sum_{w=0}^{k-1} (-B_{k-w} \xi^{k-w-1} + E_{k-w}) \Psi_w. \tag{8}$$

Letting $\xi = (\frac{1}{2}n)y$, we look for a solution to Eq. (8) of the form

$$\Psi_k(y) = e^{-y/2} y^l u_k(y). \tag{9}$$

Substituting Eq. (9) into Eq. (8), we obtain the inhomogeneous Laguerre differential equation in u_k as

$$y u_k'' + (\alpha + 1 - y) u_k' + q u_k$$

$$= \sum_{w=0}^{k-1} (B_{k-w} n(\frac{1}{2}ny)^{k-w} - \frac{1}{2}n^2 y E_{k-w}) u_w, \quad (10)$$

where the prime indicates differentiation with respect to y and

$$\alpha = 2l + 1, \quad q = n - l - 1. \quad (11)$$

The homogeneous solution of Eq. (10) is the associated Laguerre polynomial

$$u_0(y) = L_q^\alpha(y). \quad (12)$$

Let us note that $L_j^\alpha(y)$ satisfies the relation

$$yL_j^\alpha(y) = -(\alpha + j)^2 L_{j-1}^\alpha + (\alpha + 2j + 1)L_j^\alpha - [(j + 1)/(\alpha + j + 1)]L_{j+1}^\alpha. \quad (13)$$

Successive applications of this formula indicate

$$S(i, j, k - w) = (-1)^{i+j} \frac{(j + \alpha)!}{(i + \alpha)!} \sum_{\sigma_{\min}}^{\sigma_{\max}} \frac{[\alpha + (k - w) + \sigma]!}{\sigma!(i - \sigma)!(j - \sigma)! [\sigma + (k - w) - i]! [\sigma + (k - w) - j]!},$$

where σ_{\min} is the larger of $i - (k - w)$ or $j - (k - w)$, and σ_{\max} is the smaller of i or j . A tabulation of various values of $\Gamma(i, j, k - w)$ appears in the Appendix.

Let us now look for the solution, in any order k , as a sum of associated Laguerre polynomials of the form

$$u_k = \sum_j A_{k,j} L_j^\alpha. \quad (17)$$

Since L_j^α satisfies the homogeneous part of Eq. (10) with q replaced by j , we obtain

$$\sum_j (q - j)A_{k,j} L_j^\alpha = \sum_{w=0}^{k-1} [B_{k-w} n(\frac{1}{2}n)^{k-w} \sum_j A_{w,j} \times \sum_{i=j-(k-w)}^{j+(k-w)} \Gamma(i, j, k-w) L_i^\alpha - \frac{1}{2}n^2 E_{k-w} \times \sum_j A_{w,j} \sum_{i=j-1}^{j+1} \Gamma(i, j, 1) L_i^\alpha], \quad (18)$$

where $A_{0,j} = \delta_{j,q}$. Working out a few low-order results leads one to a s th-order perturbation wave function for the (n, l) or (q, α) state which is a finite sum of Laguerre polynomials

$$u_s = \sum_{j=q-s}^{q+s} A_{s,j} L_j^\alpha. \quad (19)$$

Therefore, our final equation for determining the $A_{i,j}$'s and the E_j 's is obtained by including the proper limits on the j summations:

that

$$y^{k-w} L_j^\alpha(y) = \sum_{i=j-(k-w)}^{j+(k-w)} \Gamma(i, j, k-w) L_i^\alpha(y), \quad (14)$$

whereby making use of the normalization properties of the Laguerre polynomials, one readily obtains

$$\Gamma(i, j, k-w) = \{i! / [(i + \alpha)!]^3\} \times \int_0^\infty e^{-y} y^{k-w+\alpha} L_i^\alpha(y) L_j^\alpha(y) dy. \quad (15)$$

The above integral has been evaluated⁴ to obtain

$$\Gamma(i, j, k-w) = \{i! [(k-w)!]^2 / (i + \alpha)!\} S(i, j, k-w), \quad (16)$$

where

$$\sum_{i=q-k}^{q+k} (q-i)A_{k,i} L_i^\alpha = \sum_{w=0}^{k-1} \sum_{j=q-w}^{q+w} [B_{k-w} n(\frac{1}{2}n)^{k-w} \sum_{i=j-(k-w)}^{j+(k-w)} \Gamma(i, j, k-w) L_i^\alpha - n(\frac{1}{2}n) E_{k-w} \sum_{i=j-1}^{j+1} \Gamma(i, j, 1) L_i^\alpha] A_{w,j}. \quad (20)$$

We now proceed to solve Eq. (20) through successive orders. For $k=1$ we obtain

$$\sum_{i=q-1}^{q+1} (q-i)A_{1,i} L_i^\alpha = \frac{1}{2}n^2 (B_1 - E_1) \sum_{i=q-1}^{q+1} \Gamma(i, q, 1) L_i^\alpha, \quad (21)$$

from which we obtain

$$E_1 = B_1 \quad (22)$$

in order that the coefficient of the L_q^α term on right-hand side of Eq. (21) is zero. It then follows that $A_{1,q-1} = A_{1,q+1} = 0$. We choose $A_{1,q} = 0$ also. The above result occurs since the first-order perturbation is a constant B_1 . For second order ($k=2$), we set the coefficient of the L_q^α term equal to zero first to obtain the energy E_2 as

$$E_2 = \frac{1}{2}B_2 n \frac{\Gamma(q, q, 2)}{\Gamma(q, q, 1)} = \frac{1}{2}B_2 [3n^2 - l(l+1)]. \quad (23)$$

We obtain the coefficients of the Laguerre polynomials entering the second-order wave function as

$$A_{2,q-2} = \frac{1}{8}B_2 n^3 \Gamma(q-2, q, 2) = \frac{1}{8}B_2 n^3 (n+l)^2 (l+n-1)^2, \quad (24a)$$

$$A_{2,q-1} = \frac{1}{4} B_2 n^3 \left(\Gamma(q-1, q, 2) - \frac{\Gamma(q, q, 2)}{\Gamma(q, q, 1)} \Gamma(q-1, q, 1) \right) \\ = -\frac{1}{4} B_2 n^2 (n+l)^2 [n(n-2) + l(l-1)], \quad (24b)$$

$$A_{2,q+1} = -\frac{1}{4} B_2 n^3 \left(\Gamma(q+1, q, 2) - \frac{\Gamma(q, q, 2)}{\Gamma(q, q, 1)} \Gamma(q+1, q, 1) \right) \\ = \frac{1}{4} B_2 n^2 \frac{n-l}{n+l+1} [n(n+2) + l(l+1)], \quad (24c)$$

$$A_{2,q+2} = -\frac{1}{8} B_2 n^3 \Gamma(q+2, q, 2) = -\frac{1}{8} B_2 n^3 \frac{(n-l+1)(n-l)}{(n+l+2)(n+l+1)}, \quad (24d)$$

where we have again chosen the coefficient of the homogeneous term equal to zero.

Proceeding in higher order in the same way, one obtains in third order

$$E_3 = \left(\frac{1}{2}n\right)^2 B_3 \frac{\Gamma(q, q, 3)}{\Gamma(q, q, 1)}; \quad (25)$$

$$A_{3,q-3} = \frac{1}{8} B_3 n \left(\frac{1}{2}n\right)^3 \Gamma(q-3, q, 3), \quad (26a)$$

$$A_{3,q-2} = \frac{1}{2} B_3 n \left(\frac{1}{2}n\right)^3 \Gamma(q-2, q, 3), \quad (26b)$$

$$A_{3,q-1} = B_3 n \left(\frac{1}{2}n\right)^3 \left(\Gamma(q-1, q, 3) - \Gamma(q, q, 3) / \Gamma(q, q, 1) \Gamma(q-1, q, 1) \right), \quad (26c)$$

$$A_{3,q+1} = -B_3 n \left(\frac{1}{2}n\right)^3 \\ \times \left(\Gamma(q+1, q, 3) - \frac{\Gamma(q, q, 3)}{\Gamma(q, q, 1)} \Gamma(q-1, q, 1) \right), \quad (26d)$$

$$A_{3,q+2} = -\frac{1}{2} B_3 n \left(\frac{1}{2}n\right)^3 \Gamma(q+2, q, 3), \quad (26e)$$

$$A_{3,q+3} = -\frac{1}{8} B_3 n \left(\frac{1}{2}n\right)^3 \Gamma(q+3, q, 3). \quad (26f)$$

Using the appropriate values of Γ in the Appendix, the third-order energy correction [Eq. (25)] becomes

$$E_3 = \frac{1}{2} n^2 B_3 [5n^2 - 3l(l+1) + 1]. \quad (27)$$

The final expression for the fourth-order energy is

$$E_4 = B_4 \left\{ \frac{1}{8} n^2 [35n^2(n^2-1) - 30n^2(l+2)(l-1) + 3l(l+2)(l+1)(l-1)] \right. \\ \left. + B_2^2 \left\{ \frac{1}{32} n^3 [(n-l-1)(n-l-2) \times (n+l)(n+l-1) - (n-l+1)(n-l)(n+l+2)(n+l+1)] \right. \right. \\ \left. \left. + \frac{1}{16} n [(n+l)(n-l-1)[n(n-2) + l(l+1)]^2 - (n-l)(n+l+1)[n(n+2) + l(l+1)]^2] \right\} \right\}. \quad (28)$$

Equation (28) is a new result for a general n, l state. Correct results for an arbitrary n, l state for the problem of the screened Coulomb potential where

$$B_t (-1)^{t+1} / t! \quad (29)$$

have been derived correctly through third order by

Smith.⁵ Calculations through tenth order have been obtained for the ground state and to fifth order for states with $l=n-1$ and the 2S state by the present authors.¹ For the screened Coulomb potential, using Eq. (29) in Eq. (28), E_4 is observed to go over properly to the authors's earlier results for the states above.

It is clear that Eq. (20) may be utilized to obtain higher-order perturbation-theory results in a straightforward way for any arbitrary state and central-field potential of the assumed analytic form.

III. PADÉ APPROXIMANTS

The usefulness of high-order perturbation-theory results can be markedly extended by reexpressing the original perturbation-theory expansion (to k th order) as a series of rational fractions, Padé approximants, of the form

$$E \approx \sum_{i=0}^k E_i \epsilon^i \approx R_{m/n}^{(k)}(\epsilon) = \sum_{j=0}^m a_j \epsilon^j / \sum_{l=0}^n b_l \epsilon^l, \quad (30)$$

subject to the condition that

$$m+n=k. \quad (31)$$

Equating coefficients in Eq. (30), we find that

$$\sum_{j=0}^s b_j E_{s-j} = a_s \quad (s=0, 1, \dots, k), \quad (32)$$

where $a_s = 0$ for $s > m$, and $b_j = 0$ for $j > n$. The a 's and b 's can be uniquely determined from Eq. (32) once we choose

$$a_0 = E_0. \quad (33)$$

The utilization of Padé approximants has been shown to be effective in greatly accelerating the convergence of many slowly convergent sequences and in inducing convergence in many divergent sequences.⁶

We will now apply this technique to our previously calculated results⁷ for the ground-state energy of an electron in a screened Coulomb potential to tenth order in perturbation theory. An analysis of that expansion showed it to be divergent. We were, however, able to show very good agreement with numerical integration calculations for $\epsilon \leq 0.4$. Note that for the original perturbation series, an $\epsilon = 0.8956$ led to a fifth-order correction which was larger than the fourth-order correction. Therefore, the series was terminated after four terms. This gave a value of -2 times the energy equal to -0.3064 , whereas the correct result is 0.0501 . Now by reexpressing our entire tenth-order perturbation series as an $R_{55}^{(10)}$ approximant (see Table I), we find agreement up to the third significant figure with numerical integration results. Thus, obtaining high-order results and utilizing Padé-

TABLE I. Tabulation of diagonal terms $R_{n,n}^{(k)}$ of the Padé table in order of increasing k , the order of perturbation theory.

$\epsilon = \lambda/Z$	$R_{11}^{(2)}$	$R_{22}^{(4)}$	$R_{33}^{(6)}$	$R_{44}^{(8)}$	$R_{55}^{(10)}$	$-\frac{1}{2} E_{\text{NI}^a}/Z^2$	$-\frac{1}{2} E_{\text{var}^b}/Z^2$
0.0100	0.9802	0.9802	0.9802	0.9802	0.9802	0.9801	...
0.1000	0.8140	0.8142	0.8141	0.8141	0.8141	0.8141	...
0.2000	0.6522	0.6471	0.6536	0.6536	0.6536	0.6536	...
0.2017	0.6496	0.6447	0.6511	0.6511	0.6511	0.6510*	...
0.2500	0.5789	0.5758	0.5819	0.5818	0.5818	0.5818	0.5818
0.3000	0.5102	0.5970	0.5153	0.5153	0.5153	...	0.5153
0.4000	0.3846	0.3810	0.3970	0.3968	0.3968	...	0.3968
0.5000	0.2727	0.2783	0.2972	0.2963	0.2962	0.2962	0.2962
0.6000	0.1724	0.1671	0.2148	0.2124	0.2123	...	0.2123
0.7000	0.0820	0.0758	0.1492	0.1441	0.1437	...	0.1437
0.7222	0.0631	0.0568	0.1370	0.1309	0.1305	0.1304*	...
0.8000	0.0000	-0.0070	0.1006	0.0903	0.0895	...	0.0894
0.8956	-0.0715	-0.0793	0.0723	0.0517	0.0503	0.0501*	...
0.9000	-0.0746	-0.0825	0.0692	0.0503	0.0488
1.0000	-0.1429	-0.1515	0.0561	0.0235	0.0210	0.0206	...

^a" E_{NI} " refers to the result of numerical integrations of Harwood (Ref. 10) as well as those of Rouse (Ref. 9) indicated by *.

^b" E_{var} " refers to the variational results of Harris (Ref. 11).

approximant procedures leads to eigenvalues in close agreement with the numerically integrated ones, even for divergent series and for nonperturbative values of ϵ ($\epsilon \sim 1$).

Typically the $R_{mn}^{(k)}$ results comprise a Padé table. Generally superior accuracy is obtained by considering the diagonal elements of the table⁸ – that is, those entries for which the degrees of the polynomials in both the numerator and the denominator are the same. Thus, in our table, we have utilized second-, fourth-, sixth-, eighth-, and tenth-order perturbation-theory results to obtain the diagonal approximant sequence $R_{11}^{(2)}$, $R_{22}^{(4)}$, $R_{33}^{(6)}$, $R_{44}^{(8)}$, and $R_{55}^{(10)}$. It is observed that the $R_{55}^{(10)}$ results agree to four figures with numerical^{9,10} and many-parameter variational calculations¹¹ for $\epsilon \leq 0.7$. Even for $\epsilon = 1$, agreement to two significant figures is found utilizing the tenth-order result.

ACKNOWLEDGMENT

We would like to thank James H. Renken of Sandia Laboratories for pointing out the importance of nonlinear transformations to induce convergence in divergent series.

APPENDIX: EVALUATION OF $\Gamma(i, j, k-w)$

The tabulation of various values of Γ requires evaluation of Eq. (16), namely

$$\Gamma(i, j, k-w) = \{i! [(k-w)!]^2 / (i+\alpha)!\} S(i, j, k-w), \quad (\text{A1})$$

where

$$S(i, j, k-w) = (-1)^{i+j} \frac{(j+\alpha)!}{(i+\alpha)!} \times \sum_{\sigma_{\min}}^{\sigma_{\max}} \frac{\{\alpha + (k-w) + \sigma\}!}{\sigma! (i-\sigma)! (j-\sigma)! \{\sigma + (k-w) - i\}! \{\sigma + (k-w) - j\}!}. \quad (\text{A2})$$

Since $S(i, j, k-w)$ obeys a reciprocity relation with respect to i and j (including σ_{\min} and σ_{\max}) that is

$$S(i, j, k-w) = S(j, i, k-w), \quad (\text{A3})$$

it then follows from Eq. (A1) that

$$\Gamma(j, i, k-w) = \frac{j!}{i!} \left(\frac{(i+\alpha)!}{(j+\alpha)!} \right)^3 \Gamma(i, j, k-w). \quad (\text{A4})$$

This expression, in addition to giving $\Gamma(j, i, k-w)$ in terms of $\Gamma(i, j, k-w)$, is also useful for obtaining $\Gamma(j+q, j, k-w)$ as a function of $\Gamma(j-q, j, k-w)$ ($q = \text{positive integer}$). In this regard, letting $i = j - q$, (A4) becomes

$$\Gamma(j, j-q, k-w) = \frac{j!}{(j-q)!} \left(\frac{(j-q+\alpha)!}{(j+\alpha)!} \right)^3 \times \Gamma(j-q, j, k-w). \quad (\text{A5})$$

Moreover, replacing j by $j+q$ reduces Eq. (A5) to

$$\Gamma(j+q, j, k-w) = \frac{(j+q)!}{j!} \left(\frac{(j+\alpha)!}{(j+\alpha+q)!} \right)^3 \times [\Gamma(j-q, j, k-w)_{j=j+q}]. \quad (\text{A6})$$

Thus, Eq. (A1) together with Eqs. (A4) and (A6) facilitate generating all nonvanishing Γ 's of interest.

Inspection of Eq. (14) shows that, for a given j and $(k-w)$, i varies from $j-(k-w)$ to $j+(k-w)$ indicating that there are $2(k-w)+1$ nonvanishing Γ 's. For example, with $(k-w)=1$, i ranges from $j-1$ to $j+1$. It then follows by direct application of Eqs. (A1) and (A6) that

$$\Gamma(j-1, j, 1) = -(\alpha+j)^2, \quad (\text{A7a})$$

$$\Gamma(j, j, 1) = \alpha+2j+1, \quad (\text{A7b})$$

$$\Gamma(j+1, j, 1) = -(j+1)/(j+\alpha+1), \quad (\text{A7c})$$

all other $\Gamma(i, j, 1)$ being zero. These coefficients are found to be in complete agreement with those of the recursive relation in Eq. (13). Since $\alpha=2l+1$ and $j=n-l-1$, Eq. (A7) can be written in terms of n, l as

$$\Gamma(j-1, j, 1) = -(l+n)^2 \quad (\text{A8a})$$

$$\Gamma(j, j, 1) = 2n, \quad (\text{A8b})$$

$$\Gamma(j+1, j, 1) = -(n-l)/(n-l+1). \quad (\text{A8c})$$

Various other Γ 's needed to complete the fourth-order results are, for $k-w=2$,

$$\Gamma(j-2, j, 2) = (n+l)^2(n+l-1)^2, \quad (\text{A9a})$$

$$\Gamma(j-1, j, 2) = -2(n+l)^2(2n-1), \quad (\text{A9b})$$

$$\Gamma(j, j, 2) = 2[3n^2 - l(l+1)], \quad (\text{A9c})$$

$$\Gamma(j+1, j, 2) = -2(n-l)(2n+1)/(n+l+1), \quad (\text{A9d})$$

$$\Gamma(j+2, j, 2) = (n-l)(n-l+1)/(n+l+2)(n+l+1); \quad (\text{A9e})$$

for $k-w=3$,

$$\Gamma(j-3, j, 3) = -(n+l)^2(n+l-1)^2(n+l-2)^2, \quad (\text{A10a})$$

$$\Gamma(j-2, j, 3) = 6(n+l)^2(n+l-1)^2(n-1), \quad (\text{A10b})$$

$$\Gamma(j-1, j, 3) = 3(n+l)^2 \{ (n-l-2)(n-l-3) + 3(n-l-2)(n+l+1) + (n+l+2)(n+l+1) \}, \quad (\text{A10c})$$

$$\Gamma(j, j, 3) = 4n[5n^2 - 3l(l+1) + 1], \quad (\text{A10d})$$

$$\Gamma(j+1, j, 3) = -[3(n-l)/(n+l+1)](n-l-1) \times (n-l-2) + 3(n-l-1)(n+l+2) + (n+l+3)(n+l+2), \quad (\text{A10e})$$

$$\Gamma(j+2, j, 3) = 6(n-l+1)(n-l)(n+1)/(n+l+2)(n+l+1), \quad (\text{A10f})$$

$$\Gamma(j+3, j, 3) = -(n-l+2)(n-l+1)(n-l) \times [(n+l+3)(n+l+2)(n+l+1)]^{-1}; \quad (\text{A10g})$$

and for $k-w=4$,

$$\Gamma(j, j, 4) = 2n[35n^2(n^2-1) - 30n^2(l+2) \times (l-1) + 3(l+2)(l+1)l(l-1)]. \quad (\text{A11})$$

*Research supported by the Science Development Program of the National Science Foundation.

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