

Higher-order perturbation theory for the bound states of the Dirac equation with a Yukawa-type potential

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The method of calculating higher orders of perturbation theory based on perturbation of the Fock operator with a purely discrete spectrum is generalized to the case of the Dirac equation with a potential of the Yukawa type. Corrections to any order of perturbation theory in the energy of an arbitrary bound state are given as finite polynomials which are determined through recurrence relations derived from the dynamical symmetry of the unperturbed problem. We propose a modified Padé approximant method which can be used to transform a divergent perturbation series into a rapidly convergent sequence for all bound and quasistationary states of the system.

1. INTRODUCTION

The quantum-mechanical problem of the motion of a particle in a central field of the form

$$U(r) = -Zr^{-1}V(\lambda r), \quad V(0) = 1, \quad (1)$$

where $V(x)$ is an entire analytic function of the variable $x = \lambda r$, is often encountered in nuclear theory and in plasma physics. For example, the Yukawa potential is of the form (1) with $V(x) = \exp(-x)$. Another well known case is the form $V(x) = 1 - x^2$.

Recent developments¹⁻³ in higher-order perturbation theory permit an analytic solution to the problem and the functional properties of the solution can be studied over wide ranges of the quantum numbers and parameters of the problem. In the nonrelativistic limit, the solution for a potential of type (1) has been obtained to high orders in perturbation theory³⁻⁷ with respect to the parameter λ . With the help of generalized summation methods for formally divergent series,⁸⁻¹⁰ the region of applicability of perturbation theory can be significantly widened and the energy levels can be obtained up to the ionization threshold^{3,5,7,11} and also the quasistationary states can be calculated.^{7,12}

For large values of Z , relativistic effects must be taken into account. Earlier,¹³ with the help of the method of Sturm expansions, closed-form expressions for the perturbation corrections to the bound states of the Dirac equation were obtained for a wide class of perturbing potentials. In the case of the potential (1), the first three orders of perturbation theory have been computed analytically¹⁴ for arbitrary values of the quantum numbers.

However the difficulty in calculating the perturbation terms grows rapidly with order, and a rather large number of terms in the perturbation series is necessary to get a solution good over wide ranges of the parameter λ .

In the present paper the higher orders of perturbation theory are calculated by a method based on the dynamical symmetry of the unperturbed Fock operator with a purely discrete spectrum. The method is equally suitable for the ground state and for arbitrary excited states of the Dirac equation. A general analytical expression is obtained for the expansion coefficients in the perturbation series in λ . With

the help of generalized summation methods, the energies of the bound and quasistationary states can be calculated accurately for all values of the quantum numbers n , l , and j .

2. PERTURBATION THEORY FOR THE DIRAC OPERATOR

We look for the stationary-state wave function of the Dirac equation in the form¹⁵

$$\Psi(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} f_1(r) \Omega_{jlm} \\ i^{l+l'} f_2(r) \Omega_{j'l'm} \end{pmatrix},$$

where l and j are the orbital and total angular momenta of the system, Ω_{jlm} are the spherical spinors, and $l' = 2j - l$. After separating out the angular variables and applying the scale transformation $r \rightarrow Zr$, the Dirac equation with potential (1) reduces to a set of two equations for the radial functions f_1 and f_2 :

$$\begin{aligned} \frac{df_1}{dr} + \frac{k}{r} f_1 &= \beta [-\beta^{-2} - E - r^{-1}V(\epsilon r)] f_2, \\ \frac{df_2}{dr} - \frac{k}{r} f_2 &= \beta [-\beta^{-2} + E + r^{-1}V(\epsilon r)] f_1. \end{aligned} \quad (2)$$

We use a system of units such that $\hbar = e = m = 1$. Here $k = l(l+1) - j(j+1) - 1/4\beta = \alpha Z$, and α is the fine structure constant. E is the energy divided by Z^2 and $\epsilon = \lambda/Z$.

From the assumption that $V(x)$ is analytic, we can use the expansion

$$r^{-1}V(\epsilon r) = r^{-1} + \sum_{i=1}^{\infty} V_i \epsilon^i r^{i-1} = r^{-1} + \delta V_\epsilon(r), \quad (3)$$

where the V_i are constant coefficients.

The eigenfunctions and the eigenvalues E are also expanded as power series in ϵ :

$$E = E_0 + \delta E, \quad \delta E = \sum_{N=1}^{\infty} E_N \epsilon^N, \quad (4)$$

where E_0 is the unperturbed eigenvalue of system (2) with the potential $V_0(r) = r^{-1}$ and δE is the correction due to the perturbation δV_ϵ .

Following the approach taken in Ref. 13, we transform to a set of equations for functions $F(x)$ and $G(x)$, related to f_1

and f_2 by

$$F(x) = (2-2E_c)^{1/2} f_1(\nu x/2) + (2+2E_c)^{1/2} f_2(\nu x/2),$$

$$G(x) = -(2-2E_c)^{1/2} f_1(\nu x/2) + (2+2E_c)^{1/2} f_2(\nu x/2),$$

where $E_c = \beta^2 E_0$, $\nu = \beta(1-E_c^2)^{-1/2}$, $x = 2\nu^{-1}r$. Eliminating one of the functions, say $G(x)$, from the above pair of equations, we find a single second-order equation for the function $F(x)$. The substitution

$$F(x) \rightarrow y(x) = [\nu - k + w(x)]^{-1/2} F(x), \quad (5)$$

where

$$w(x) = (\nu^2 x/2) [\delta E + \delta V_r(\nu x/2)], \quad (6)$$

converts this to the self-adjoint form

$$(L-N)Y(x) = W(x)Y(x), \quad (7)$$

where $N = E_c \nu + 1/2$ and L is a self-adjoint operator given by

$$L = -\frac{d}{dx} x \frac{d}{dx} + \frac{s^2}{4x} + \frac{x}{4}, \quad (8)$$

with $s = 2(k^2 - \beta^2)^{1/2}$. The unperturbed equation

$$(L-N)y^{(0)}(x) = 0 \quad (9)$$

corresponds to a Coulomb field and has a purely discrete spectrum of eigenvalues given by (see Ref. 16) $N_p = p + (s+1)/2$, where $p = 0, 1, 2, \dots$ is the radial quantum number. Setting $N = N_p$, we obtain

$$\nu = \{ [p + (k^2 - \beta^2)^{1/2}]^2 + \beta^2 \}^{1/2}$$

and the Sommerfeld formula for the unperturbed energies $E_0 = \beta^{-2}(1 - \beta^2/\nu^2)^{1/2}$.

The operator W on the right-hand side of (7) is due to the perturbation. We have

$$W(x) = E_c [w(x) - w'(x)] + (1-E_c^2)x^{-1}w(x)[2\nu + w(x)] + A(x)[2E_c(\nu + w(x)) - x + 1] - xA^2(x) + xA'(x), \quad (10)$$

where $w(x)$ is given by (6),

$$A(x) = w'(x)/2[\nu - k + w(x)], \quad w'(x) = dw/dx,$$

$$A'(x) = dA/dx.$$

Using (10), we expand W in a power series in ε :

$$W(x) = \sum_{m=1}^{\infty} W_m(x) \varepsilon^m. \quad (11)$$

The functions $W_m(x)$ are independent of ε , and according to (3), (4), and (6), are polynomials of degree m in x with coefficients dependent on E_1, E_2, \dots, E_m .

We seek a solution of (7) in the form

$$Y(x) = \sum_N \varepsilon^N \sum_{p=0}^{\infty} C_p^{(N)} y_p(x), \quad C_p^{(0)} = \delta_{pp_0}, \quad (12)$$

where the $C_p^{(N)}$ are the expansion coefficients of the N th order corrected function with respect to the complete set of eigenfunctions $\{y_p\}$, and p_0 is the radial quantum number of the unperturbed function $y_{p_0}(x)$,

$$y_p(x) = \left[\frac{p!}{\Gamma(p+s+1)} \right]^{1/2} x^{s/2} e^{-x/2} L_p^{(s)}(x),$$

where $L_p^{(s)}$ are the Laguerre polynomials.

Substituting (11) and (12) into equation (7), multiplying by $y_q(x)$ from the left, and integrating with respect to x , we obtain

$$(q-p_0)C_q^{(N)} = \sum_{m=1}^N \sum_{\substack{p=q-m \\ (p>0)}}^{q+m} W_m(q,p)C_p^{(N-m)}, \quad (13)$$

where

$$W_m(q,p) = \langle y_q | W_m | y_p \rangle.$$

Because of the dynamical symmetry of the unperturbed problem,¹⁷ for any integer p, q, m , we have $W_m(p,q) = 0$ if $|q-p| > m$, and hence the sums over m and p on the right-hand side of (13) are finite, so that in each order $C_p^{(N)} = 0$ for $|p-p_0| > N_0$.

The coefficients $C_q^{(N)}$ can be calculated from (13) if the coefficients $C_p^{(N_0)}$ ($N_0 < N$) and matrix elements $W_m(q,p)$ ($m \leq N$) are known. To obtain the N th-order correction to the energy, we use the relation

$$W_N(p_0, p_0) = - \sum_{m=1}^{N-1} \sum_{\substack{p=p_0-m \\ (p>0)}}^{p_0+m} W_m(p_0, p) C_p^{(N-m)}, \quad (14)$$

which follows from (13) with $q = p_0$. Since $W_N(p_0, p_0)$ depends linearly on E_N , relation (14) leads directly to an expression for E_N in terms of E_j and the coefficients $C_p^{(i)}$ for $i, j \leq N-1$ through a simple recurrence procedure. As a result, E_N can be written as a polynomial involving ν^2 , k , and E_c :

$$E_N = 2^{-\alpha_N} \sum_{i_1=M}^{N-1} \sum_{i_2=0}^{2(N-i_1-1)} \sum_{i_3=0}^{2(i_1-M)+i_2} B_{i_1 i_2 i_3}^{(N)} \nu^{2i_1} k^{i_2} E_c^{i_3}, \quad (15)$$

where the α_N are integers, M is the integral part of $(N-1)/2$, and the index i_3 takes values such that the sum $i_2 + i_3 + N$ is odd,

$$B_{i_1 i_2 i_3}^{(N)} = \sum_{\kappa_1, \kappa_2, \dots, \kappa_N} \gamma_{i_1 i_2 i_3}^{(N)}(\kappa_1, \kappa_2, \dots, \kappa_N) V_1^{\kappa_1} V_2^{\kappa_2} \dots V_N^{\kappa_N}, \quad (16)$$

where $\kappa_j \geq 0$, $\gamma_{i_1 i_2 i_3}^{(N)}(\kappa_1, \kappa_2, \dots, \kappa_N)$ is an integer, and $\sum_{j=1}^N \kappa_j = N$.

When $p = 0$, $\nu^2 = k^2$ and E_N are polynomials involving only two variables E_c and k . Explicit analytical expressions for the first several orders of perturbation-theory corrections to the energy of an arbitrary state are presented in the Appendix.

3. SUMMATION OF THE PERTURBATION SERIES FOR BOUND AND QUASISTATIONARY STATES

In most cases the perturbation series will have bounded radii of convergence or actually be asymptotic series. Therefore when the expansion parameter is sufficiently large, it is necessary to employ generalized summation methods to the series.

In the case of the Dirac equation with a Yukawa potential

$$U(r) = -Zr^{-1}e^{-\lambda r} \quad (V_i = (-1)^i/i!)$$

with use of (13) and (14) we calculated 26 of the expansion coefficients (4) for all states with quantum numbers $n = 1, 2, 3$ for $\beta = 0$ (the nonrelativistic limit), 10α , 20α , 40α , 80α , 110α , and the limiting value $\beta = 137|k|/\alpha$ ($\alpha^{-1} = 137.036$). In all cases the signs of E_n were alternating and $|E_n|$ rapidly increased with increasing N . The dependence of $|E_n|$ on β turned out to be a monotonic decrease. For example, in the $1s_{1/2}$ state for $Z = \beta/\alpha = 0, 40, 80, 110, 137$, the quantity E_{25} was respectively equal to $1.021 \cdot 10^{12}$, $6.911 \cdot 10^{11}$, $1.779 \cdot 10^{11}$, $1.921 \cdot 10^{10}$, and $8.423 \cdot 10^6$.

The perturbation series were summed using the method of Padé approximants.⁸ The usual Padé approximants $[M/L]$ to the function $f(\varepsilon)$ satisfy a linear equation

$$Q_L(\varepsilon)f^{[M/L]}(\varepsilon) - P_M(\varepsilon) = 0, \quad Q_L(0) = 1, \quad (17)$$

where $P_M(\varepsilon)$ and $Q_L(\varepsilon)$ are polynomials of degree M and L whose coefficients are determined from the condition

$$Q_L(\varepsilon)f(\varepsilon) - P_M(\varepsilon) = o(\varepsilon^{M+L}).$$

The method gives good results in the nonrelativistic case ($\beta = 0$).^{5,7} This method was used on the Dirac equation to calculate the energies of the bound states for all values of ε up to threshold.

In discussing the dependence of E on ε it is convenient to use the scale transformation $E \rightarrow \tilde{E}' = n^2 E'$, $\varepsilon \rightarrow \tilde{\varepsilon} = n^2 \varepsilon$, where $E' = E - \beta^2$. For fixed l and j and different n , the functions $\tilde{E}'(\tilde{\varepsilon})$ are very close to one another. The dependence of \tilde{E}' on $\tilde{\varepsilon}$ is shown in Fig. 1 for the states $1s_{1/2}$, $2s_{1/2}$, $3s_{1/2}$ with $\beta/\alpha = 0, 80, 110$. In the nonrelativistic case ($\beta = 0$) all three curves are identical to within the accuracy of the figure.

The critical values $\varepsilon = \varepsilon_c$ corresponding to a continuous energy spectrum are shown in Table I. The nonrelativistic values ε_c^0 are given in the second column. Relativistic values ε_c are given in columns 3, 4, and 5 for $\beta/\alpha = 40, 80, 110$, respectively. The corresponding values of λ_c are $\varepsilon_c Z$. For small Z the values ε_c can be approximated closely by the formula

$$\varepsilon_c \approx \varepsilon_c^0 + \beta^2 \delta \varepsilon_c. \quad (18)$$

The coefficients $\delta \varepsilon_c$ are given in the last column of Table I. With the help of (18), ε_c can be determined to an accuracy of

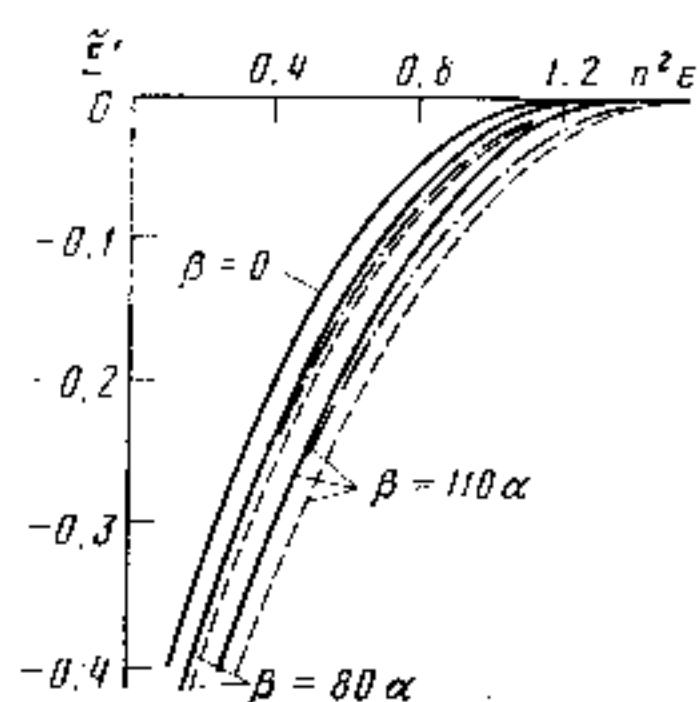


FIG. 1. Dependence of the energy of the s -levels on the screening parameter for different values of β . $\tilde{E}'_{l,j}$ is given by the solid curves, $\tilde{E}'_{2s,1/2}$ by the dotted curves, and $\tilde{E}'_{3s,1/2}$ by the dash-dot curves. Here $\tilde{E}' = (n/Z)^2(E - \beta^2)$ atomic units.

within 2% or less for Z values in the interval $0 < Z < 80$ for all states shown in Table I.

When $\varepsilon > \varepsilon_c$ and $l \neq 0$, because of the centrifugal barrier quasistationary states arise⁷ causing poles in the Padé approximants in the interval $\varepsilon_c \infty$ and the sequence of the Padé approximants in the interval (ε_c, α) and the sequence of the Padé approximants diverges. In order to find the energies in this region it is necessary to construct a multivalued analytic function which would give the real and imaginary parts of the energy for $\varepsilon > \varepsilon_c$. This can be done using the usual "linear" Padé approximants satisfying (17) by transforming the independent variable.⁷ If such a transformation is carried out with the help of a multivalued analytic function containing the parameter ε_c explicitly, then the energy and width of the Breit-Wigner resonance can be actually determined.¹²

In general, when there are both bound and quasistationary states, a sufficiently general summation method is required which does not assume *a priori* information on the threshold value of ε . The multi-valued function can be approximated by a single analytical expression using an approach which is in a certain sense a generalization of the Padé approximant method. In contrast to the usual Padé approximants, which satisfy the linear relation (17), we shall consider modified approximants which are solutions of nonlinear equations with polynomial coefficients determined from the expansion of the function to be approximated in a Taylor series.

TABLE I. Relativistic values of the critical screening parameter $\varepsilon_c(Z) = \lambda_c(z)/z$, atomic units.

n/j	$\varepsilon_c^0(Z=0)$	$\varepsilon_c(40)$	$\varepsilon_c(80)$	$\varepsilon_c(110)$	$\delta \varepsilon_c$
$1s_{1/2}$	1.1906	1.2050	1.2557	1.342	0.162
$2s_{1/2}$	0.31021	0.31676	0.3408	0.3848	0.0736
$2p_{3/2}$	0.220	0.221	0.223	0.225	0.008
$2p_{1/2}$	0.220	0.224	0.239	0.265	0.05
$3s_{1/2}$	0.13945	0.1421	0.1516	0.1686	0.0298
$3p_{3/2}$	0.113	0.114	0.115	0.117	0.0061
$3p_{1/2}$	0.113	0.115	0.121	0.133	0.021
$3d_{5/2}$	0.0913	0.0914	0.0919	0.0924	0.014
$3d_{3/2}$	0.0913	0.0918	0.0930	0.0946	0.005

TABLE II. Convergence of the "quadratic" approximants to the energy of the $2p$ state.

N	$E^{[N, N, N] \cdot 10^3}$		N	$E^{[N, N, N] \cdot 10^3}$	
	$\varepsilon=0,23$	0,26		$\varepsilon=0,23$	0,26
9	1,033 (0,409)	3,888 (3,40)	15	1,152 (0,407)	3,817 (3,37)
11	1,177 (0,382)	3,802 (3,38)	16	1,152 (0,407)	3,817 (3,37)
13	1,151 (0,411)	3,816 (3,36)			

For example, we consider the "quadratic" diagonal approximants $[N, N, N]$ satisfying the equation

$$P_N(\varepsilon) [E^{[N, N, N]}(\varepsilon)]^2 + Q_N(\varepsilon) E^{[N, N, N]}(\varepsilon) + R_N(\varepsilon) = 0, \quad (19)$$

where $P_N(\varepsilon)$, $Q_N(\varepsilon)$, and $R_N(\varepsilon)$ are polynomials of degree N determined from the conditions

$$P_N(\varepsilon) [E(\varepsilon)]^2 + Q_N(\varepsilon) E(\varepsilon) + R_N(\varepsilon) = o(\varepsilon^{2N+1}), \quad P_N(0) = 1. \quad (20)$$

In (20) the function $E(\varepsilon)$ is represented by the Taylor series (4) in powers of ε with known coefficients. The $3N + 2$ unknown coefficients of the polynomials P_N , Q_N , R_N are found by the solutions of a set of linear equations.

The convergence of the approximants to the energy of the $2p_{3/2}$ state for $\beta = 0$ and for values $\varepsilon = 0.23$ and 0.26 is demonstrated in Table II, where values of one branch of the function $E^{[N, N, N]}(\varepsilon)$ are given. The imaginary part of the function is shown in parentheses. The values of $\text{Re } E'(\varepsilon)$ and $\text{Im } E'(\varepsilon)$ for the $2p$ state for $\varepsilon > \varepsilon_c$ completely correspond to results obtained by the method of conformal mapping.¹²

According to the general results of Refs. 18 and 19, the dependence of $\text{Im } E'_{nl}$ on ε for $l \neq 0$ close to threshold is accurately described by the relation

$$\text{Im } E'_{nl}(\varepsilon) \approx C_0(nl) (\varepsilon - \varepsilon_c)^{l+1/2}. \quad (21)$$

For the $2p_{3/2}$ and $3p_{3/2}$ states at $\beta = 0$ we have $C_0(2p) = 0.42$ and $C_0(3p) = 0.36$.

We also considered approximants of higher degree (third, fourth, and fifth degree). In all cases the results were found to be self-consistent.

In Fig. 2 the dependence of the magnitude of the doublet splitting of the $2p$ levels ($E_{2p_{3/2}} - E_{2p_{1/2}}$) is shown as a function of ε divided by Z^2 . The results obtained using Padé approximants $[8/8]$ and $[13/12]$ differ by less than 10^{-4} for all Z .

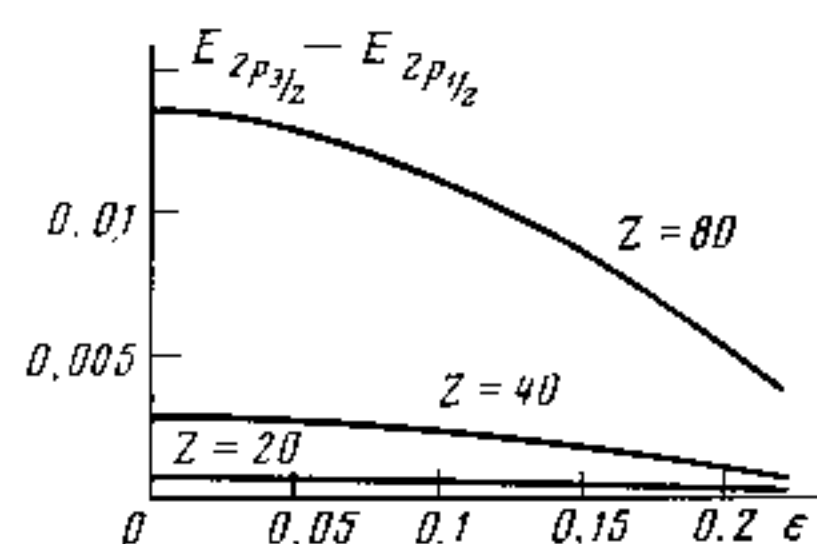


FIG. 2. Magnitude of the doublet splitting of the $2p$ level as a function of ε (in atomic units).

APPENDIX

From the recurrence relations (13) and (14) we obtain directly

$$\begin{aligned} E_1 &= -V_1; \quad E_2 = 2^{-1} V_2 (k + k^2 E_c - 3v^2 E_c); \\ E_3 &= 2^{-1} V_3 v^2 [k^2 - 1 + k E_c (3 + 2k E_c) - v^2 (1 + 4E_c^2)]; \\ E_4 &= 2^{-2} v^2 \{ 6V_4 k + 3k^2 E_c (V_4 + V_2^2) + 2k^3 (V_2^2 - 3V_4) \\ &\quad + k^3 E_c^2 V_2^2 (4 + k E_c) + k^4 E_c (2V_2^2 - 3V_4) \\ &\quad + v^2 [6k V_4 (1 + 4E_c^2) - 5E_c (5V_4 + V_2^2) \\ &\quad + 6k^2 E_c (3V_4 + V_2^2) + 6k^2 E_c^3 (2V_4 - V_2^2)] \\ &\quad + v^4 E_c [-3(5V_4 + 4V_2^2) + 5E_c^2 (V_2^2 - 4V_4)] \}; \\ E_5 &= 2^{-3} v^4 \{ -12V_5 + 10k E_c (5V_5 + V_2 V_3) \\ &\quad + k^2 (15V_5 + V_2 V_3) + 4k^2 E_c^2 (5V_5 + 6V_2 V_3) \\ &\quad + 4k^4 E_c^2 (2V_2 V_3 - 3V_5) + 8k^4 E_c^4 V_2 V_3 \\ &\quad - 30k^3 E_c (V_5 - E_c^2 V_2 V_3) - k^4 (3V_5 + V_2 V_3) \\ &\quad + v^2 [6k E_c (5V_5 + 4V_2 V_3) - 3(1 + 6E_c^2) (5V_5 + 3V_2 V_3) \\ &\quad + 2k^2 (3V_5 + 5V_2 V_3) + 10k E_c^3 (4V_5 - V_2 V_3) \\ &\quad + 12k^2 E_c^2 (4V_5 + 3V_2 V_3) + 16k^2 E_c^4 (V_5 - 2V_2 V_3)] \\ &\quad + v^4 [24E_c^4 (V_2 V_3 - V_5) - 3(V_5 + 3V_2 V_3) \\ &\quad - 12E_c^2 (3V_5 + 5V_2 V_3)] \}. \end{aligned}$$

The expressions for E_1 , E_2 , E_3 obtained in Ref. 14 agree with our results.

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