

Bound state energies for the exponential cosine screened Coulomb potential

Sameer M. Ikhdaïr¹, Ramazan Sever²

¹ Department of Electrical Engineering, Near East University, Lefkoşa, Mersin 10, Turkey

² Department of Physics, Middle East Technical University, 06531 Ankara, Turkey

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Abstract. The energy eigenvalues of bound states of an electron in the general exponential cosine screened Coulomb potential are obtained using the shifted $1/N$ expansion method. The energies for the states from $1s$ to $8k$ are calculated from six to eight significant figures. The energy eigenvalues for the $1s$, $2s-2p$, $3s-3d$, and $4s-4f$ states are also presented as a function of the screening parameter λ . Results are compared with the ones obtained by other workers. The agreement reduces roughly for large λ . It is also observed that the convergence of the expansion series increases remarkably as l increases.

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I. Introduction

Screened Coulomb potentials are known to adequately describe the effective interaction in many-body atomic phenomena. The general exponential cosine screened Coulomb potential (GECSCP),

$$V(r) = -\frac{1}{r} e^{-\lambda r} \cos(\varepsilon \lambda r),$$

where ε is a constant, is important in this class of potentials [1–4].

The Schrödinger equation for such a potential does not admit exact solutions. So various approximate methods both numerical and analytical have been developed. It has applications in various fields of physics such as plasma physics, nuclear physics and solid state physics [5–18]. Lam and Varshni [5] have employed perturbation and variation methods to obtain the energy eigenvalues, the critical screening parameter and the number of bound states for the GECSCP. Further, the energy eigenvalues of the ECSCP [6] have been recalculated for the $1s$ state using the ground-states logarithmic perturbation theory [7, 8] and the Pade approximant method. The critical screening parameter λ_c for the s states has been studied

[9]. Lai [10] has been shown that the problem of screened Coulomb potentials can be solved to very high accuracy by using the hypervirial relations [11, 13] and the Pade approximant method. Lai has also reported [14] that the bound-states energies of the GECSCP for all eigenstates can be accurately determined within the framework of the same hypervirial Pade scheme. Dutt [15] investigated the problem of GECSCP to compute the energies for various s -states using the Ecker-Weizel approximation. He also extended the work of [1] with more complete problems and determined λ_c in the $1s$ state analytically [16]. Singh and Varshni [17] employed a numerical method to calculate the critical screening parameters and some energy eigenvalues for the $1s$ to $8k$ states. Sever and Tezcan [18] studied the problem of the GECSCP in the context of the large- N expansion and obtained energies of the ground state and the first excited state and the corresponding wave functions.

In this work, we investigate the bound-states of the more general GECSCP using the shifted $1/N$ expansion technique [19] which has been proved itself in solving the quantum mechanical problems. In Sect. II, we formulate the problem for any bound-state. In Sect. III, we discuss and compare our results with the other findings and results obtained by using the other methods for the sake of comparison. Finally Sect. IV is devoted for our conclusions.

II. The method

The N -dimensional radial Schrödinger equation for the GECSCP in atomic units ($\hbar = m = c = e = 1$) has the general form

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{[\bar{k} - (1-a)][\bar{k} - (3-a)]}{8r^2} - \frac{e^{-\lambda r}}{r} \cos(\varepsilon \lambda r) \right] \chi_{n,l}(r) = E_{n,l} \chi_{n,l}(r), \quad (1)$$

where $\bar{k} = N + 2l - a$, a is the so-called shifting parameter. We follow the prescription of the shifted $1/N$ expansion introduced by Imbo et al. [19] and make use of the expansions of $V(r)$ and E developed recently by us [20] to solve (1) for its bound-state energies. The energy eigenvalues are given by an expansion in powers of $1/\bar{k}$ as follows

$$E_{n,l} = \frac{\bar{k}^2}{r_0^2} \left[\frac{1}{8} - \frac{1}{4(1 + \lambda r_0 + \varepsilon \lambda r_0 \tan(\varepsilon \lambda r_0))} + \frac{\gamma^{(1)}}{\bar{k}^2} + \frac{\gamma^{(2)}}{\bar{k}^3} + O\left[\frac{1}{\bar{k}^4}\right] \right], \quad (2)$$

where $\gamma^{(1)}$ and $\gamma^{(2)}$ are defined in [21]. The quantities used in these definitions are listed in Appendix A.

The quantity r_0 is chosen so as to minimize the leading term, E_0 [20]. That is,

$$\frac{dE_0}{dr_0} = 0 \quad \text{and} \quad \frac{d^2E_0}{dr_0^2} > 0. \quad (3)$$

and therefore it satisfies the equation

$$(2l+1) + (2n_r+1)\bar{\omega} = 2\sqrt{r_0 \cos(\varepsilon \lambda r_0) e^{-\lambda r_0} (1 + \lambda r_0 + \varepsilon \lambda r_0 \tan(\varepsilon \lambda r_0))}, \quad (4)$$

where

$$\bar{\omega} \equiv 2\omega = \left(\frac{1 + \lambda r_0 - \lambda^2 r_0^2 + \varepsilon^2 \lambda^2 r_0^2 + \varepsilon \tan(\varepsilon \lambda r_0) (\lambda r_0 - 2\lambda^2 r_0^2)}{1 + \lambda r_0 + \varepsilon \lambda r_0 \tan(\varepsilon \lambda r_0)} \right)^{1/2}. \quad (5)$$

Once r_0 is determined, the task of obtaining the energy eigenvalues from the algebraic expression (2) and the other related equations become relatively simple and straight-forward. In (2) and (4), n_r and $n = (n_r + l + 1)$ are the radial and principal quantum numbers, respectively. The shifting parameter a is defined by

$$a = 2 - (2n_r + 1)\bar{\omega}, \quad (6)$$

Table 1. Critical screening parameter and energy eigenvalues for $\lambda/\lambda_c = 0.2, 0.4, 0.6,$ and 0.8 for states $1s$ to $8k$. Energies are in atomic units

State	λ_c	$-E_{n,l}$			
		$\lambda/\lambda_c = 0.2$	0.4	0.6	0.8
1s	0.720 524 085 88	0.358 409 88	0.229 165 57	0.120 212 67	0.042 203 71
2s	0.166 617 60	0.092 132 33	0.061 608 30	0.035 025 99	0.013 718 66
3s	0.072 436 99	0.041 255 06	0.027 928 33	0.016 259 67	0.006 797 35
4s	0.040 427 22	0.023 266 77	0.015 819 07	0.009 288 66	0.003 979 19
5s	0.025 787 30	0.014 907 19	0.010 154 02	0.005 984 67	0.002 592 94
6s	0.017 878 28	0.010 357 86	0.007 061 75	0.004 170 25	0.001 818 10
7s	0.013 122 87	0.007 612 19	0.005 192 52	0.003 069 96	0.001 343 64
8s	0.010 041 42	0.005 829 18	0.003 977 58	0.002 353 44	0.001 032 79
2p	0.148 205 03	0.095 594 23	0.067 435 68	0.041 453 00	0.018 504 59
3p	0.068 712 14	0.041 953 12	0.029 086 74	0.017 483 65	0.007 587 69
4p	0.039 263 40	0.023 484 29	0.016 175 11	0.009 646 77	0.004 163 42
5p	0.025 315 62	0.014 995 15	0.010 296 24	0.006 120 49	0.002 642 42
6p	0.017 652 07	0.010 399 98	0.007 129 04	0.004 231 16	0.001 830 09
7p	0.013 001 07	0.007 634 83	0.005 228 30	0.003 100 56	0.001 343 89
8p	0.009 970 09	0.005 842 43	0.003 998 28	0.002 370 10	0.001 029 36
3d	0.063 581 54	0.042 918 63	0.030 710 91	0.019 266 56	0.008 890 31
4d	0.037 405 05	0.023 832 89	0.016 756 04	0.010 271 31	0.004 594 56
5d	0.024 500 01	0.015 147 85	0.010 548 91	0.006 386 61	0.002 813 19
6d	0.017 242 90	0.010 476 48	0.007 254 85	0.004 360 91	0.001 906 28
7d	0.012 774 70	0.007 677 11	0.005 297 44	0.003 170 34	0.001 380 73
8d	0.009 835 21	0.005 867 76	0.004 039 22	0.002 410 50	0.001 048 10
4f	0.035 241 24	0.024 240 68	0.017 443 83	0.011 028 52	0.005 148 49
5f	0.023 482 16	0.015 339 08	0.010 868 90	0.006 733 76	0.003 058 97
6f	0.016 708 15	0.010 576 75	0.007 421 69	0.004 539 50	0.002 027 82
7f	0.012 469 38	0.007 734 29	0.005 392 13	0.003 270 36	0.001 445 72
8f	0.009 649 19	0.005 902 40	0.004 096 61	0.002 470 32	0.001 084 95
5g	0.022 371 42	0.015 548 64	0.011 223 13	0.007 124 83	0.003 345 99
6g	0.016 099 48	0.010 691 27	0.007 613 88	0.004 749 17	0.002 178 17
7g	0.012 110 84	0.007 801 61	0.005 504 54	0.003 391 74	0.001 530 49
8g	0.009 425 57	0.005 944 33	0.004 166 34	0.002 544 87	0.001 135 47
6h	0.015 455 48	0.010 812 85	0.007 819 75	0.004 976 95	0.002 345 81
7h	0.011 720 49	0.007 875 11	0.005 628 20	0.003 527 16	0.001 628 35
8h	0.009 176 57	0.005 991 13	0.004 244 70	0.002 629 95	0.001 195 75
7i	0.011 314 42	0.007 951 82	0.005 758 24	0.003 671 30	0.001 734 65
8i	0.008 912 13	0.006 040 96	0.004 328 69	0.002 722 20	0.001 262 76
8k	0.008 639 85	0.006 092 42	0.004 416 01	0.002 819 10	0.001 334 36

III. Results and discussions

We display the critical screening parameters λ_c and binding energies $-E_{n,l}$ at $\lambda/\lambda_c=0.2, 0.4, 0.6,$ and 0.8 for the $1s$ to $8k$ states in Table 1. We have compared our results with those of [17]. We observe the exact agreement with the other findings when $\lambda/\lambda_c=0.2$ and 0.4 and highly accurate result for $\lambda/\lambda_c=0.6$ and 0.8 . As in [5], it was also noticed that our results become exact with increasing quantum numbers. In Table 2 we list E_{1s} and E_{2p} values calculated for various screening parameters between 0 and λ_c . In Tables 3, 4, we present the calculated energy eigenvalues $E_{n,l}$ as a function of screening parameter λ for the $1s, 2s-2p, 3s-3d,$ and $4s-4f$ states respectively. Our estimated values of the energy eigenvalues are compared with those of the Pade approximation $E[10, 10]$ and $E[10, 11]$ by Lai [14] and the perturbation and variational calculations by Lam and Varshni [5]. As

Table 2. Energy eigenvalues as a function of screening parameter λ for the $1s$ and $2p$ states in atomic units

λ	$-E_{1s}$	$-E_{2p}$
0.00	0.500 000 00	0.125 000 06
0.02	0.480 007 83	0.105 074 64
0.04	0.460 061 01	0.085 559 07
0.06	0.440 200 57	0.066 777 29
0.08	0.420 463 86	0.048 996 93
0.10	0.400 884 21	0.032 470 11
0.12	0.381 492 73	0.017 488 58
0.13	0.371 875 64	0.010 707 76
0.14	0.362 316 55	0.004 519 88

clear from Tables 3–6, the estimated values from the shifted $1/N$ expansion method for various values of screening parameter λ coincide, except for the values of λ very close to the critical screening parameter λ_c .

Table 3. Energy eigenvalues as a function of screening parameter λ for the $1s$ state in atomic units

λ	$E[10, 10]$	$E[10, 11]$	Perturbation	Variational	Shifted
0.50	-0.077 680	-0.077 679	-0.068 047	-0.077 606	-0.078 532 70
0.40	-0.142 439	-0.142 439	-0.139 153	-0.142 418	-0.142 487 11
0.30	-0.219 416	-0.219 416	-0.218 619	-0.219 411	-0.219 391 58
0.20	-0.306 335	-0.306 335	-0.306 235	-0.306 334	-0.306 326 33
0.10	-0.400 885	-0.400 885	-0.400 883	-0.400 885	-0.400 884 21
0.08	-0.420 464	-0.420 464	-0.420 464	-0.420 464	-0.420 463 86
0.06	-0.440 201	-0.440 201	-0.440 201	-0.440 201	-0.440 200 39

Table 4. Energy eigenvalues as a function of screening parameter λ for the $2s$ and $2p$ states in atomic units

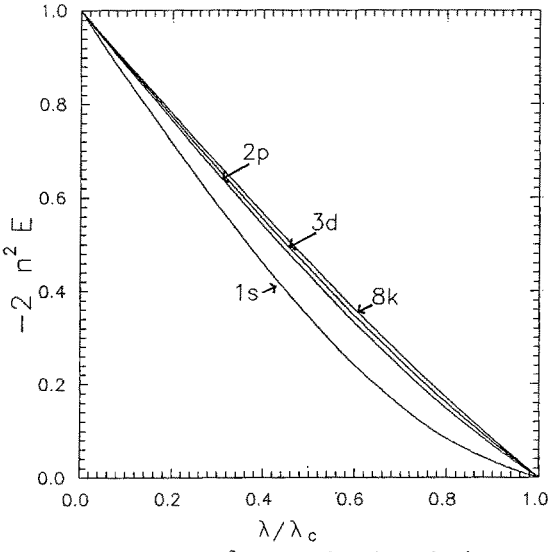
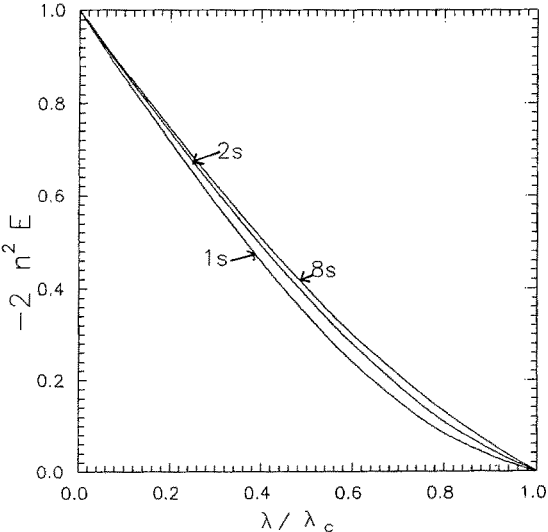
State	λ	$E[10, 10]$	$E[10, 11]$	Perturbation	Variational	Shifted
$2s$	0.10	-0.034 941	-0.034 941	-0.034 425	-0.034 935	-0.035 004 67
$2p$		-0.032 469	-0.032 469	-0.032 042		-0.032 470 15
$2s$	0.08	-0.050 387	-0.050 387	-0.050 222	-0.050 384	-0.050 408 25
$2p$		-0.048 997	-0.048 997			-0.048 996 93
$2s$	0.06	-0.067 421	-0.067 421	-0.067 385	-0.067 421	-0.067 426 08
$2p$		-0.066 778	-0.066 778			-0.066 777 29
$2s$	0.04	-0.085 769	-0.085 769	-0.085 767	-0.085 769	-0.085 769 59
$2p$		-0.085 591	-0.085 591			-0.085 559 13
$2s$	0.02	-0.105 104	-0.105 104	-0.105 104	-0.105 104	-0.105 103 61
$2p$		-0.105 075	-0.105 075	-0.105 075		-0.105 074 64

Table 5. Energy eigenvalues as a function of screening parameter λ for the $3s, 3p$ and $3d$ states in atomic units

State	λ	$E[10, 10]$	$E[10, 11]$	Perturbation	Variational	Shifted
$3s$	0.06	-0.005 461	-0.005 462	-0.004 538	-0.005 454	-0.005 666 38
$3p$		-0.004 471	-0.004 472			-0.004 492 33
$3d$		-0.002 308	-0.002 309			-0.002 313 56
$3s$	0.05	-0.011 576	-0.011 576			-0.011 685 44
$3p$		-0.010 929	-0.010 929	-0.010 538		-0.010 939 85
$3d$		-0.009 555	-0.009 555	-0.009 292		-0.009 555 42
$3s$	0.04	-0.018 823	-0.018 823	-0.018 707	-0.018 822	-0.018 867 16
$3p$		-0.018 453	-0.018 453			-0.018 457 05
$3d$		-0.017 682	-0.017 682			-0.017 682 08
$3s$	0.02	-0.036 025	-0.036 025	-0.036 022	-0.036 025	-0.036 027 38
$3p$		-0.035 968	-0.035 968	-0.035 965		-0.035 967 71
$3d$		-0.035 851	-0.035 851	-0.035 849		-0.035 850 66

Table 6. Energy eigenvalues as a function of screening parameter λ for the $4s$, $4p$, $4d$ and $4f$ states in atomic units

State	λ	$E[10, 10]$	$E[10, 11]$	Perturbation	Variational	Shifted
$4s$	0.04	-0.000 119	-0.000 125	+0.001 079	-0.000 118	-0.000 322 73
$4s$	0.03	-0.005 270	-0.005 270			-0.005 375 32
$4p$		-0.005 033	-0.005 033			-0.005 059 64
$4d$		-0.004 539	-0.004 539			-0.004 541 86
$4f$		-0.003 748	-0.003 748			-0.003 748 34
$4s$	0.02	-0.012 572	-0.012 572	-0.012 539	-0.012 572	-0.012 592 33
$4p$		-0.012 486	-0.012 486	-0.012 454		-0.012 490 69
$4d$		-0.012 310	-0.012 310	-0.012 283		-0.012 310 65
$4f$		-0.012 038	-0.012 038	-0.012 019		-0.012 038 16
$4s$	0.01	-0.021 438	-0.021 438	-0.021 436	-0.021 437	-0.021 438 62
$4p$		-0.021 424	-0.021 424	-0.021 424		-0.021 424 62
$4d$		-0.021 398	-0.021 398	-0.021 397		-0.021 397 99
$4f$		-0.021 358	-0.021 358	-0.021 357		-0.021 357 83

**Fig. 1.** Quantity $(-2n^2 E)$ as a function of λ/λ_c for $1s$, $2p$, $3d$, and $8k$ states. Curves for $4f$, $5g$, $6h$, and $7j$ states lie so close to the curve for the $8k$ state that they cannot be shown separately on the scale of the diagram**Fig. 2.** Quantity $(-2n^2 E)$ as a function of λ/λ_c for $1s$, $2s$, and $8s$ states. Curves for $3s-7s$ states lie so close to the curve for the $8s$ state that they cannot be shown separately on the scale of the diagram

The accuracy as well as the convergence increases as the principal and angular quantum numbers increase.

Figures 1 and 2 show that binding energies as a function of the screening parameter become flatter with increasing quantum numbers. This point is clear when we plot $-2n^2 E$ against λ/λ_c for states with maximum angular momentum $l=n-1$ and for s states respectively. These plots show a rapid approach to a limiting behavior for large quantum numbers. Similar behavior is exhibited by states with other values of l .

Appendix A. The values of ϵ_j 's, δ_j 's and $\gamma^{(1)}$ and $\gamma^{(2)}$ for ECSCP are

$$\delta_1 = -\frac{(1-a)(3-a)}{4}, \quad \delta_2 = -\frac{3}{2}\delta_1, \quad (\text{A1})$$

$$\delta_3 = (2-a), \quad \delta_4 = -\frac{5}{4}\delta_3, \quad (\text{A2})$$

$$\epsilon_1 = \frac{1}{2}\delta_3, \quad \epsilon_2 = -\frac{3}{4}\delta_3, \quad (\text{A3})$$

$$\begin{aligned} \epsilon_3 = & -\frac{1}{2} + \frac{r_0}{k^2} e^{-\lambda r_0} \cos(\epsilon \lambda r_0) [1 + \lambda r_0 + \frac{1}{2} \lambda^2 r_0^2 + \frac{1}{6} \lambda^3 r_0^3 \\ & + \epsilon \tan(\epsilon \lambda r_0) (\lambda r_0 + \lambda^2 r_0^2 + \frac{1}{2} \lambda^3 r_0^3) \\ & - \frac{1}{2} \epsilon^2 (\lambda^2 r_0^2 + \lambda^3 r_0^3) - \frac{1}{6} \epsilon^3 \tan(\epsilon \lambda r_0) \lambda^3 r_0^3], \quad (\text{A4}) \end{aligned}$$

$$\begin{aligned} \epsilon_4 = & \frac{5}{8} - \frac{r_0}{k^2} e^{-\lambda r_0} \cos(\epsilon \lambda r_0) \\ & \times [1 + \lambda r_0 + \frac{1}{2} \lambda^2 r_0^2 + \frac{1}{6} \lambda^3 r_0^3 + \frac{1}{24} \lambda^4 r_0^4 \\ & + \epsilon \tan(\epsilon \lambda r_0) (\lambda r_0 + \lambda^2 r_0^2 + \frac{1}{2} \lambda^3 r_0^3 + \frac{1}{6} \lambda^4 r_0^4) \\ & - \frac{1}{2} \epsilon^2 (\lambda^2 r_0^2 + \lambda^3 r_0^3 + \frac{1}{2} \lambda^4 r_0^4) \\ & - \frac{1}{6} \epsilon^3 \tan(\epsilon \lambda r_0) (\lambda^3 r_0^3 + \lambda^4 r_0^4) + \frac{1}{24} \epsilon^4 \lambda^4 r_0^4], \quad (\text{A5}) \end{aligned}$$

$$\begin{aligned} \delta_5 = & -\frac{3}{4} + \frac{r_0}{k^2} e^{-\lambda r_0} \cos(\epsilon \lambda r_0) [1 + \lambda r_0 + \frac{1}{2} \lambda^2 r_0^2 \\ & + \frac{1}{6} \lambda^3 r_0^3 + \frac{1}{24} \lambda^4 r_0^4 + \frac{1}{120} \lambda^5 r_0^5 + \epsilon \tan(\epsilon \lambda r_0) \\ & \times (\lambda r_0 + \lambda^2 r_0^2 + \frac{1}{2} \lambda^3 r_0^3 + \frac{1}{6} \lambda^4 r_0^4 + \frac{1}{24} \lambda^5 r_0^5) \\ & - \frac{1}{2} \epsilon^2 (\lambda^2 r_0^2 + \lambda^3 r_0^3 + \frac{1}{2} \lambda^4 r_0^4 + \frac{1}{6} \lambda^5 r_0^5) \end{aligned}$$

$$-\frac{1}{6}\varepsilon^3 \tan(\varepsilon\lambda r_0)(\lambda^3 r_0^3 + \lambda^4 r_0^4 + \frac{1}{2}\lambda^5 r_0^5) + \frac{1}{24}\varepsilon^4(\lambda^4 r_0^4 + \lambda^5 r_0^5) + \frac{1}{120}\varepsilon^5 \tan(\varepsilon\lambda r_0)\lambda^5 r_0^5], \quad (\text{A6})$$

$$\delta_6 = \frac{7}{8} - \frac{r_0}{k^2} e^{-\lambda r_0} \cos(\varepsilon\lambda r_0) [1 + \lambda r_0 + \frac{1}{2}\lambda^2 r_0^2 + \frac{1}{6}\lambda^3 r_0^3 + \frac{1}{24}\lambda^4 r_0^4 + \frac{1}{120}\lambda^5 r_0^5 + \frac{1}{720}\lambda^6 r_0^6 + \varepsilon \tan(\varepsilon\lambda r_0)(\lambda r_0 + \lambda^2 r_0^2 + \frac{1}{2}\lambda^3 r_0^3 + \frac{1}{6}\lambda^4 r_0^4 + \frac{1}{24}\lambda^5 r_0^5 + \frac{1}{120}\lambda^6 r_0^6) - \frac{1}{2}\varepsilon^2(\lambda^2 r_0^2 + \lambda^3 r_0^3 + \frac{1}{2}\lambda^4 r_0^4 + \frac{1}{6}\lambda^5 r_0^5 + \frac{1}{24}\lambda^6 r_0^6) - \frac{1}{6}\varepsilon^3 \tan(\varepsilon\lambda r_0)(\lambda^3 r_0^3 + \lambda^4 r_0^4 + \frac{1}{2}\lambda^5 r_0^5 + \frac{1}{6}\lambda^6 r_0^6) + \frac{1}{24}\varepsilon^4(\lambda^4 r_0^4 + \lambda^5 r_0^5 + \frac{1}{2}\lambda^6 r_0^6) + \frac{1}{120}\varepsilon^5 \tan(\varepsilon\lambda r_0)(\lambda^5 r_0^5 + \lambda^6 r_0^6) - \frac{1}{720}\varepsilon^6 \lambda^6 r_0^6], \quad (\text{A7})$$

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