Resonance transitions of Zn-like ions from the multiconfiguration relativistic random-phase approximation

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Excitation energies and oscillator strengths from the $^1S_0$ ground state to the first $^1P_1^\circ$ and $^3P_1^\circ$ excited states of Zn-like ions are calculated by using the multiconfiguration relativistic random-phase approximation. Results are compared with those from other theories and with experiment. Predicted values for highly stripped ions are listed.

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I. INTRODUCTION

Excitation energies and oscillator strengths for resonance transitions in highly stripped ions are needed for estimating the energy loss through impurity ions in plasmas and for plasma diagnostics. Precision spectroscopy both in astrophysical and in laboratory beam-foil measurements also demands accurate theoretical values. At present, a complete treatment of electron-electron correlations poses a formidable obstacle in theoretical calculations. In recent years, the relativistic random-phase approximation (RRPA) [1–3] and multiconfiguration

TABLE I. Excitation energies (in cm^{-1}) of the transition $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$ for Zn-like ions.

Ion	HF[a]	MCHF[a]	MCDF	RRPA[b]	RRPA[c]	MCRRPA	Experiment
Ga^{1+}	66 084	69 244	75 788	67 484	68 821	70 001	70 700[d]
Ge^{2+}	88 141	90 160	99 536	89 764	91 313	92 207	91 873[d]
As^{3+}	108 157	109 496	121 311		112 316	112 975	112 022[d]
Br^{5+}	145 490	146 060	162 753	150 985	152 538	153 133	151 274[d]
Kr^{6+}	163 421	163 728	183 136		172 493	173 028	170 832[e]
Rb^{7+}			203 528		192 782	192 992	190 502[f]
Nb^{11+}			287 157		275 175	275 298	271 939[f,g]
Mo^{12+}	266 662	266 223	308 946	294 554	296 458	296 827	293 333[f,g]
							293 255[h]
Ag^{17+}			426 290		412 803	413 222	409 271[i]
Cd^{18+}			451 870		438 070	438 672	434 696[i]
I^{23+}			593 910		579 205	580 294	576 495[i]
Xe^{24+}	466 383	465 286	625 630	608 663	610 629	611 944	607 903[h]
Cs^{25+}			658 640		643 640	644 953	641 313[i]
Ba^{26+}			693 000		677 869	679 296	675 950[j]
							675 804[i]
Tb^{35+}			1 077 570		1 061 566	1 064 029	
Hf^{42+}			1 502 530		1 486 144	1 489 390	
Ta^{43+}			1 574 890		1 558 466	1 561 750	1 563 722[j]
W^{44+}	794 937	793 840	1 650 390	1 634 448	1 633 803	1 637 317	1 639 882[j]
Pt^{48+}			1 989 730		1 973 168	1 976 921	
Au^{49+}			2 084 590	2 070 579	2 067 875	2 071 835	2 081 339[k]
Hg^{50+}			2 183 810		2 167 068	2 171 119	
Pb^{52+}			2 396 210		2 379 434	2 383 665	2 398 714[k]
Rn^{56+}			2 882 990		2 866 164	2 870 764	
U^{62+}			3 799 440	3 802 906	3 782 477	3 787 707	3 820 439[k]

[a]Fischer and Hansen, Ref. [23].
[b]Shorer and Dalgarno, Ref. [24], with QED corrections.
[c]Present results.
[d]Moore, Ref. [25].
[e]Fawcett, Jones, and Wilson, Ref. [26].
[f]Reader and Acquista, Ref. [27].
[g]Litzén and Ando, Ref. [28].
[h]Hinnov, Ref. [29].
[i]Acquista and Reader, Ref. [30].
[j]Reader and Luther, Ref. [31].
[k]Seely *et al.*, Ref. [32].

Dirac-Fock (MCDF) [4,5] have played two of the major roles in attacking the correlation problem in relativistic calculations and have produced extensive data on a variety of atoms and ions. Although it is possible to treat open-shell systems from the relativistic equation-of-motion approach [6], where the RRPA type as well as other correlations can be accounted for, the associated numerical techniques are still under development. In the meantime, the RRPA can be improved upon by using a multiconfiguration wave function as the reference state. The electron-electron correlation effects owing to the presence of "real" doubly excited configuration in the initial states are thereby included. This approach is called the multiconfiguration relativistic random-phase approximation (MCRRPA) [7]. In essence, it has certain features of the MCDF, while preserving all of the advantages, especially the gauge invariance of the RRPA. A detailed derivation of the MCRRPA theory has been given, and applications of the theory to photoexcitations of Be-, Mg-, Zn-, Cd-, Hg-, and Pb-like ions [8–12] and to photoionization of Be, Mg, Zn, and Sr atoms [13–17] have been reported and are in excellent agreement with experiment.

In this paper we present excitation energies and oscillator strengths from the $^1S_0$ ground state to the first $^1P_1^\circ$ and $^3P_1^\circ$ excited states of Zn-like ions by using the multiconfiguration relativistic random-phase approximation. Results are compared with other theories and experiment. In Sec. II we give a brief account of the MCRRPA theory. Results and discussion are presented in Sec. III.

II. THE MCRRPA THEORY

The MCRRPA theory is based on an approximate relativistic Hamiltonian

$$H(t)=H_0+V(t)\ . \tag{1}$$

Here the time-independent part H_0 is composed of single-electron Dirac Hamiltonians h_n and Coulomb terms e^2/r_{nm}, and $V(t)$ is a harmonic time-dependent

TABLE II. Oscillator strengths of the transition $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$ for Zn-like ions.

Ion	HF[a]	MCHF[a] (outer)	MCDF[a] (full)	RRPA[b]	RRPA	MCRRPA	Experiment
Ga^{1+}	2.53	1.97	1.71	1.97	2.022	1.983	1.85±0.15[c]
Ge^{2+}	2.51	1.96	1.71	1.98	2.048	1.979	1.85±0.2[c]
As^{3+}	2.40	1.90	1.67		2.010	1.935	1.56±0.23[c]
Br^{5+}	2.19	1.78	1.58	1.84	1.899	1.831	0.82±0.12[d]
							0.82±0.07[e]
Kr^{6+}	2.10	1.72	1.54		1.846	1.781	0.81±0.09[f]
							0.94±0.04[g]
							0.81±0.09[e]
Rb^{7+}					1.801	1.732	
Nb^{11+}					1.621	1.564	
Mo^{12+}	1.69	1.42	1.30	1.54	1.579	1.527	
Ag^{17+}					1.418	1.373	
Cd^{18+}					1.390	1.348	
I^{23+}					1.277	1.242	
Xe^{24+}	1.22	1.05	0.98	1.24	1.258	1.225	
Cs^{25+}					1.242	1.210	
Ba^{26+}					1.227	1.196	
Tb^{35+}					1.147	1.127	
Hf^{42+}					1.147	1.133	
Ta^{43+}					1.151	1.137	
W^{44+}	0.84	0.73	0.70	1.15	1.155	1.143	
Pt^{48+}					1.182	1.171	
Au^{49+}				1.19	1.190	1.180	
Hg^{50+}					1.199	1.190	
Pb^{52+}					1.220	1.212	
Rn^{56+}					1.269	1.262	
U^{62+}				1.37	1.361	1.356	

[a]Fischer and Hansen, Ref. [23].
[b]Shorer and Dalgarno, Ref. [24].
[c]Andersen *et al.*, Ref. [33].
[d]Pinnington, Kernahan, and Donnelly, Ref. [34].
[e]Knystautas and Drouin, Ref. [35].
[f]Druetta and Buchet, Ref. [36].
[g]Irwin *et al.*, Ref. [37].

external potential which induces transitions between atomic states:

$$H_0 = \sum_{n=1}^{N} h_n + \sum_{n<m}^{N} \frac{e^2}{r_{nm}} , \tag{2}$$

$$V(t) = v_+ e^{-i\omega t} + v_- e^{i\omega t} , \tag{3}$$

where the perturbing fields $v_\pm$ are sums of electric and magnetic multipole potentials [7].

Our point of departure is the time-dependent variational principle. We describe the many-electron system as a superposition of configuration wave functions with time-dependent weights. Since the external perturbation may have components with nonvanishing angular momentum and with odd parity, the atomic wave function contains terms of mixed angular momentum and parity. Applying the variational principle we derive time-dependent multiconfiguration Dirac-Fock equations describing the response of the atom to the external field. Terms independent of the external field lead to the usual stationary multiconfiguration Dirac-Fock description of an atomic state. Those terms proportional to the external field lead to equations describing the linear response of the atomic state to the external field; in the sequel we refer to these linear-response equations as the MCRRPA equations. If we start from a single-configuration reference state, the MCRRPA equations reduce to the usual RRPA equations. The MCRRPA equations may alternatively be derived from an equation-of-motion point of view [6].

Because of the near degeneracy of orbitals $4s_{1/2}$, $4p_{1/2}$, and $4p_{3/2}$, the $^1S_0$ ground states of Zn-like ions are not described well by a single-configuration wave function. Therefore in the present MCRRPA formulation, the reference state is given by a multiconfiguration wave

TABLE III. Excitation energies (in cm^{-1}) and oscillator strengths of the transition $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^o$ for Zn-like ions. Numbers in brackets represent powers of 10.

	Excitation energies			Oscillator strengths		
Ion	MCDF	MCRRPA	Experiment	MCRRPA	MCHF[h] (outer)	MCHF[h] (full)
Zn	29 249	28 440	32 501[a]	9.549[−5]		
Ga^{1+}	44 974	43 970	47 816[a]	3.803[−4]		
Ge^{2+}	59 861	58 758	62 496[a]	8.781[−4]		
As^{3+}	74 435	73 262	76 962[a]	1.617[−3]		
Br^{5+}	103 276	101 997	106 431[a]	3.922[−3]		
			105 675[b]			
Kr^{6+}	117 690	116 365	120 080[c]	5.540[−3]		
Rb^{7+}	132 150	130 782	134 522[d]	7.500[−3]		
Nb^{11+}	190 874	189 334	193 084[e]	1.904[−2]		
Mo^{12+}	205 836	204 246	207 980[e]	2.286[−2]	1.6[−2]	1.5[−2]
Ag^{17+}	282 560	280 663	284 251[f]	4.663[−2]		
Cd^{18+}	298 290	296 318	299 838[f]	5.203[−2]		
I^{23+}	378 780	376 390		7.954[−2]		
Xe^{24+}	395 220	392 714	396 040[g]	8.479[−2]	7.5[−2]	7.0[−2]
Cs^{25+}	411 780	409 209		8.989[−2]		
Ba^{26+}	428 450	425 793		9.478[−2]		
Tb^{35+}	583 290	579 989		1.274[−1]		
Hf^{42+}	709 840	706 294		1.394[−1]		
Ta^{43+}	728 380	724 822		1.403[−1]		
W^{44+}	747 070	743 507		1.411[−1]	1.78[−1]	1.71[−1]
Pt^{48+}	822 960	819 405		1.430[−1]		
Au^{49+}	842 250	838 693		1.432[−1]		
Hg^{50+}	861 640	858 112		1.433[−1]		
Pb^{52+}	900 820	897 334		1.432[−1]		
Rn^{56+}	980 600	977 258		1.421[−1]		
U^{62+}	1 103 630	1 100 588		1.388[−1]		

[a]Moore, Ref. [25].
[b]Curtis *et al.*, Ref. [38].
[c]Pinnington, Ansbacher, and Kernahan, Ref. [39].
[d] Litzén and Reader, Ref. [40].
[e]Litzén and Ando, Ref. [28].
[f]Churilov, Ryabtsev, and Wyart, Ref. [41].
[g]Hinnov *et al.*, Ref. [42].
[h]Ficher and Hansen, Ref. [23].

function of the form

$$\Psi(t)=C_1(4s^2_{1/2})_0+C_2(4p^2_{1/2})_0+C_3(4p^2_{3/2})_0\ , \qquad (4)$$

where the symbol $(4l_j^2)_0$ designates a Slater determinant constructed from the $4l_j$ valence orbital and core orbitals, and the subscript 0 denotes the total angular momentum quantum number $J=0$. The parameters C_a $(a=1,2,3)$ in the above equation are configuration weight coefficients. The core and valence orbitals and the configuration weights are determined by solving the MCDF equations numerically [4] with Fermi nuclear charge distribution. The Breit interaction and Lamb shift contributions are also evaluated perturbatively as corrections to the excitation energies in the present calculation. The method of evaluation is similar to that used in a series of MCDF calculations [18–22].

III. RESULTS AND DISCUSSION

Tables I and II give the excitation energies and oscillator strengths, respectively, of the transition $(4s^2)^1S_0\rightarrow(4s4p)^1P_1^\circ$ in Zn-like ions from the MCRRPA. Comparisons are made with those from other theories and with experiment. In Table II the large discrepancy between theories and experiment for Br^{5+} and Kr^{6+} may be due to an improper account of cascade effects in the measured lifetime, although core polarization effects could reduce the theoretical values. Similar comparisons for the transition $(4s^2)^1S_0\rightarrow(4s4p)^3P_1^\circ$ are shown in Table III. By subtracting the energies of the ground state $^1S_0$, calculated by using Eq. (4) as the reference state in the MCDF equations, from the energies of $^1P_1^\circ$ and $^3P_1^\circ$, calculated from

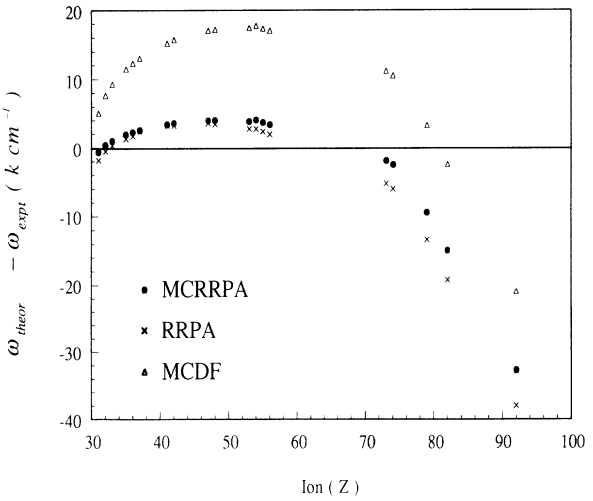

FIG. 1. Comparison of excitation energies from experiment and theories for the transition $(4s^2)^1S_0\rightarrow(4s4p)^1P_1^\circ$ in Zn-like ions. The data are given in Table VI.

TABLE IV. Various contributions to the MCDF excitation energies (in cm^{-1}) of the transition $(4s^2)^1S_0\rightarrow(4s4p)^1P_1^\circ$ for Zn-like ions. The MCDF value is the sum of Coulomb, Breit, and Lamb contributions.

Ion	MCDF	Coulomb	Breit	Lamb
Ga^{1+}	75 788	75 836	−26	−22
Ge^{2+}	99 536	99 603	−24	−43
As^{3+}	121 311	121 399	−22	−68
Br^{5+}	162 753	162 899	−14	−132
Kr^{6+}	183 136	183 315	−7	−172
Rb^{7+}	203 528	203 748	0	−220
Nb^{11+}	287 157	287 607	37	−487
Mo^{12+}	308 946	309 476	47	−577
Ag^{17+}	426 290	427 392	105	−1207
Cd^{18+}	451 870	453 131	117	−1378
I^{23+}	593 910	596 260	170	−2520
Xe^{24+}	625 630	628 270	180	−2820
Cs^{25+}	658 640	661 596	190	−3146
Ba^{26+}	693 000	696 301	200	−3501
Tb^{35+}	1 077 570	1 085 780	220	−8430
Hf^{42+}	1 502 530	1 517 630	270	−15 370
Ta^{43+}	1 574 890	1 591 310	240	−16 660
W^{44+}	1 650 390	1 668 410	10	−18 030
Pt^{48+}	1 989 730	2 014 510	−260	−24 520
Au^{49+}	2 084 590	2 111 350	−350	−26 410
Hg^{50+}	2 183 810	2 212 680	−460	−28 410
Pb^{52+}	2 396 210	2 429 700	−710	−32 780
Rn^{56+}	2 882 990	2 927 490	−1400	−43 100
U^{62+}	3 799 440	3 865 740	−3140	−63 160

TABLE V. Various contributions to the MCDF excitation energies (in cm^{-1}) of the transition $(4s^2)^1S_0\rightarrow(4s4p)^3P_1^\circ$ for Zn-like ions. The MCDF value is the sum of Coulomb, Breit, and Lamb contributions.

Ion	MCDF	Coulomb	Breit	Lamb
Zn	29 249	29 272	−10	−13
Ga^{1+}	44 974	45 002	−1	−27
Ge^{2+}	59 861	59 895	12	−46
As^{3+}	74 435	74 477	27	−69
Br^{5+}	103 276	103 339	68	−131
Kr^{6+}	117 690	117 765	95	−170
Rb^{7+}	132 150	132 241	126	−217
Nb^{11+}	190 874	191 050	308	−484
Mo^{12+}	205 836	206 042	369	−575
Ag^{17+}	282 560	282 989	791	−1220
Cd^{18+}	298 290	298 785	902	−1397
I^{23+}	378 780	379 759	1610	−2589
Xe^{24+}	395 220	396 342	1780	−2902
Cs^{25+}	411 780	413 065	1960	−3245
Ba^{26+}	428 450	429 908	2160	−3618
Tb^{35+}	583 290	587 580	4520	−8810
Hf^{42+}	709 840	718 770	7190	−16 120
Ta^{43+}	728 380	738 220	7640	−17 480
W^{44+}	747 070	757 860	8140	−18 930
Pt^{48+}	822 960	838 500	10 230	−25 770
Au^{49+}	842 250	859 210	10 810	−27 770
Hg^{50+}	861 640	880 110	11 420	−29 890
Pb^{52+}	900 820	922 650	12 690	−34 520
Rn^{56+}	980 600	1 010 540	15 540	−45 480
U^{62+}	1 103 630	1 149 940	20 680	−66 990

TABLE VI. Differences in excitation energies (in cm^{-1}) of various theories as compared with experiment for the two transitions $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$ and $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$ in Zn-like ions.

	$(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$					$(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$	
Ion	HF	MCHF	MCDF	RRPA	MCRRPA	MCDF	MCRRPA
Zn						−3229	−4061
Ga^{1+}	−4616	−1456	5088	−1879	−699	−2842	−3846
Ge^{2+}	−3732	−1713	7663	−560	334	−2635	−3738
As^{3+}	−3865	−2526	9289	294	953	−2527	−3700
Br^{5+}	−5784	−5214	11 479	1264	1859	−2399	−3678
Kr^{6+}	−7411	−7104	12 304	1661	2196	−2390	−3715
Rb^{7+}			13 026	2280	2490	−2372	−3740
Nb^{11+}			15 218	3236	3359	−2210	−3750
Mo^{12+}	−26 593	−27 032	15 691	3203	3572	−2144	−3734
Ag^{17+}			17 019	3532	3951	−1691	−3588
Cd^{18+}			17 174	3374	3976	−1548	−3520
I^{23+}			17 415	2710	3798		
Xe^{24+}	−141 520	−142 617	17 727	2726	4041	−820	−3326
Cs^{25+}			17 327	2327	3640		
Ba^{26+}			17 050	1919	3346		
Ta^{43+}			11 168	−5256	−1972		
W^{44+}	−844 945	−846 042	10 508	−6079	−2565		
Au^{49+}			3251	−13 464	−9505		
Pb^{52+}			−2504	−19 280	−15 049		
U^{62+}			−20 999	−37 962	−32 732		

TABLE VII. Predicted excitation energies (in cm^{-1}) of the transitions $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$ and $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$ for Zn-like ions.

	$(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$	$(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$	
Ion	Predicted values[a]	Predicted values[a]	Predicted values[b]
Zn		32 331	
Ga^{1+}	70 767	47 833	
Ge^{2+}	92 062	62 596	62 518
As^{3+}	112 075	77 074	76 899
Br^{5+}	151 111	105 757	105 747
Kr^{6+}	170 603	120 100	120 183
Rb^{7+}	190 250	134 491	134 642
Nb^{11+}	271 875	192 943	193 108
Mo^{12+}	293 331	207 830	207 955
Ag^{17+}	409 577	284 125	283 600
Cd^{18+}	435 013	299 756	299 046
I^{23+}	576 576	379 710	377 870
Xe^{24+}	608 223	396 011	393 963
Cs^{25+}	641 236	412 483	410 123
Ba^{26+}	675 595	429 044	426 462
Tb^{35+}	1 061 662	583 038	
Hf^{42+}	1 491 027	709 194	
Ta^{43+}	1 564 266	727 702	
W^{44+}	1 640 796	746 366	
Pt^{48+}	1 985 121	822 183	
Au^{49+}	2 081 430	841 450	
Hg^{50+}	2 182 191	860 849	
Pb^{52+}	2 397 923	900 032	
Rn^{56+}	2 892 159	979 878	
U^{62+}	3 820 553	1 103 096	

[a]Present results.
[b]Curtis, Ref. [43].

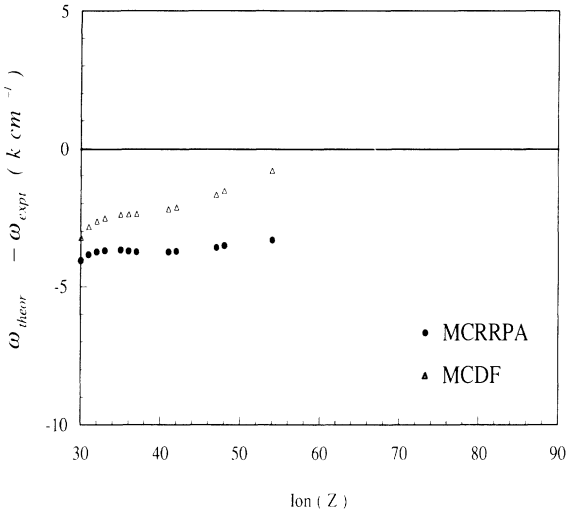

FIG. 2. Comparison of excitation energies from experiment and theories for the transition $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$ in Zn-like ions. The data are given in Table VI.

$$\Psi(t) = C_4(4s_{1/2}4p_{1/2})_1 + C_5(4s_{1/2}4p_{3/2})_1 , \quad (5)$$

we derived the excitation energies of the MCDF theory shown in Tables I and III. Each atomic state is optimized separately. The contributions of the Breit interaction and Lamb shift are listed in Tables IV and V for respective transitions. All the present MCDF, RRPA, and MCRRPA results contain these quantum electrodynamic and field-theoretic contributions.

Table VI gives the differences in excitation energies of various theories as compared with experiment. The lack of relativistic effects in the Hartree-Fock theory (HF) and multiconfiguration Hartree-Fock theory (MCHF) causes the errors in both theories to increase drastically for highly stripped ions. It is of interest to note that among various theories while the MCRRPA results for the transition $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$ agree better with experiment, the MCRRPA results for the transition $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$ are worse than the MCDF results. Data in Table VI are also shown in Figs. 1 and 2. Judging from the differences between the theories and experiment, there seems to be some irregularities in the experimental results for both transitions. On the theoretical side, the self-energy corrections may need to be reexamined in addition to correlation effects. Table VII lists the predicted excitation energies for the transitions $(4s^2)^1S_0 \rightarrow (4s4p)^1P_1^\circ$ and $(4s^2)^1S_0 \rightarrow (4s4p)^3P_1^\circ$, obtained by the regression analysis of the differences between the MCRRPA and experiment. Although the agreement between the MCRRPA and experiment for Zn-like ions is not as good as that for Be-like ions [8], the present method does offer a systematic way to obtain excitation energies for highly stripped ions where both the relativistic and correlation effects play important roles.

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