# Doubly excited nonautoionizing *P*, *D*, and *F* states of helium with Coulomb and screened Coulomb potentials

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We have investigated the doubly excited  ${}^{1,3}P^{\text{e}}$ ,  ${}^{1,3}D^{\text{o}}$ , and  ${}^{1,3}F^{\text{e}}$  nonautoionizing states of helium atom with Coulomb and screened Coulomb (Yukawa) potentials in the framework of Ritz variational principle. Highly accurate correlated exponential wave functions with exponents generated by a quasirandom process are used to represent the correlation effect. For the Coulomb case, the metastable bound-excited 2pnp  ${}^{1}P^{\text{e}}$  ( $3 \le n \le 5$ ), 2pnp  ${}^{3}P^{\text{e}}$  ( $2 \le n \le 5$ ), 2pnd  ${}^{1,3}D^{\text{o}}$  ( $3 \le n \le 9$ ), and 2pnf  ${}^{1,3}F^{\text{e}}$  ( $4 \le n \le 9$ ) states energies are reported. Our upper-bound results for the 2pnd  ${}^{1}D^{\text{o}}$  ( $3 \le n \le 7$ ), 2pnf  ${}^{1}F^{\text{e}}$  ( $4 \le n \le 8$ ),  ${}^{3}D^{\text{o}}$  and  ${}^{3}F^{\text{e}}$  states are the lowest values up to this date. For the screened Coulomb case, the lower-lying metastable bound states energies for different screening parameters and for each spin states are also reported.

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### I. INTRODUCTION

The study of the electron-electron correlation in helium plays an important role in the investigation of doubly excited states of helium atom as the two electrons are strongly correlated for such states. The importance of the electronelectron correlation become apparent after the pioneering observation of one-photon two-electron spectra of ground state of helium in the field of synchrotron radiation [1]. With the advanced experimental techniques [2,3], it becomes challenging to theoreticians to come up with more accurate results. Due to angular-momentum and parity conservation rules, the autoionization of doubly excited states below N=2 threshold of He is completely forbidden in LS approximation if the state has parity  $(-1)^{(L+1)}$ . The states with such "unnatural" parity do not interact with continuum; the Rayleigh-Ritz variational principle is applicable to obtain upper bound to respective exact state energies variationally. For a treatment of doubly excited quasibound states (resonances or "natural" parity states), readers are referred to our earlier works [4,5].

In the present investigation, we report the results for doubly excited states with unnatural parities lying below the He<sup>+</sup> (N=2) threshold. Our aim is to investigate the nonautoionizing doubly excited P, D, and F unnaturally parity states of neutral helium in the framework of the Ritz variational principle using highly correlated exponential basis functions. The helium atom with pure Coulomb and screened Coulomb (Yukawa) potentials is investigated. Several experimental investigations have been performed to observe the wavelengths of the  ${}^{3}P^{e} \rightarrow {}^{3}P^{o}$  and  ${}^{3}P^{e} \rightarrow {}^{3}D^{o}$  transitions of helium ([6,7], and references therein). Few theoretical investigations on the doubly excited metastable bound unnatural parity states of helium have been reported in the literatures [8-20]. The accurate 2pnp<sup>1,3</sup>P<sup>e</sup> metastable bound states energies of helium atom have been reported by Hilger et al. [14] using Hylleraas-configuration interaction-(CI)type basis functions. Recently, Mukherjee and Mukherjee reported the  $2p^{2} {}^{3}P^{e}$ [15] and  $2pnd^{1,3}D^{\circ}$  states [16] of He, using correlated wave functions. It is important to mention here that the  $2p^{2} {}^{3}P^{e}$  state eigenenergies reported by Hilger *et al.* [14] are more accurate than the reported results of Mukherjee and Mukherjee [15]. Details of the calculations with unnatural parity states can be found in the earlier works ([8–20], and references therein).

In the present work, we have obtained an accurate energy for the  $2pnp^{-1,3}P^{e}$ ,  $2pnd^{-1,3}D^{o}$ , and  $2pnf^{-1,3}F^{e}$  states of He using highly correlated exponential basis functions. Recently, we have reported the unnatural parity states of helium atom in which the Coulomb potential is replaced by screened Coulomb potentials [18–20] and CI-type basis functions were employed. In the present work, we have investigated the  $2p^2$  $^{1,3}P^{\rm e}$ ,  $^{2}p3p$   $^{1,3}P^{\rm e}$ ,  $^{2}p3p$   $^{1,3}D^{\rm o}$ , and  $^{2}p4f$   $^{1,3}F^{\rm e}$  states of helium with screened Coulomb (Yukawa) potentials using correlated basis functions. Our present results obtained by using correlated exponential functions are compared with our earlier works employing CI-type basis functions. Several of the Dand F-states energies obtained from the present work are the lowest in the literature and, due to the upper-bound principle, they are closer to the exact results. Our P-wave results are comparable with the reported results of Higler *et al.* [14]. Convergence of our calculations is examined with increasing number of terms in the basis expansions and with different sets of nonlinear variational parameters. The present study on the doubly excited metastable bound states of He employing highly correlated exponential wave functions could be used for the benchmark purpose in future investigations. All calculations have been performed in quadruple precision arithmetic (32 significant figures) on the IBM and ALPHA-DEC work stations in the UNIX, FEDORA, and CENT operating systems.

## **II. CALCULATIONS**

The nonrelativistic Hamiltonian describing the screened helium atom characterized by a parameter  $\mu$  is given by

TABLE I. Nonrelativistic energy eigenvalues -E (a.u.) and effective quantum numbers  $(n^*)$  for the  $2pnp^{-1,3}P^e$   $(3 \le n \le 5)$  states of helium.

	Present calculations						
n	-E n*		<i>n</i> *	-Е			
	500	600	700				
$^{3}P^{e}$							
2	$0.7105001556782^{a}$	0.7105001556783 <sup>a</sup>	0.7105001556783	<sup>a</sup> 1.5411992588340	0.7105001556567833 <sup>b</sup>		
					0.71050015565678 <sup>c</sup>		
					0.710500152070 <sup>d</sup>		
3	0.567812898706	0.567812898723	0.567812898724	2.7153689503058	0.56781289872515 <sup>b</sup>		
					0.56781130 <sup>e</sup>		
1	0.5358671786	0.5358671881	0.5358671887	3.73367346552	0.53586718876821 <sup>b</sup>		
5	0.5222539	0.52225436	0.52225457	4.73996788	0.52225457570723 <sup>b</sup>		
ı	400	500	600	$n^*$	-E		
		1	pe				
3	0.580246472580	0.580246472593	0.580246472594	2.496157741675	0.58024647259438 <sup>b</sup>		
					0.5802464636 <sup>e</sup>		
					$0.580246463^{\rm f}$		
1	0.5400415797	0.54004159008	0.54004159009	3.53369729835	0.540041590093851 <sup>b</sup>		
					0.540041588 <sup>f</sup>		
5	0.5241764	0.5241788	0.5241790	4.5474280	0.5241789818141 <sup>b</sup>		
					0.524178980 <sup>f</sup>		

<sup>a</sup>Values taken from our work [29].

<sup>b</sup>Reference [14].

<sup>c</sup>Reference [15].

<sup>d</sup>Reference [9].

<sup>e</sup>Reference [11].

<sup>f</sup>Reference [17].

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - 2\left[\frac{\exp(-\mu r_1)}{r_1} + \frac{\exp(-\mu r_2)}{r_2}\right] + \frac{\exp(-\mu r_{12})}{r_{12}},$$
(1)

where  $r_1$  and  $r_2$  are the radial coordinates of the two electrons and  $r_{12}$  is their relative distance. When the helium atom is placed in vacuum, we have  $\mu=0$ . In plasma physics, the parameter  $\mu$  (=1/ $\lambda$ ,  $\lambda$  is called the Debye length) is known as the Debye screening parameter.

For the  ${}^{1,3}P$ ,  ${}^{1,3}D$ , and  ${}^{1,3}F$  unnatural parity states of the helium atom, we employ highly correlated wave functions [21–23]

$$\Psi = (1 + S_{pn}\hat{P}_{12})\sum_{i=1}^{N}\sum_{l_1=\varepsilon}^{L}A_i(-1)^{\varepsilon}\boldsymbol{\mathcal{Y}}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2)$$
$$\times \exp(-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}), \qquad (2)$$

$$\boldsymbol{\mathcal{Y}}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) = r_1^{l_1} r_2^{l_2} \sum_{m_1,m_2} C_{l_1m_1,l_2m_2}^{LM} Y_{l_1m_1}(\hat{r}_1) Y_{l_1m_2}(\hat{r}_2), \quad (3)$$

where the functions  $\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1, \mathbf{r}_2)$  are the bipolar harmonics or Schwartz harmonics,  $\hat{r}_{j} = \mathbf{r}_{j}/r_{j}$  (j=1, 2),  $Y_{l_{j}m_{i}}(\hat{r}_{j})$  denotes the usual spherical harmonics,  $C_{l_{1}m_{1},l_{2}m_{2}}^{LM}$  are the Clebsch-Gordan coefficients,  $\alpha_{i}, \beta_{i}, \gamma_{i}$  are the nonlinear variation parameters,  $A_{i}(i=1,\ldots,N)$  are the linear-expansion coefficients,  $l_{1}+l_{2}$  $=L+\varepsilon, \varepsilon=1$ , and L=1 for P states, L=2 for D states, 3 for Fstates,  $S_{pn}=1$  indicates singlet states and  $S_{pn}=-1$  assigns triplet states, N is number of basis terms, and the operator  $\hat{P}_{12}$  is the permutation of the two identical particles 1 and 2. For F states, in Eq. (3), we consider  $l_{1}=\text{mod}(i/L)+\varepsilon$ , where mod(i/L) denotes the remainder of the integer division i/L. The nonlinear variational parameters  $\alpha_{i}, \beta_{i}$  and  $\gamma_{i}$  are chosen from a quasirandom process [22–25]. The nonlinear parameters  $\alpha_{i}, \beta_{i}$  and  $\gamma_{i}$  are chosen from the three positive intervals  $[A_{1}, A_{2}], [B_{1}, B_{2}]$ , and  $[C_{1}, C_{2}]$ ,

$$\alpha_i = \eta \langle \langle i(i+1)\sqrt{2}/2 \rangle \rangle (A_2 - A_1) + A_1 ],$$

$$\beta_i = \eta [\langle \langle i(i+1)\sqrt{3/2} \rangle \rangle (B_2 - B_1) + B_1],$$

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TABLE II. Nonrelativistic energy eigenvalues -E (a.u.) and effective quantum numbers  $(n^*)$  for the  $2pnd^{-1,3}D^0$  ( $3 \le n \le 9$ ) states of helium along with the wavelengths for the  $2p^{2-3}P^e \rightarrow {}^{3}D^0$  (TPD) and  $2p3p^{-1}P^e \rightarrow {}^{1}D^0$  (SPD) transitions (in angstrom).

	Present calculations $-E$			Other calculations $-E$				
п	800	900	1100	$n^*$	SPD	Ref. [16]	Ref. [17]	Ref. [10]
				$^{1}D^{\mathrm{o}}$				
3	0.563800420459	0.563800420462	0.563800420462	2.799453330	27704.70	0.56380042	0.563800349	0.563800405
4	0.534576385554	0.534576385555	0.534576385556	3.802727506	9976.618	0.53457638	0.534576361	0.534576015
5	0.521659015465	0.521659015466	0.521659015466	4.804693035	7776.972	0.52165901	0.521659004	0.521642770
6	0.51483359305	0.51483359320	0.51483359321	5.80579664	6965.494	0.51483359	0.514833587	0.51426906
7	0.5107926122	0.5107926187	0.5107926191	6.8064644	6560.226	0.51078723	0.510792615	
8	0.50820309	0.50820369	0.50820375	7.8069	6324.48	0.50801458	0.508203761	
9	0.506431	0.506442	0.506445	8.808	6173.8		0.506446070	
n	800	900	1100	$n^*$	TPD	Ref. [17]	Ref. [10]	
				$^{3}D^{0}$				
3	0.559328263093	0.559328263095	0.559328263096	2.903047789	3014.006	0.55932826	0.55932825	
4	0.532678601894	0.532678601895	0.532678601895	3.911589470	2562.305	0.53267860	0.532678075	
5	0.520703462027	0.520703462027	0.520703462028	4.91432093	2400.64	0.52070345	0.520693865	
6	0.5142883063	0.51428830660	0.51428830662	5.9155431	2322.15	0.514288303	0.51423578	
7	0.510452848	0.5104528561	0.5104528567	6.91620	2277.63	0.51045267		
8	0.5079769	0.5079779	0.5079780	7.9166	2249.79	0.50794530		
9	0.506267	0.506284	0.506287	8.918	2231.2			

$$\gamma_i = \eta [\langle \langle i(i+1)\sqrt{5/2} \rangle \rangle (C_2 - C_1) + C_1], \tag{4}$$

where the symbol  $\langle \langle ... \rangle \rangle$  denotes the fractional part of a real number,  $\eta$  is a scaling factor. As used in the earlier works [22–26], we set  $\eta$ =1. The exponential wave functions supported by the quasirandom process are widely used in several other works ([4,22–26], references therein). In this work, according to our computational scheme, it was found that the better and straight forward optimization can be obtained by setting  $A_1$ =0,  $B_1$ =0, and  $C_1$ =0. From here, we will mention  $A_2$ =A,  $B_2$ =B, and  $C_2$ =C. To evaluate necessary integrals, we follow the works of Calais and Löwdin [27], Drake [28], and Frolov and Smith, Jr. [21].

#### **III. RESULTS AND DISCUSSIONS**

We present our results for Coulomb and screened Coulomb interactions in two different subsections.

#### A. Results with Coulomb interaction

The optimized energies obtained from our calculations are presented in Tables I–III. From Table I, it is clear that the <sup>1,3</sup> $P^{e}$  energies are comparable with the best reported results [14]. Our <sup>1</sup> $D^{o}$  (n=3, 4, 5, 6) and <sup>3</sup> $D^{o}$  states energies presented in Table II are lower than the available results in the literature [16,17]. Our calculated results for the doubly excited <sup>1,3</sup> $F^{e}$  metastable bound states energies are presented in Table III, and such *F*-states energies obtained from the present calculations are comparable with our earlier work with CI-type basis functions. We have also presented the

convergence of the  ${}^{1,3}F^{e}$  states calculations in Table III. In our optimization, first we have optimized the eigenenergies for fixed number of terms in the wave functions for different sets of nonlinear parameters and then checked the convergence with the increasing number of basis terms. The results presented in Table I for P, Table II for D states, and Table III for F states are obtained with (2.84, 2.34, 0.3), (1.64, 0.84, 0.84)0.12), and (1.40, 0.22, 0.3) as optimized (A, B, C) parameter values, respectively. We have also use different sets of nonlinear parameters to check the convergence for higher number of terms, for example,  $2p^{2} {}^{3}P^{e}$ ,  $2p3p {}^{1}P^{e}$  states energies with 600 and 700 terms wave functions will be the same to all quoted digits in Table I also for parameter choice (2.84, 1.44, 0.8). The 2pnf  ${}^{1,3}F^{e}$   $(4 \le n \le 5)$  states energies are more accurate (lower) (for example, the  $2p4f^{-1,3}F^{e}$ eigenvalues are -0.531 995 436 952 6 energy and -0.531 991 326 348 9, respectively, using 1700-term basis functions) with parameters (1.84, 0.44, 0.2) than the results in Table III, and the  $2p3d^{-1,3}D^{\circ}$  energies seem more accurate (the values are  $-0.563\ 800\ 420\ 462\ 4$  for  ${}^{1}D^{0}$  and -0.559 328 263 097 3 for <sup>3</sup>D° states using 800-term wave functions) for the optimized parameters (2.84, 1.44, 0.2) with respect to (1.64, 0.84, 0.12) parameters used to generate Table II. We found that the parameter choices (2.84, 1.44, 0.8) for P states (2.84, 1.44, 0.2) for D states, and (1.84, (0.44, 0.2) for F states are not suitable to produce the best results for the higher values of the quantum number n. From the present optimization in the framework of the Ritz principle, it appears that the best parameter sets for all n are (2.84, 2.34, 0.3), (1.64, 0.84, 0.12), and (1.40, 0.22, 0.3),respectively, for P, D, and F states. To obtain the best upper TABLE III. Nonrelativistic energy eigenvalues -E (a.u.) and effective quantum numbers ( $n^*$ ) for the  $2pnf^{-1,3}F^e$  ( $3 \le n \le 9$ ) states of helium.

	Present results						
			-E				
n	1000	1200	1400	1600	1800		
			$^{1}F^{e}$				
4	0.53199543633	0.53199543679	0.53199543691	0.53199543694	0.5319954369461		
5	0.52038567050	0.52038567091	0.52038567101	0.52038567104	0.5203856710447		
6	0.51411321700	0.51411321805	0.51411321814	0.51411321817	0.5141132181756		
7	0.5103456999	0.5103457333	0.5103457371	0.5103457378	0.510345737802		
8	0.50790703	0.50790738	0.50790747	0.50790752	0.5079075428		
9	0.506209	0.506227	0.506235	0.5062378	0.506239511		
n	1000	1200	1400	1600	1800		
			$^{3}F^{e}$				
4	0.53199132569	0.53199132618	0.53199132630	0.53199132633	0.5319913263420		
5	0.52038285872	0.52038285914	0.52038285924	0.52038285927	0.5203828592800		
6	0.51411142787	0.51411142898	0.51411142908	0.51411142911	0.5141114291158		
7	0.5103445236	0.5103445598	0.5103445636	0.5103445644	0.510344564666		
8	0.50790620	0.50790658	0.50790667	0.507906714	0.507906741		
9	0.506207	0.506226	0.506234	0.5062370	0.50623893		
		Present results		Othe	r results		
		-E		-E			
n	2000	2200	$n^*$				
		$^{1}F^{e}$		Ref. [20] <sup>a</sup>	Ref. [17]		
4	0.5319954369491	0.5319954369509	3.953128934	0.5319954	0.531995404		
5	0.5203856710470	0.5203856710486	4.952477329	0.520385	0.520385649		
6	0.5141132181769	0.5141132181781	5.952124058	0.514113	0.514113204		
7	0.510345738036	0.510345738040	6.95191196		0.510345728		
8	0.5079075475	0.5079075482	7.95177491		0.507907542		
9	0.506239628	0.506239653	8.9516848		0.506239653		
n	2000	2200	$n^*$				
		$^{3}F^{e}$					
4	0.5319913263442	0.5319913263465	3.953382897	0.5319913			
5	0.5203828592823	0.5203828592839	4.952818909	0.5203828			
6	0.5141114291171	0.5141114291180	5.952501354	0.5141114			
7	0.510344564681	0.510344564686	6.95230621				
8	0.5079067453	0.5079067461	7.9521782				
9	0.506239057	0.506239088	8.952090				

<sup>a</sup>Our earlier work using CI-type basis functions.

bound with precision for each n, the energy level for each states should be optimized separately for the optimized choice of (A, B, C) in the framework of the Hylleraas-Undheim theorem. The present study is optimized in such a way that a particular set of optimized values of the nonlinear parameters can produce reasonably accurate energy levels for a particular partial-wave state. In Tables I–III, we have compared the results of Mihelič [17]. It is should be mentioned here that the  ${}^{1}P^{e}$ ,  ${}^{1}D^{o}$ , and  ${}^{1}F^{e}$  states energies of Mihelič [17] (presented in Tables I–III) were obtained in the context of resonance studies in dc electric field performed by a complex rotation method. To the best of our knowledge, there are no other results available in the literature on  $F^{e}$ states using correlated wave functions. TABLE IV. Unnatural parity P, D, and F bound states energies of the screened helium atom for different screening parameters along with the He<sup>+</sup>(2P) threshold energies.

λ	<sup>3</sup> P <sup>e</sup>	$^{1}P^{e}$	$^{1}D^{0}$	$-E^+_{\operatorname{He}(2P)}$
$\infty$	0.7105001556783, 0.71049955 <sup>a</sup>	0.580246472594, 0.58024645 <sup>a</sup>	0.5638004204575, 0.56380037 <sup>b</sup>	0.5000000000
100	0.6808807258575, 0.6808075 <sup>a</sup>	0.550899895763, 0.55080696 <sup>a</sup>	0.534448084917, 0.534357 <sup>b</sup>	0.4802475576
50	0.6520088035026, 0.651729 <sup>a</sup>	0.522806598165, 0.52245923 <sup>a</sup>	$0.506342548021, 0.506002^{b}$	0.4609808964
20	0.569696595978, 0.5681235 <sup>a</sup>	0.44540813084, 0.443627855 <sup>a</sup>	0.429011272975, 0.4272665 <sup>b</sup>	0.4059698543
15	0.526642274736, 0.5239985 <sup>a</sup>	0.4065111192, 0.40367417 <sup>a</sup>	0.390381642130, 0.3876165 <sup>b</sup>	0.3771352488
10	0.445977530750, 0.440635 <sup>a</sup>	0.3367132303, 0.366328185 <sup>a</sup>		0.3229615482
8	0.390050878574, 0.382315 <sup>a</sup>	0.29091301		0.2852504022
6	0.305159478008			0.2276682968
5	0.244468549420			0.1861375619
4	0.165096713911			0.1310729742
3.5	0.1168605596			0.0969010609
3	0.063691959			0.0579343171
λ	$^{3}D^{0}$	${}^{1}F^{e}$	<sup>3</sup> F <sup>e</sup>	He <sup>+</sup> (2 <i>P</i> )
$\infty$	0.5593282630905, 0.5593280 <sup>b</sup>	0.531995436, 0.5319954 <sup>c</sup>	0.531991326, 0.5319913 <sup>c</sup>	0.5000000000
100	0.530003005430, 0.5299317 <sup>b</sup>	0.503056068, 0.502956 <sup>c</sup>	0.503052113, 0.502952 <sup>c</sup>	0.4802475576
50	0.502075144728, 0.50171035 <sup>b</sup>	0.476090624, 0.4757375 <sup>c</sup>	0.476087092, 0.4757337 <sup>c</sup>	0.4609808964
20	0.425641977303, 0.42381195 <sup>b</sup>	0.4060876	0.4060871	0.4059698543
15	0.387728831214, 0.38483495 <sup>b</sup>			0.3771352488

<sup>a</sup>Other results using CI-type basis functions (Ref. [18]).

<sup>b</sup>Other results using CI-type basis functions (Ref. [19]).

<sup>c</sup>Other results using CI-type basis functions (Ref. [20]).

We have calculated the effective quantum number  $(n^*)$  for  ${}^{1,3}P^{\text{e}}$ ,  ${}^{1,3}D^{\text{o}}$ , and  ${}^{1,3}F^{\text{e}}$  metastable bound states using the formula [12],

$$E = -\frac{1}{2} \left[ \left( \frac{Z}{N} \right)^2 + \left( \frac{Z-1}{n^*} \right)^2 \right],\tag{5}$$

where *N*, *E*, and *Z* denote the inner electron quantum number, the energy of the state below the total ionization, and the atomic number, respectively. We present the effective quantum number in Tables I–III. The wavelengths for  $2p^2 {}^{3}P^{e} \rightarrow {}^{3}D^{o}$  and  $2p3p {}^{1}P^{e} \rightarrow {}^{1}D^{o}$  transitions in helium are presented in Tables I and II. They were obtained by converting the transition energies in a.u. to angstrom (in Å) by considering the standard conversion units (1 a.u. of energy corresponds to a wavelength of 455.633 Å) [4,19].

#### B. Results with screened Coulomb interaction

In our earlier works [18–20], we have investigated the unnatural parity states of helium with screened Coulomb (Yukawa) potentials using CI-type basis functions. An atom with screened Coulomb potentials experiences various perturbations due to screening environments and, depending on screening strengths, this leads to atomic wave functions which are different from the unscreened case. It can be observed from the perturbation theory that the screening is a repulsive perturbation for which all the isolated energy levels are displaced upward and ultimately into the continuum. In general, by writing the screened Coulomb potential as

$$-\frac{z}{r}\exp(-r/\lambda)\approx-\frac{z}{r}+\frac{z}{\lambda}-\frac{zr}{2\lambda^2}+\cdots,$$
 (6)

*z* being the nuclear charge, one can observe that all the matrix element will be reduced due to screening and the first-order correction upshifts all bound levels equally without changing the wave functions [30]. The effect of the perturbation potential in the lowest order in  $r/\lambda$  is given by  $\Delta V = -\frac{zr}{2\lambda^2}$ . The effect of first-order corrections on the energy levels has been reported in our earlier works [5]. In the earlier study [18–20] using CI-type basis functions, we made some approximations on the electron-electron screening and the Hamiltonian. In that work [5,18–20], we have included the electron-nucleus screening, explicitly, but approximated the electron-screened Coulomb potential in the form of Eq. (5) by the following expansion, i.e.,

$$\frac{e^{-\mu r_{12}}}{r_{12}} \equiv \sum_{n=0}^{m} (-1)^n \mu^n \frac{r_{12}^{n-1}}{n!}.$$
(7)

Furthermore, for the electron-electron screening term given in Eq. (7), we have approximated  $r_{12} \approx r_1 + r_2$ , assuming the two electrons are located on the opposite sides of the nucleus. Details validity of such approximations can be found from our earlier works [5,18–20]. In the present work, we calculate the lowest  ${}^{1,3}P^{\text{e}}$ ,  ${}^{1,3}D^{\text{o}}$ , and  ${}^{1,3}F^{\text{e}}$  states below the He<sup>+</sup>(2P) threshold using the correlated wave function to

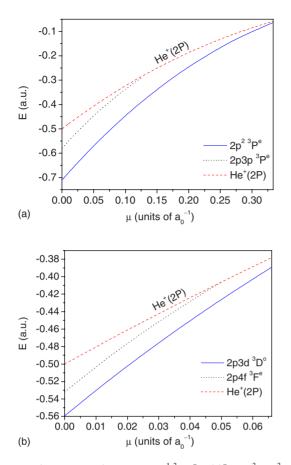


FIG. 1. (Color online) The bound  ${}^{1,3}P^{e}$  [in (a)] and  ${}^{3}D^{0}$ ,  ${}^{3}F^{e}$  [in (b)] states energies as functions of the screening parameter,  $\mu$  along with the He<sup>+</sup>(2P) threshold.

compare the present results with our earlier studies [18–20]. We have used 700-term wave functions for  ${}^{3}P^{e}$ ,  ${}^{1,3}D^{o}$  states, 600-term for  ${}^{1}P^{e}$  states, and 1000-term for  ${}^{1,3}F^{e}$  states. The lowest  ${}^{1,3}P^{e}$ ,  ${}^{1,3}D^{o}$ , and  ${}^{1,3}F^{e}$  states energies for different screening parameters obtained from our calculations are presented in Table IV and in Fig. 1. The eigenenergy  $E(\lambda)$  are

fairly convergent up to the quoted digits. From Table I, it is clear that the energy eigenvalues for each screening parameters are greatly improved compared to our earlier reported results using CI-type basis functions [18–20]. From Fig.1 and Table IV, it appears that the eigenenergies are approaching the He<sup>+</sup>(2*P*) threshold with increasing screening parameters  $\mu$  or decreasing  $\lambda$ .

## **IV. CONCLUSIONS**

In the present work, we have obtained accurate 2pnp  $^{1}P^{e}$  $(3 \le n \le 5)$ ,  $2pnp^{3}P^{e}$   $(2 \le n \le 5)$ ,  $2pnd^{1,3}D^{o}$   $(3 \le n \le 9)$ , and  $2pnf^{1,3}F^{e}$  ( $4 \le n \le 9$ ) states energies by employing exponential wave functions with exponents generated by a widely used quasirandom process. The P-state energies are comparable to the best published results. The  $2pnd^{-1}D^{\circ}$  ( $3 \le n$  $\leq$ 7), 2pnf <sup>1</sup>F<sup>e</sup> ( $4\leq n\leq 8$ ), and <sup>3</sup>D<sup>o</sup> and <sup>3</sup>F<sup>e</sup> states energies reported by the present work are so far the lowest results. We have presented the effective quantum number and the wavelengths for the  $2p^2 {}^{3}P^{e} \rightarrow {}^{3}D^{o}$  and  $2p3p {}^{1}P^{e} \rightarrow {}^{1}D^{o}$  transitions. The effect for the screened Coulomb (Yukawa) potentials on the lowest P-, D-, and F-wave unnatural parity states are also investigated using correlated exponential wave functions. With the improved experimental techniques [2,3] and the recent advancement in laser plasmas, and with the broad applications of screened Coulomb potentials in different areas of physics and chemistry, we believe our results can serve as a benchmark reference for future investigations to the research communities of atomic physics, chemical physics, plasma physics, astrophysics, and few-body physics.

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