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Resonances for positron–helium and positron–lithium systems in kappa-distribution plasma*

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S-wave resonances of positron–helium and positron–lithium systems in kappa-distribution plasmas are investigated using Hylleraas-type wave functions in the framework of the stabilization method. A model potential approach is used to represent the interactions between the outer electron, the positron and the core. The resonance parameters (position and width) of positron–helium and positron–lithium systems below the Ps(2s) threshold are reported as a function of screening parameter and spectral index of plasma.

Keywords: positron–atom scattering, kappa-distribution plasmas, model potential approach, variational method

PACS: 34.80.Uv, 52.20.–j, 95.30.Dr **DOI:** 10.1088/1674-1056/27/12/123402

1. Introduction

This study aims to present the resonances in positron–atom scattering with kappa-distribution plasmas. During the past few years, the applicability of Lorentzian (or kappa) distribution functions in astrophysical and space environments, such as solar-wind, solar corona, planetary magnetospheres, planetary nebula, supernova magnetospheres has been studied extensively[1–8] (references therein). In astrophysical and space plasma environments, the velocity distributions of inner particles can be well-described by non-Maxwellian or Lorentzian distribution. The kappa distribution function which was first shown by Vasyliunas[9] can be described in the following form:[10–20]

$$f_\kappa(v) = n\left(\frac{m}{2\pi\kappa E_\kappa}\right)^{3/2}\frac{\Gamma(\kappa+1)}{\Gamma(\kappa-1/2)}\left(1+\frac{mv^2}{2\kappa E_\kappa}\right)^{-(\kappa+1)}, \quad (1)$$

where κ is the spectral index of the plasma, m and v are the mass and velocity of the plasma electron, $E_\kappa = [(1-3/2\kappa)E_T]$ is the characteristic energy in generalized Lorentzian plasma, $E_T = k_B T_e$, k_B is the Boltzmann constant, T_e is the electron temperature, and n is the number density. The effective potential for two-body system in kappa-distribution plasma having charges q_a and q_b can be written as

$$V(r,\mu_\kappa) = \frac{q_a q_b}{r}\exp(-r\mu_\kappa), \quad (2)$$

where μ_κ is the effective screening parameter in kappa-distribution plasma, and μ_κ can be written as $\mu_k = \sqrt{\frac{\kappa-1/2}{\kappa-3/2}}\mu_D$, $\mu_D = 1/\lambda_D$ is the Debye screening parameter, λ_D is the standard Debye length in Maxwellian plasma. In the limit $\kappa \to \infty$, the kappa distribution functions become a simple Maxwellian function.

In this work, we are mainly interested in describing the behavior of resonance parameters (positions and widths) of positronic helium and positronic lithium under the influence of kappa-distribution plasmas. Resonances in positron–helium system using the model potential approach were first studied by Kar and Ho[21], who used the stabilization method (SM). Ren *et al.*[22] have performed a three-body calculation for the S-wave resonances in the positron–helium scattering in the hyperspherical coordinates by using the SM. Yu *et al.*[23] reported their investigation on resonances in e^+–He scattering by using the momentum-space coupled-channel optical method. The first theoretical study of resonance phenomena for positron–lithium scattering in a vacuum was carried out by Ward *et al.*[24], who used the close-coupling approach. Roy and Ho[25,26] calculated the resonance parameters in positron–lithium scattering using the SM based on the model potential approach and Hylleraas-type basis functions. Han *et al.*[27] calculated S-wave resonances in positronic lithium using the SM in the framework of hyperspherical coordinate. Liu *et al.*[28] have calculated the resonances for positronic Li using the momentum-space coupled-channel optical method. In plasma environments, the recent calculations of S-wave resonances in positron–helium system and positron–lithium sys-

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tem under the Debye screening were performed by Ghoshal and Ho[29,30] using SM.

In the present investigation, we use the stabilization method[31–33] to extract the S-wave resonance parameters (both positions and widths) for the proposed systems below the Ps(2s) threshold. Hylleraas-type wave functions are used to represent the correlation effects between the outer electron, the positron and the core. We obtain the resonance parameters for different values of spectral index κ and Debye screening parameter $\mu_{\rm D}$. All of the calculations are performed on IBM machines by using quadruple precision arithmetic in the CENT operating system.

2. Calculations

The non-relativistic Hamiltonian for positron–helium and positron–lithium systems in kappa-distribution plasma is given by[14,15,21,25,26]

$$H = T + V_{\mu_\kappa}, \tag{3}$$

with

$$T = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2, \tag{4}$$

$$V_{\mu_\kappa} = V_{e^-}(r_1)\exp(-r_1\mu_\kappa) + V_{e^+}(r_2)\exp(-r_2\mu_\kappa) - \frac{1}{r_{12}}\exp(-r_{12}\mu_\kappa), \tag{5}$$

where r_1 and r_2 denote, respectively, the radial coordinate of electron and positron with respect to core. The $V_{e^-}(r_1)$ and $V_{e^+}(r_2)$ are used to represent the model potentials for interactions between the active electron and the respective ionic cores, and the positron and the respective cores, respectively. The well-tested explicit expressions for $V_{e^-}(r_1)$ and $V_{e^+}(r_2)$ can be considered as[34–41]

$$V_{e^-}(r_1) = -\frac{Z}{r_1} + A\left[\frac{1}{r_1} - \frac{1}{r_1}(1+Br_1)\exp(-2Br_1)\right], \tag{6}$$

$$V_{e^+}(r_2) = \frac{Z}{r_2} - A\left[\frac{1}{r_2} - \frac{1}{r_2}(1+Cr_2)\exp(-2Cr_2)\right], \tag{7}$$

where $A = Z - 1$. In this study, we set $B = 1.6559$, $C = 1.7212$ for e^+–Li[25] system and $B = C = 2.601$ for e^+–He[21] system. Using these model potentials, the energies for the (1s2s ^{1}S, 1s2p ^{1}P) states of helium and ($1s^2$2s ^{2}S, $1s^2$2p ^{2}P) states of lithium obtained from this calculations for free-atomic system are (-0.14595, -0.12548) a.u. (the unit a.u. is short for atomic unit) and (-0.19814, -0.12993) a.u., respectively, which are in good agreement with the experimental values (-0.14595, 0.12383) a.u.[21] and (-0.19814, -0.13024) a.u..[25] It is important to mention here that we set the same values of the parameters B and C in the model potentials for the free-atomic systems and the screening environments as recommended in the earlier studies.[38,39,42,43]

To represent the correlation effect between the electron, positron and the core, we consider the Hylleraas-type basis functions in the form of[44–46]

$$\left\{r_1^{l_i} r_2^{m_i} r_{12}^{n_i} e^{-\alpha(r_1+r_2)} : l_i + m_i + n_i \le \omega;\ \ i = 1,\ldots,N\right\}, \tag{8}$$

where l_i, m_i, and n_i are positive integers or zero, and α is the nonlinear variational parameter, N is the number of basis terms. Here, N has been conveniently chosen to be the well-known relation $N = (\omega+1)(\omega+2)(\omega+3)/6$.[47–50] Note that we use the wave-functions (8) to calculate the S-state only and the total angular momentum is zero for the S-wave.

To calculate the Ps(2s) and He^+(1s) threshold energy, we employ the Slater-type wavefunctions:

$$\varphi_{nlm} = r^{n+l-1}\exp(-\lambda r)Y_{lm}(\theta,\phi), \quad n = 1,2,3,\ldots; l = 0,1,2,\ldots \tag{9}$$

Exploiting the model potential approach, we estimate the $1s^2$2s ^{2}S state energy of Li by using wavefunctions (9).

3. Results and discussion

In the present calculation, we have employed the SM[21,22,25–27,29–33,50–53] to extract the resonance states of positron–helium and positron–lithium systems in kappa-distribution plasma. To extract resonance parameters with using the SM, in the first step, one needs to determine the energy levels precisely. In this work, we calculate the energy levels by diagonalizing the Hamiltonian with basis set (8). After calculating the energy levels $E(\alpha,\mu,\kappa)$ for varying α for different values of μ and κ, we construct the stabilization diagrams by plotting $E(\alpha,\mu,\kappa)$ versus α for fixed μ and κ. The resonance positions can be identified by observing the slowly decreasing energy levels at avoided crossings (*e.g.*, as marked in red, see Fig. 1) in the stabilization diagrams. To extract the resonance energy $E_{\rm r}$ and width Γ for a particular resonance state, we calculate the density of the resonance states by using the well-known formula[32]

$$\rho_n(E) = \left|\frac{En(\alpha_{i+1},\mu,\kappa) - En(\alpha_{i-1},\mu,\kappa)}{\alpha_{i+1} - \alpha_{i-1}}\right|^{-1}_{En(\alpha_i,\mu,\kappa)=E}, \tag{10}$$

where the index i is the i-th varied value for α_i, and the index n is for the n-th resonance. The α_{i-1} and α_{i+1} are the $(i-1)$-th and $(i+1)$-th varied α values next to α_i. Once the density of resonance states has been calculated by using formula (10), we plot the density of states versus $E(\alpha,\mu,\kappa)$ and use the standard Lorentzian fitting formula having the baseline offset y_0 and total area A

$$\rho_n(E) = y_0 + \frac{A}{\pi}\frac{\Gamma/2}{(E-E_{\rm r}) + (\Gamma/2)^2}, \tag{11}$$

where $E_{\rm r}$ is the center of the peak and Γ denotes the full width at the half height of the peak. It is interesting to point out

that we obtain the resonance energy E_r and total width Γ by observing the best fitting in all the fittings at the avoided crossings for a particular resonance. In this way, we obtain the resonance parameters (E_r, Γ) for each κ and μ. We perform the calculations with $\omega = 13$ and $N = 560$ for different α values within 0.2–0.4. Figures 1 and 2 show the stabilization diagram and the best fitting of the density resonance state below the Ps(2s) threshold in positron–helium system in kappa-distribution plasma for $\kappa = 6$, $\mu_D = 0.01$.

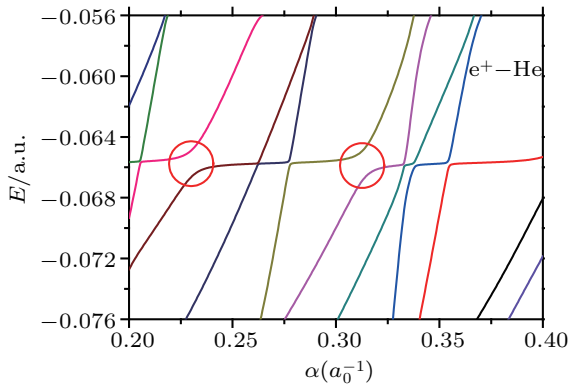


Fig. 1. (color online) Stabilization plot for the lowest S-wave resonance in positron–helium system in kappa-distribution plasma for $\kappa = 6$, $\mu_D = 0.01$ (in unit a.u.). Red circles indicate avoided crossings.

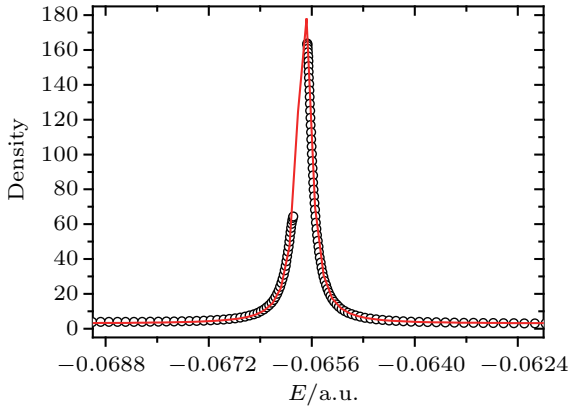


Fig. 2. (color online) The best fitting (solid line) of calculated density of resonance states (circles) to the Lorentzian form for S-wave resonance of positron–helium system below Ps(2s) threshold in kappa distribution plasma for $\kappa = 6$, $\mu_D = 0.01$ (in unit a.u.).

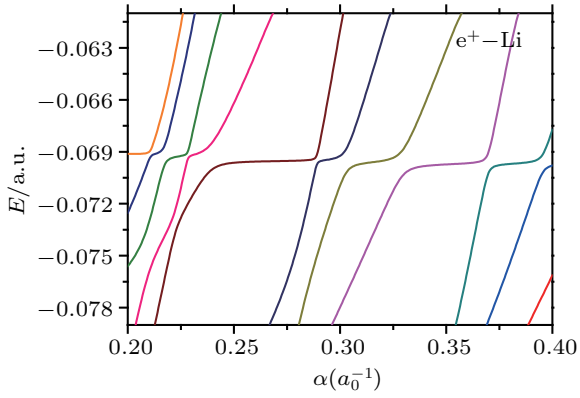


Fig. 3. (color online) Stabilization plot for the lowest S-wave resonance of positron–lithium system in kappa-distribution plasma for $\kappa = 6$, $\mu_D = 0.01$ (in unit a.u.).

Similarly, Figures 3 and 4 show the stabilization diagram and the best fitting of the density resonance state below the Ps(2s) threshold in positron–lithium system in kappa-distribution plasma for $\kappa = 6$, $\mu_D = 0.01$. All of the values of resonance parameters obtained from this work for different κ and μ_D are shown in Tables 1 and 2 and Figs. 5–8. To show the convergence with increasing the number of terms in the basis functions, we also include the results for $\omega = 12$ and $N = 455$ for selected screening parameters in Tables 1 and 2.

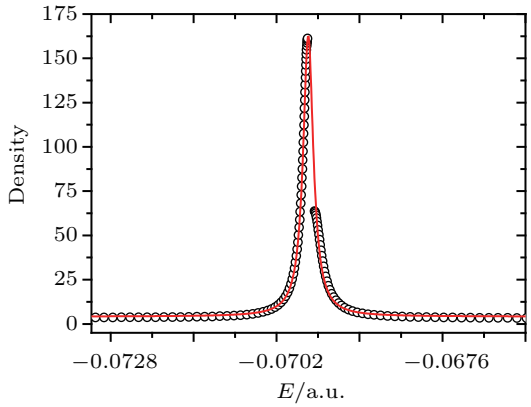


Fig. 4. (color online) The best fitting (solid line) of calculated density of resonance states (circles) to the Lorentzian form for S-wave resonance of positron–lithium system below Ps(2s) threshold in kappa distribution plasma for $\kappa = 6$, $\mu_D = 0.01$ (in unit a.u.).

Table 1 shows the $He^+(1s\ ^2S)$ state energies, $He(1s^2\ ^1S)$ energies, the lowest resonance parameters for positron–helium system and the Ps(2s) threshold energies in kappa-distribution plasma in terms of κ and μ_D. Similarly, Table 2 displays the $Li(1s^22s\ ^2S)$ state energies, the lowest resonance parameters for positron–lithium system and the Ps(2s) threshold energies in kappa-distribution plasmas in terms of κ and μ_D. In the tables, the energies are listed both in atomic units (a.u.) and electron volts (eV), and the resonance widths are presented in units a.u. and meV. To convert energies into eV, we estimate the energies of ground states of the respective atomic systems. As our model potential is related to the He^+ core, the energy of the He^+ core (as shown in Table 1 for each screening parameter) should be added to our results (as shown in Table 1) to obtain the total energy of a resonance. The total resonance energies E_r and Ps(2s) threshold are converted into eV as measured from the $He(1s^2\ ^1S)$ energies. We calculate the He $(1s^2\ ^1S)$ energies for each screening parameters by using the Hylleraas-type basis functions in Eq. (8) within the framework of Ritz variational method. The He $(1s^2\ ^1S)$ eigen energies are listed in Table 1. In Table 2, we convert the resonance energies E_r and Ps(2s) threshold into eV relative to $Li(1s^22s\ ^2S)$ state energies. We calculate the $Li(1s^22s\ ^2S)$ energies by using the Slater-type orbitals (9) in the framework of model potential approach and the $Li(1s^22s\ ^2S)$ energies for different screening parameters are listed in Table 2. Figures 5 and 6 display the surface plots of resonance energy E_r and width

Γ for positron–helium system each as a function of spectral index κ and Debye screening parameter μ_D. Figures 7 and 8 exhibit the same plots for positronic Li. It is seen evident from the figures and tables that the resonance parameters (in unit of eV) increase with κ increasing and decreases with μ_D increasing.

Table 1. Values of S-wave resonance energy E_r and width Γ for positron–helium system below the Ps(2s) threshold in kappa-distribution plasma for selected spectral index κ and Debye screening parameter μ_D.

μ_D	κ	He^+ ($1s\ ^2S$)	He ($1s^2\ ^1S$)	E_r		Γ		Ps(2s) threshold	
		a.u.	a.u.	a.u.	eV	(10^{-4}) a.u.	meV	a.u.	eV
0.01	2	−1.96558	−2.85211	−0.059885	22.494	2.48	6.75	−0.046852	22.849
	4	−1.97644	−2.86839	−0.064983	22.503	2.50	6.80	−0.051466	22.871
	6	−1.97798	−2.87070	−0.065718	22.504	2.50	6.80	−0.052143	22.873
	8	−1.97860	−2.87163	−0.066016	22.504	2.50	6.80	−0.052419	22.874
				−0.066002[a]	22.505[a]	2.50[a]	6.80[a]		
	10	−1.97894	−2.87214	−0.066177	22.504	2.50	6.80	−0.052568	22.875
0.02	2	−1.93161	−2.80116	−0.044997	22.437	2.30	6.26	−0.034144	22.733
	4	−1.95309	−2.83337	−0.054212	22.478	2.43	6.61	−0.041884	22.814
	6	−1.95614	−2.83795	−0.055579	22.483	2.45	6.67	−0.043066	22.823
	8	−1.95738	−2.83980	−0.056135	22.484	2.45	6.67	−0.043549	22.827
	10	−1.95805	−2.84080	−0.056437	22.485	2.45	6.67	−0.043813	22.829
0.03	2	−1.89807	−2.75089	−0.032109	22.333	2.01	5.47	−0.023920	22.556
	4	−1.92994	−2.79866	−0.044312	22.433	2.29	6.23	−0.033584	22.725
	6	−1.93448	−2.80547	−0.046189	22.444	2.32	6.31	−0.035124	22.745
	8	−1.93632	−2.80823	−0.046957	22.448	2.34	6.37	−0.035759	22.753
				−0.046941[a]	22.449[a]	2.31[a]	6.29[a]		
	10	−1.93732	−2.80972	−0.047376	22.450	2.34	6.37	−0.036105	22.757
0.04	2	−1.86496	−2.70127	−0.021356	22.176	1.64	4.46	−0.015849	22.326
	4	−1.90700	−2.76427	−0.035351	22.366	2.10	5.71	−0.026431	22.608
	6	−1.91300	−2.77327	−0.037611	22.386	2.15	5.85	−0.028205	22.642
	8	−1.91543	−2.77691	−0.038542	22.393	2.18	5.93	−0.028942	22.655
	10	−1.91675	−2.77889	−0.039051	22.397	2.19	5.96	−0.029346	22.661
0.05	2	−1.83227	−2.65230	−0.012807	21.966	1.26	3.43	−0.009671	22.051
	4	−1.88425	−2.73019	−0.027376	22.274	1.87	5.09	−0.020320	22.466
	6	−1.89170	−2.74134	−0.029884	22.307	1.95	5.31	−0.022217	22.515
	8	−1.89471	−2.74585	−0.030927	22.319	1.98	5.39	−0.023013	22.534
				−0.030909[a]	22.320[a]	1.91[a]	5.20[a]		
	10	−1.89634	−2.74830	−0.031498	22.326	1.99	5.42	−0.023451	22.545
0.06	2	−1.79999	−2.60396	−0.006515	21.700	0.98	2.67	−0.0051722	21.736
	4	−1.86171	−2.69640	−0.020413	22.158	1.61	4.38	−0.015158	22.301
	6	−1.87056	−2.70967	−0.023034	22.207	1.71	4.65	−0.017083	22.369
	8	−1.87415	−2.71505	−0.024136	22.225	1.75	4.76	−0.017900	22.395
	10	−1.87609	−2.71796	−0.024745	22.235	1.77	4.82	−0.018351	22.409

[a] Present results with $\omega = 12$ and $N = 455$.

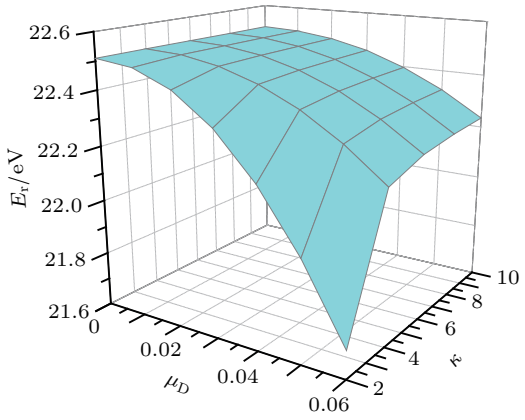


Fig. 5. (color online) Resonance energy for positron–helium system as a function of spectral index κ and Debye screening parameter μ_D (in unit eV).

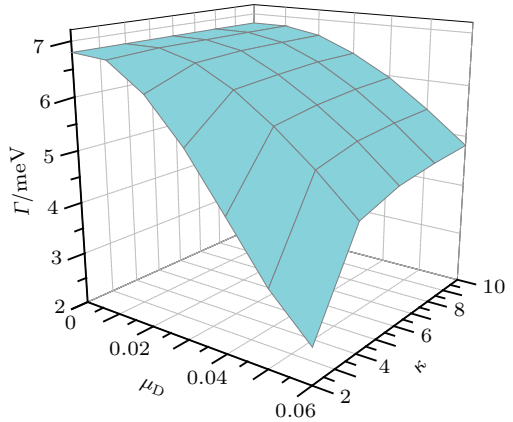


Fig. 6. (color online) Resonance width for positron–helium system as a function of spectral index κ and Debye screening parameter μ_D (in unit meV).

Table 2. Values of S-wave resonance energy E_r and width Γ for positron–lithium system below the Ps(2s) threshold in kappa-distribution plasma for selected spectral index κ and Debye screening parameter μ_D.

μ_D	κ	Li ($1s^2 2s\ ^2S$)	E_r		Γ		Ps(2s) threshold	
		a.u.	a.u.	eV	(10^{-4}) a.u.	meV	a.u.	eV
0.01	2	−0.18102	−0.063902	3.187	1.92	5.22	−0.046852	3.651
	4	−0.18633	−0.068972	3.193	1.94	5.28	−0.051466	3.670
	6	−0.18709	−0.069703	3.194	1.94	5.28	−0.052143	3.672
	8	−0.18739	−0.070000	3.194	1.94	5.28	−0.052419	3.673
			−0.069885[a]	3.197[a]	1.94[a]	5.28[a]		
	10	−0.18756	−0.070161	3.195	1.94	5.28	−0.052568	3.673
0.02	2	−0.16498	−0.049131	3.152	1.76	4.79	−0.034144	3.560
	4	−0.17502	−0.058268	3.177	1.89	5.14	−0.041884	3.623
	6	−0.17648	−0.059625	3.180	1.91	5.20	−0.043066	3.630
	8	−0.17707	−0.060177	3.181	1.91	5.20	−0.043549	3.633
	10	−0.17739	−0.060477	3.181	1.91	5.20	−0.043813	3.635
0.03	2	−0.14994	−0.036368	3.090	1.31	3.56	−0.023920	3.429
	4	−0.16421	−0.048452	3.150	1.73	4.71	−0.033584	3.555
	6	−0.16630	−0.050313	3.156	1.78	4.84	−0.035124	3.569
	8	−0.16715	−0.051075	3.159	1.79	4.87	−0.035759	3.575
			−0.050957[a]	3.162[a]	1.70[a]	4.63[a]		
	10	−0.16761	−0.051488	3.160	1.80	4.90	−0.036105	3.578
0.04	2	−0.13586	−0.025686	2.998	0.632	1.72	−0.015849	3.266
	4	−0.15387	−0.039578	3.110	1.46	3.97	−0.026431	3.468
	6	−0.15654	−0.041816	3.122	1.54	4.19	−0.028205	3.492
	8	−0.15763	−0.042739	3.126	1.56	4.24	−0.028942	3.502
	10	−0.15822	−0.043242	3.129	1.58	4.30	−0.029346	3.507
0.05	2	−0.12269	−0.017105	2.873	0.079	0.21	−0.009671	3.075
	4	−0.14398	−0.031674	3.056	1.06	2.88	−0.020320	3.365
	6	−0.14718	−0.034160	3.075	1.20	3.27	−0.022217	3.400
	8	−0.14848	−0.035195	3.083	1.25	3.40	−0.023013	3.414
			−0.035076[a]	3.086[a]	1.25[a]	3.40[a]		
	10	−0.14919	−0.035762	3.087	1.28	3.48	−0.023451	3.422
0.06	2	−0.11037	−0.010418	2.720	0.0079	0.021	−0.0051722	2.863
	4	−0.13452	−0.024745	2.987	0.561	1.53	−0.015158	3.248
	6	−0.13820	−0.027357	3.016	0.763	2.08	−0.017083	3.296
	8	−0.13970	−0.028455	3.027	0.835	2.27	−0.017900	3.314
	10	−0.14052	−0.029060	3.033	0.886	2.41	−0.018351	3.324

[a]Present results with $\omega = 12$ and $N = 455$.

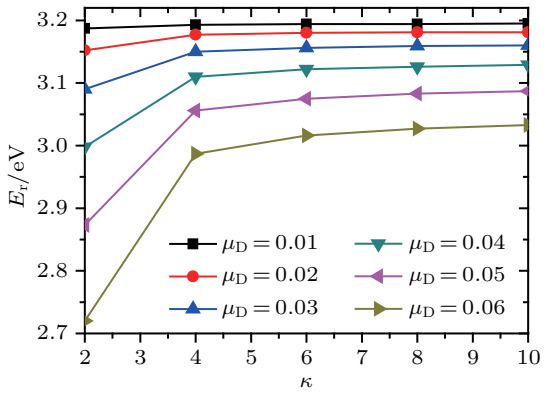


Fig. 7. (color online) Plots of resonance energy for positron–lithium system as function of spectral index κ for different values of Debye screening parameter μ_D (in unit eV).

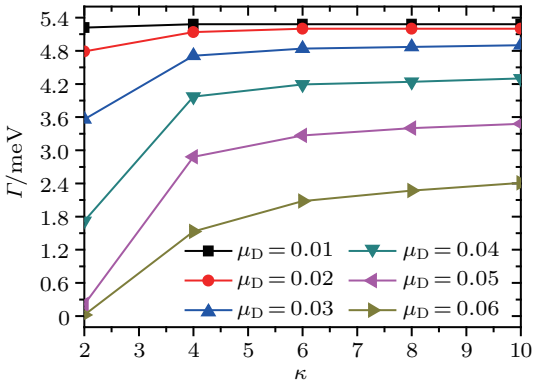


Fig. 8. (color online) Plots of resonance width for positron–lithium system as function of spectral index κ for different values of Debye screening parameter μ_D (in unit meV).

For the free-atomic system, the resonance parameters (E_r, Γ) (in atomic units) of positron–helium system estimated from this calculation are (−0.076505, 0.00025) which is in agreement with the resonance parameters (−0.07653, 0.00025), (−0.07654, 0.00023), (0.07667, 0.00143), and (−0.076495, 0.00023) reported respectively by Kar and Ho,[21] Ren *et al.*,[22] Yu *et al.*,[23] Ghoshal and Ho.[29] The resonance parameters (E_r, Γ) (in atomic units) of positron-lithium sys-

tem obtained from this work are (−0.080476, 0.000194) which are comparable to the results (−0.080495, 0.000205), (−0.080658, 0.000202), and (−0.080454, 0.000193) reported, respectively, by Roy and Ho,[25] Han *et al.*,[27] Ghoshal and Ho.[30] Apart from this theoretical work, positronic He and Li are also of experimental interest.[54,55] For kappa-distribution plasma environments, there are no other theoretical researches of e^+–He and e^+–Li systems in the literature for comparison. At present, the theoretical results might be used for astrophysical plasma diagnostic purposes. In the future, positronic He or Li may be of experimental interest due to importance of kappa-distribution plasma in astrophysics and stellar atmosphere.

4. Summary and conclusions

In this work, we have investigated the S-wave resonances of positron–helium and positron–lithium systems in kappa-distribution plasma based on a simple and powerful variational stabilization method. The Hylleraas-type wave functions are used to represent the correlation effect between the charged particles. A model potential approach is used to represent the interactions between the outer electron, the positron and the core. We employ the Lorentzian fitting technique to extract resonance parameters. With applicability of Lorentzian (kappa-distribution) astrophysical plasmas[1–8] and with recent progress of atomic process in kappa-distribution plasmas,[11–20] it is expected that our findings will contribute to further studies in positron–atom scattering phenomenon.

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