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Reply to "Comment on 'Doubly excited bound and resonance ($^3P^e$) states of helium'"

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In response to the comment by Kar and Ho [Phys. Rev. A **82**, 036501 (2010)], we have clarified the reason for anomaly between our and their results for the resonance states below the $N = 5$ ionization threshold of He$^+$.

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In their Comment, Kar and Ho [1] repeated their previous calculations [2] in the framework of the complex coordinate rotation (CCR) method with a different basis set in order to clarify the discrepancies between their [2] and our [3] calculated values of resonance parameters for the $^3P^e$ state below the $N = 4$ and $N = 5$ ionization thresholds of He$^+$.

TABLE I. Comparison of resonance parameters of $^3P^e$ resonance states of helium below $N = 6$ and $N = 7$ ionization thresholds of He$^+$ between our work [3] and the work of Eiglsperger *et al.* [4].

	$N = 6$				$N = 7$			
	Saha and Mukherjee [3]		Eiglsperger *et al.* [4]		Saha and Mukherjee [3]		Eiglsperger *et al.* [4]	
$^3P^e$	Energy	Width	Energy	Width	Energy	Width	Energy	Width
1	0.077 21	0.000 369	0.076 443	0.000 596	0.053 63	0.000 125	0.053 47	0.000 70
2			0.073 661	0.000 871			0.0534 029	0.000 280 3
3			0.073 387 0	0.000 739 2			0.052 228 8	0.000 367 7
4	0.070 79	0.000 483	0.070 754 5	0.000 358 1	0.051 90	0.000 280	0.052 015	0.000 430
5			0.070 218	0.000 841			0.051 024	0.000 048 2
6	0.068 25	0.000 735	0.068 631 2	0.000 586 5	0.050 85	0.000 045	0.050 847 80	0.000 012 02
7	0.067 04	0.000 275	0.067 072 5	0.000 105 0			0.050 394	0.000 530
8	0.066 65	0.000 149	0.066 527 2	0.000 368 3			0.049 773	0.000 241
9			0.066 190	0.000 655	0.049 65	0.000 02	0.049 702 6	0.000 062 3
10	0.065 45	0.000 274 5	0.065 516 9	0.000 234	0.048 60	0.000 105	0.048 578	0.000 458
11	0.065 22	0.000 070 5	0.065 294 9	0.000 094 1			0.048 461 1	0.000 156 7
12	0.064 49	0.000 005 1	0.064 495 12	0.000 008 92			0.048 404 8	0.000 157 6
13			0.063 937	0.000 256			0.048 397	0.000 174
14	0.063 83	0.000 152	0.063 814 2	0.000 388 9			0.048 275	0.000 193
15			0.063 613 8	0.000 257 2	0.047 52	0.000 295	0.047 323	0.000 366
16	0.063 58	0.000 003 425	0.063 594 605	0.000 004 761			0.047 154 83	0.000 018 55
17	0.062 72	0.000 000 336 5	0.062 721 69	0.000 003 40			0.047 070 7	0.000 285 4
18			0.062 337 2	0.000 207 3			0.046 881 8	0.000 089 3
19			0.062 326	0.000 145			0.046 750 2	0.000 103 7
20			0.062 138 9	0.000 155 5	0.046 55	0.000 015	0.046 576 57	0.000 012 32
21	0.061 87	0.000 173 5	0.061 869 1	0.000 211 0			0.046 240 2	0.000 186 2
22			0.061 300 50	0.000 005 46			0.046 110 8	0.000 204 0
23	0.061 15	0.000 125 5	0.061 275	0.000 329			0.045 970 1	0.000 096 6
24			0.061 051 0	0.000 082 6			0.045 826 8	0.000 031 4
25			0.060 972 48	0.000 018 12			0.045 814 48	0.000 005 27
26	0.060 75	0.000 092	0.060 666 9	0.000 181 3	0.045 73	0.000 075	0.045 580 6	0.000 093 1
27	0.060 28	0.000 163	0.060 361 9	0.000 221 3	0.045 19	0.000 250	0.045 348 2	0.000 385 7
28			0.060 256 92	0.000 006 81			0.045 313 7	0.000 087 3
29			0.060 114 66	0.000 025 53			0.045 169 12	0.000 008 14
30	0.059 73	0.000 234 5	0.059 797 1	0.000 153 8			0.045 070 11	0.000 000 94
31			0.059 582 5	0.000 134 9			0.045 033 07	0.000 001 8
32			0.059 470 995	0.000 012 354	0.044 84	0.000 110	0.044 785 9	0.000 218 4
33			0.059 402 6	0.000 073 9			0.044 775 9	0.000 097 4
34			0.059 365 2	0.000 027 9			0.0446000	0.0000344
35	0.059 13	0.000 267	0.059 144 9	0.000 122 5				

The controversy lies mainly with the values of resonance parameters of four $^3P^e$ states among which two states are below the $N = 4$ and two states are below the $N = 5$ threshold of He$^+$, although for a large number of resonance states below the $N = 4{,}5$ thresholds of He$^+$, there is reasonable agreement between our results [3] and those of Kar and Ho [1].

The assignment of the configuration $5p^2(^3P^e)$ to the resonance energy value of -0.126378 a.u. as reported by Kar and Ho [1] below the $N = 5$ threshold of He$^+$ is incorrect. This energy value is more negative than the energy value of -0.125 a.u. corresponding to the $N = 4$ ionization threshold of He$^+$ and therefore should lie below the $N = 4$ threshold of He$^+$. In a recent rigorous CCR method calculation, Eiglsperger *et al.* [4] reported that the energy value below the $N = 5$ threshold starts with $-0.119\,30$ a.u., which is in good conformity with our value of $-0.119\,37$ a.u. [3] and contradicts the reported value of $-0.126\,378$ a.u. obtained by Kar and Ho [1]. In their calculation, Eiglsperger *et al.* [4] have obtained as many as 11 $^3P^e$ states in the energy range from $-0.126\,888\,607\,0$ a.u. to $-0.126\,336\,013$ a.u. below the $N = 4$ ionization threshold of He$^+$. It is therefore clear that the first resonance energy value of $-0.126\,378$ a.u. below $N = 5$, as reported by Kar and Ho [1], lies in the previously mentioned energy range [4] below the $N = 4$ ionization threshold of He$^+$. Hence assignments of electronic configurations ascertained by Kar and Ho [1] and conclusions thereof are proved to be incorrect because of their improper assignment of the energy value of $-0.126\,378$ a.u. as a $5p^2(^3P^e)$ state.

Kar and Ho [1] put forward a qualitative argument to assign the electronic configuration to each resonance state by labeling individual angular momenta of two electrons. Labels denoting individual angular momenta may be good indicators of dominant contributions to various excited states, but strictly speaking, this is not exact as they do not commute with the Hamiltonian. In the case of metastable bound states, such labeling of individual angular momenta to the overall state may be done by demonstrating their contribution to the energies because of the most important configuration, as was done by Saha *et al.* [5]. In our opinion, for resonance states, it is better to report their energy values in orderly status, as previously done by Ho and Bhatia [2] and other authors [3,4], instead of labeling individual angular momenta to these states.

It is important to mention that a large number of states present in the calculation of Eiglsperger *et al.* [4] are missing in the calculation of Kar and Ho [1], although both have used the CCR method. By using the stabilization method, we [3] have obtained more numbers of resonance states than Kar and Ho [1] but fewer numbers of resonance states than Eiglsperger *et al.* [4]. Kar and Ho [1] used almost 900 numbers of terms in the wave function, and we [3] have used 1575 numbers of terms in the basis set, whereas Eiglsperger *et al.* [4] used almost 16,000 numbers of effective terms in their wave function. This suggests that the dimension of the wave function plays a crucial role in obtaining more numbers of resonance states below any hydrogenic threshold of helium rather than proving the superiority of the CCR method over the stabilization method and vice versa.

It may be noted that Eiglsperger *et al.* [4] are unable to associate our results with their results for the resonance $^3P^e$ states lying below the $N = 6$ and $N = 7$ ionization thresholds of He$^+$. Our own comparison of our data [3] with those of Eiglsperger *et al.* [4] for $^3P^e$ resonance states below the $N = 6$ and $N = 7$ ionization thresholds of He$^+$, as given in Table I shows that our results are in reasonable agreement with those of Eiglsperger *et al.* [4] as it is difficult to ensure the exact position of the resonance states since these states have some definite width. However, the reason for missing resonance $^3P^e$ states below the $N = 6{,}7$ ionization thresholds of He$^+$ in our calculation [3] is the fewer numbers of terms than given by Eiglsperger *et al.* [4] as used in the wave function, as discussed in the preceding paragraph. This warrants the immediate calculation of resonance parameters of high-lying doubly excited states in the framework of the stabilization method with a wave function of larger dimension and finer variation of the nonlinear parameter set.

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