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ENERGY LEVEL SCHEME OF $\bar{p}$ He$^+$ SYSTEM
IN AN IMPROVED ADIABATIC APPROACH

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Energy level scheme of states of $\bar{p}$ He$^+$ system is studied in the effective adiabatic approach which has been developed in our previous work [7]. Possibilities of experimental data fit by means of appropriate choice of effective potentials are discussed. Systematic calculations of the energy level system and their estimations are given.

The investigation has been performed at the Laboratory of Computing Techniques and Automation and at the Bogoliubov Laboratory of Theoretical Physics, JINR.

Схема уровней энергии $\bar{p}$ He$^+$-системы
в улучшенном адиабатическом подходе

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Схема уровней энергии $\bar{p}$ He$^+$-системы изучается в эффективном адиабатическом подходе, который был развит в нашей предыдущей работе [7]. Обсуждаются возможности фитирования экспериментальных данных с помощью подходящего выбора эффективных потенциалов. Выполнены систематические расчеты уровней энергии $\bar{p}$ He$^+$-системы и даны оценки их значений.

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1. Introduction

Recent experiments [1] using the laser-induced saturation effect have shown that the metastable states in the atomcule $\bar{p}$ He$^+$ have quantum numbers $n_{max} \approx 40$, $l_{max} \approx n_{max} - 1$, which correspond to nearly circular orbits, and the main primary population appearing at $n \approx 38$. However, an isolated atomcule has, in addition to these states, a wide range of other populated metastable states. With allowance made for these states, the total population of metastable hadronic $\bar{p}$ He$^+$ states amounts up to 30%, that is six or seven times greater than the experimental values. So, for the quantitative treatment of the obtained experimental data, first of all, the systematic calculations of the initial populations and the rotational-vibrational states of the $\bar{p}$ He$^+$ atomcule are the actual problem [2]. The previous study of

the exotic states has been performed in the crude Born–Oppenheimer (B-O) approximation [3—5] and adiabatic approximation [6].

In this paper the energy level scheme of states of $\bar{p}\,\mathrm{He}^+$ system is studied by means of the effective adiabatic approach [7].

2. An Improved Adiabatic Approximation

The adiabatic representation is based on the expansion of the Schrödinger three-body wave function $\Psi(\bar{R}, \bar{r})$ over a complete set of the Coulomb two-center problem solutions [8] in the rotational system of coordinates [9]

$$\Psi_v^J(\bar{R}, \bar{r}) = \sum_j \Phi_j^J(\bar{r}, \bar{R}) R^{-1} \chi_{jv}^J(R). \tag{1}$$

After averaging we have an infinite system of the radial equations [10]

$$\left[\frac{d^2}{dR^2} + 2M\varepsilon_{Jv} - U_{ii}^J(R) \right] \chi_{iv}^J(R) = \sum_{i \neq j} U_{ij}^J(R)\, \chi_{iv}^J(R). \tag{2}$$

Here $U_{ij}^J(R)$ are effective potentials with fixed values of the total orbital momentum J and its projection $m = m_j$ [9]:

$$U_{ii}^J(R) = 2M\left(E_i(R) - E_{1b} - \frac{2}{R} \right) + H_{ii}^{AD}(R) + \frac{J(J+1) - 2m^2}{R^2},$$

$$U_{ij}^J(R) = H_{ij}(R) + \frac{d}{dR} Q_{ij}(R) + 2Q_{ij} \frac{d}{dR} + B_{ij}^J(R),$$

$M = M_0/m_b$, M_0 is the reduced mass of nuclei, $M_0^{-1} = M_a^{-1} + M_b^{-1}$, in particular, $M_a = M_{\bar{p}}$ is the mass of antiproton, and $M_b = M_{He}$ is the mass of the Helium nucleus, m_b is the reduced electron mass, $m_b^{-1} = m_e^{-1} + M_b^{-1}$, of the separated atomic ion He^+ with the binding energy $-E_{1b} = 2$, $E_j(R)$ are eigenvalues of the Coulomb two-center problem, $-\varepsilon_{Jv}$ is the binding energy, $\varepsilon_{Jv} = E_{Jv} - E_{1b}$, and E_{Jv} is the energy of the three-body system $\bar{p}\,\mathrm{He}^+$ in the reduced atomic units $(e = \hbar = m_b = 1)$.

It should be noted that the asymptotic behavior of the effective potentials with respect to large quantum numbers may be studied by using a quasiclassical approximation [8], and the Kantorovich theorem [11] of reduction of the infinite system of equations (2) to the finite one may be proved. It makes possible to consider a finite system of equations and to use different types of approximations. One of them is usually connected with the so-called Born-Oppenheimer approximation which corresponds to the limit of infinite heavy mass of nuclei:

$$\left[\frac{d^2}{dR^2} + 2M(\varepsilon_{Jv} - U_{11}^J(R)) \right] \chi_v^J(R) = 0. \tag{3}$$

Here U_{11}^J is the B-O potential

$$U_{11}^J(R) = \left(E_1(R) - E_1^{AS} - \frac{2}{R} \right) + \frac{J(J+1)}{2MR^2},$$

$M = M_0/m_e$ is reduced nucleus mass, and $-\varepsilon_{Jv}$ is binding energy, $\varepsilon_{Jv} = E_{Jv} - E_1^{AS}$, counting out $-E_1^{AS} = 2.$ in a.u. $(e = \bar{h} = m_e = 1)$. This approximation possesses an important property. It gives a lower boundary of eigenvalues E_{Jv} of the corresponding eigenvalue problem for the system of equations (2) in accordance with the Brat'sev theorem [12]. We examine this property numerically for the $dt\mu$ molecule with orbital momenta $J = 0, 1, 2$ and obtain the following lower estimations of the energy ε_{Jv} in eV: $\varepsilon_{00} = -329.16$, $-\varepsilon_{01} = -43.66$, $\varepsilon_{10} = -239.41$, $\varepsilon_{11} = -8.52$, $\varepsilon_{20} = -106.55$, $\varepsilon_{21} = 3.40$ counting out $E_1^{AS} = -2813.25$ eV. Note

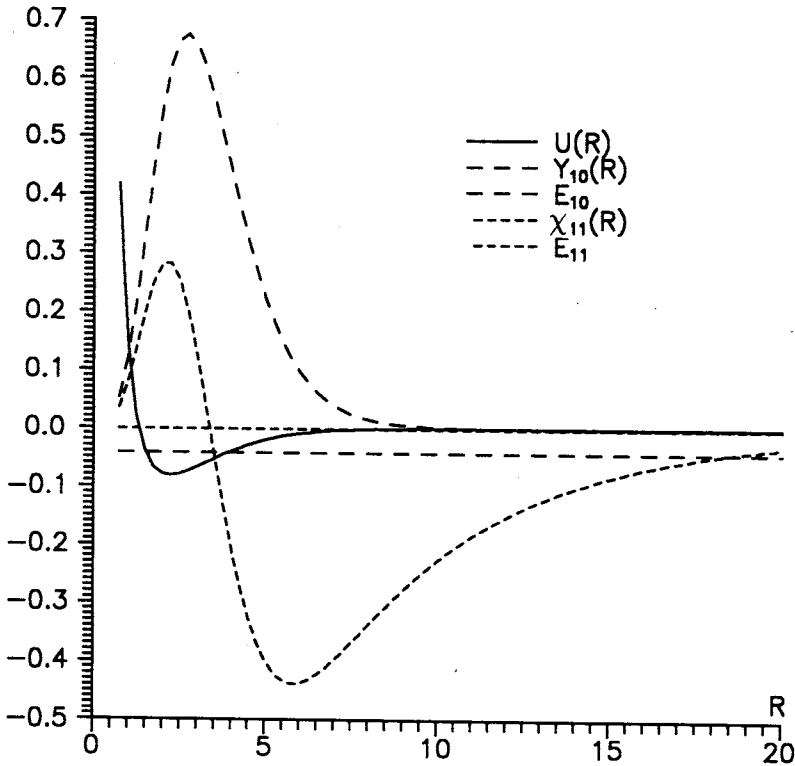

Fig.1. The potential $U(R)$, wave functions $\chi_{1i}(R)$ and energy levels E_{1i}, $i = 0, 1$ of the dtm molecule in the Born—Oppenheimer approximation
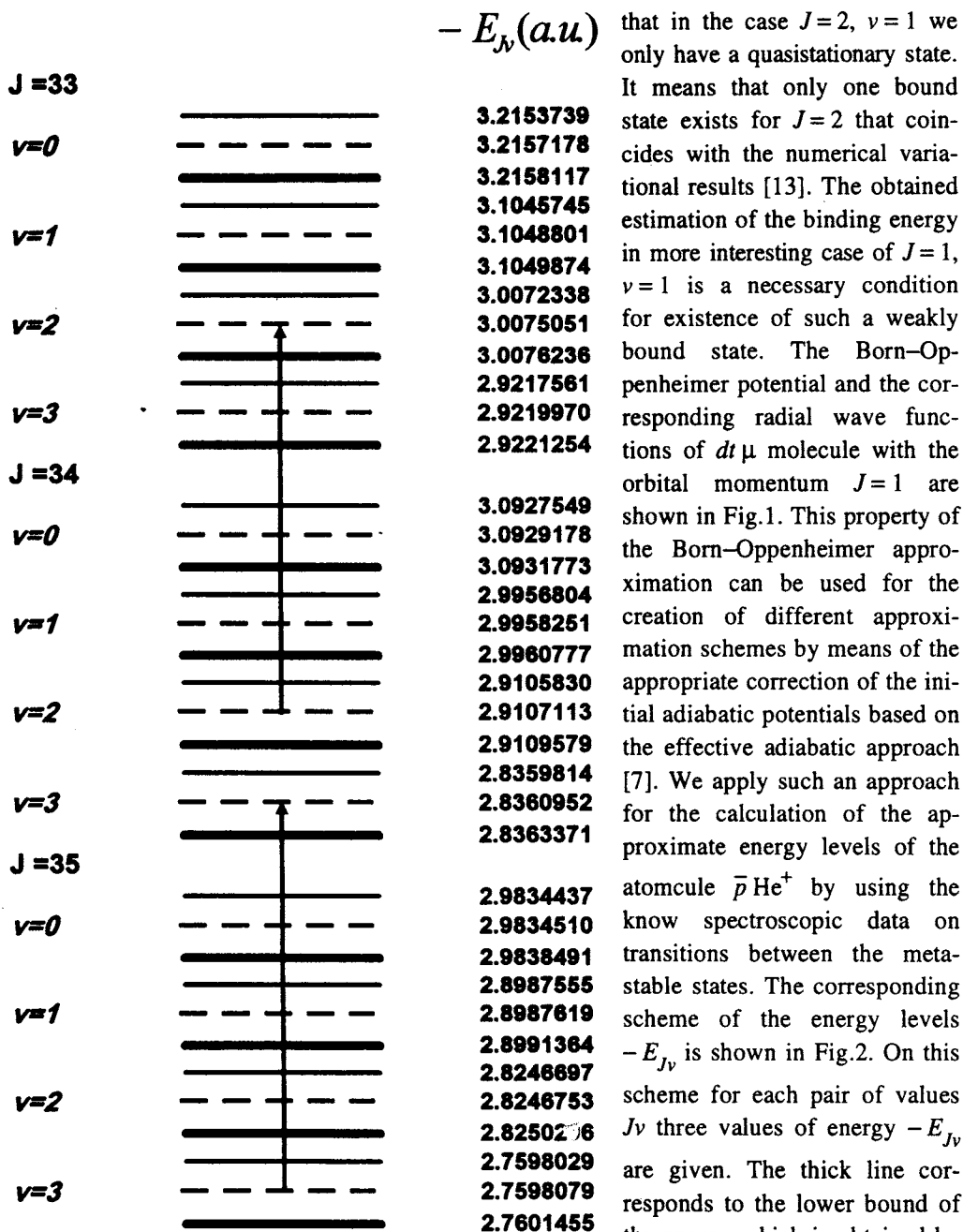
$$-E_{Jv}(a.u.)$$

J =33

v=0

v=1

v=2

v=3

3.2153739
3.2157178
3.2158117
3.1045745
3.1048801
3.1049874
3.0072338
3.0075051
3.0076236
2.9217561
2.9219970
2.9221254

J =34

v=0

v=1

v=2

v=3

3.0927549
3.0929178
3.0931773
2.9956804
2.9958251
2.9960777
2.9105830
2.9107113
2.9109579
2.8359814
2.8360952
2.8363371

J =35

v=0

v=1

v=2

v=3

2.9834437
2.9834510
2.9838491
2.8987555
2.8987819
2.8991364
2.8246697
2.8246753
2.8250236
2.7598029
2.7598079
2.7601455

Fig.2. The scheme of the energy levels $-E_{Jv}$ (in a.u.) of the $\bar{p}\,^4He^+$ atomcule

that in the case $J=2$, $v=1$ we only have a quasistationary state. It means that only one bound state exists for $J=2$ that coincides with the numerical variational results [13]. The obtained estimation of the binding energy in more interesting case of $J=1$, $v=1$ is a necessary condition for existence of such a weakly bound state. The Born–Oppenheimer potential and the corresponding radial wave functions of $dt\mu$ molecule with the orbital momentum $J=1$ are shown in Fig.1. This property of the Born–Oppenheimer approximation can be used for the creation of different approximation schemes by means of the appropriate correction of the initial adiabatic potentials based on the effective adiabatic approach [7]. We apply such an approach for the calculation of the approximate energy levels of the atomcule $\bar{p}\,He^+$ by using the know spectroscopic data on transitions between the metastable states. The corresponding scheme of the energy levels $-E_{Jv}$ is shown in Fig.2. On this scheme for each pair of values Jv three values of energy $-E_{Jv}$ are given. The thick line corresponds to the lower bound of the energy which is obtained by means of the Born–Oppenheimer approximation (3). The thin line shows the upper estimation of the energy which is

calculated by means of the effective adiabatic approximation with the true asymptotic behavior:

$$\left[\frac{d^2}{dR^2} + 2\frac{M}{\alpha}(\varepsilon_{Jv} - U_{11}^J(R)) \right]\chi_v^J(R) = 0. \tag{4}$$

Here $U_{11}^J(R)$ is the effective adiabatic potential

$$U_{11}^J(R) = \left(E_i(R) - E_1^{(as)} - \frac{2}{R} \right) + \frac{1}{2M}H_{11}(R) + \beta\frac{J(J+1)}{2MR^2},$$

the vibrational and rotational parameters α and β are approximately defined by ratio, $\alpha = \beta = M_0/M_b$, of reduced masses, $M_b^{-1} = (M_b + m_e)^{-1} + M_a^{-1}$, $M = M_0/m_b$, $-\varepsilon_{Jv}$ is binding energy, $\varepsilon_{Jv} = E_{Jv} - E_{1b}$, counting out $-E_{1b} = 2$ in the units $(e = \hbar = m_b = 1)$. In general case the parameters α and β are functions with respect to R [7,14]. Thus, for obtaining a more close upper estimation we can take into account this fact. For the typical values of orbital momentum $J \approx 30$ it leads to variations of the second order rotational correction $(2M)^{-2}J(J+1) \approx 10^{-4}$ and the third order rotational correction $(2M)^{-3}J(J+1)\sqrt{J(J+1)} \approx$ $\approx 10^{-6}$. It means that some improvement of the adiabatic potential may be achieved with the help of the appropriate correction of the values of the orbital momentum J. We suppose that such values of J may be obtained by fitting the known experimental data of transitions between the states [1]: $J = 34$, $v = 2$ to $J = 33$, $v = 2$ and $J = 35$, $v = 3$ to $J = 34$, $v = 3$. The dotted lines of the scheme (see Fig.2) correspond to the energy level values which are calculated by means of fitting values of orbital momentum J in the equations (4) with respect to these data. In the fitting process we use additional restrictions which resulted from the lower and upper adiabatic estimation obtained previously. Finally we have following values $J = 32.99735$, 33.99859, 34.99993 and values of the energy levels which are given in the right column of the scheme.

3. Results and Discussion

In the calculations, we made use of the following values of masses of particles: $M_{\bar{p}} = 1836.1527m_e$, $M_{3He^{2+}} = 5495.885m_e$, $M_{4He^{2+}} = 7294.299m_e$ and Ry $= 13.6058041$ eV. In order to fit the results of the numerical calculations of $\delta E = (E_{Jv} - E_{J'v'})$ with experimental data, the following scale factor is applied: $\lambda(J,v;J',v')[nm] = 10^9[(E_{Jv} - E_{J'v'})2R_\infty]^{-1}$, where $R_\infty = 10973731.538\,m^{-1}$ is the Rydberg constant [15]. (The approximated value of the
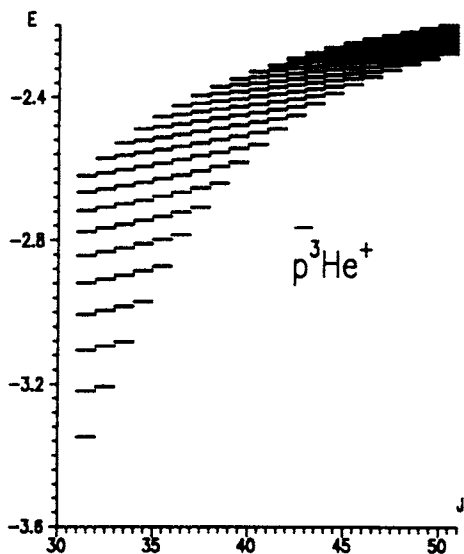
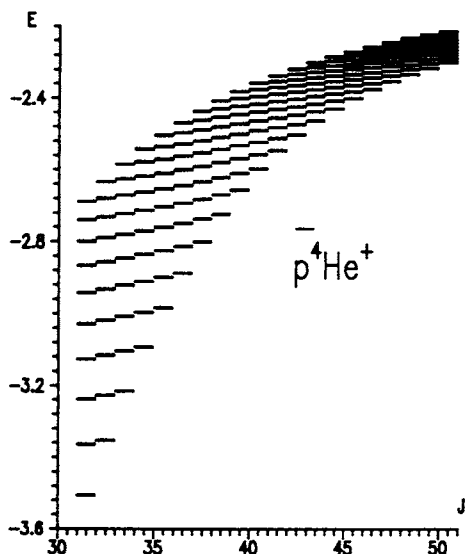Fig.3. The energy levels E^{Jv} ($J = 30$—50, $v = 0$—9) of $\bar{p}\,^3He^+$ system

Fig.4. The energy levels E^{Jv} ($J = 30$—50, $v = 0$—9) of $\bar{p}\,^4He^+$ system
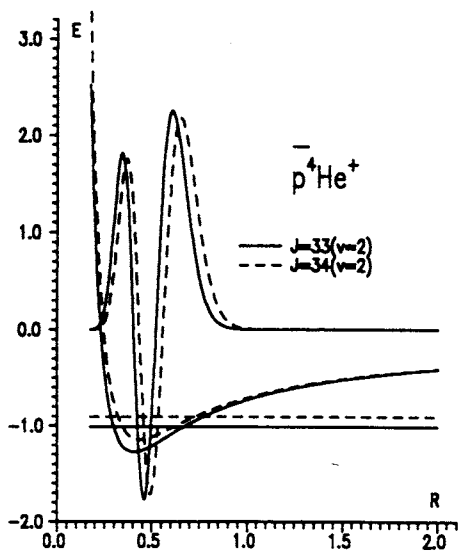

Fig.5. The potentials, wave functions and energy levels for the transition ($J = 33$, $v = 2$) to ($J = 34$, $v = 2$)
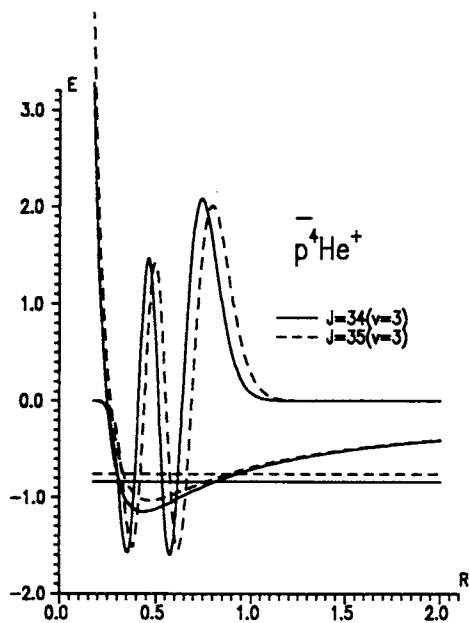
Fig.6. The potentials, wave functions and energy levels for the transition ($J = 34$, $v = 3$) to ($J = 35$, $v = 3$)

wavelength is the following: $\lambda = 45.56335 1/\delta E$). For the numerical solving of the eigenvalue problem we used calculating schemes and programs [16,17] which provide the accuracy of the numerical approximation of order 10^{-8}. The energy level schemes for the atomcule $\bar{p}\,He^+$ are shown in Figs.3,4. The adiabatic potentials and wave functions corresponding to the experimentally observed transitions $J = 34$, $v = 2$ to $J = 33$, $v = 2$ and $J = 35$, $v = 3$ to $J = 34$, $v = 3$ with wavelengths [1]: $\lambda (34, 2; 33, 2) = 470.725\,nm$, and $\lambda (35, 3; 34, 3) = = 597.259 \pm 0.002\,nm$ are shown in Figs.5,6. We give, as example, the lower estimations of the energy levels of the atomcule $\bar{p}\,He^+$ for $J = 31,..., 50$ in Tables 1,2. We suppose that the further development of the proposed approach will provide an alternative way of other cumbersome calculations.

Table 1. Energy levels E^{Jv} ($v = 0$—9) of $\bar{p}\,^3He^+$ system for $J = 31,..., 40$

	$J = 31$	$J = 32$	$J = 33$	$J = 34$	$J = 35$
$v = 0$	−3.348098	−3.207149	−3.081765	−2.970423	−2.871799
$v = 1$	−3.218832	−3.093983	−2.983073	−2.884748	−2.797815
$v = 2$	−3.105510	−2.994993	−2.896942	−2.810138	−2.733488
$v = 3$	−3.006239	−2.908440	−2.821762	−2.745093	−2.677422
$v = 4$	−2.919294	−2.832736	−2.756062	−2.688250	−2.628368
$v = 5$	−2.843107	−2.766438	−2.698514	−2.638400	−2.585237
$v = 6$	−2.776260	−2.708246	−2.647938	−2.594481	−2.547095
$v = 7$	−2.717477	−2.657007	−2.603300	−2.555584	−2.513158
$v = 8$	−2.665628	−2.611708	−2.563709	−2.520940	−2.482777
$v = 9$	−2.619721	−2.571478	−2.528410	−2.489905	−2.455417

	$J = 36$	$J = 37$	$J = 38$	$J = 39$	$J = 40$
$v = 0$	−2.784731	−2.708176	−2.641179	−2.582843	−2.532294
$v = 1$	−2.721201	−2.653926	−2.595074	−2.543773	−2.499181
$v = 2$	−2.665993	−2.606727	−2.554821	−2.509447	−2.469826
$v = 3$	−2.617819	−2.565415	−2.519399	−2.479013	−2.443555
$v = 4$	−2.575551	−2.529000	−2.487974	−2.451795	−2.419849

Table 1 (Continuation)

	J = 36	J = 37	J = 38	J = 39	J = 40
v = 5	−2.538234	−2.496666	−2.459874	−2.427263	−2.398305
v = 6	−2.505066	−2.467749	−2.434565	−2.405002	−2.378610
v = 7	−2.475389	−2.441710	−2.411620	−2.384682	−2.360514
v = 8	−2.448667	−2.418117	−2.390699	−2.366039	−2.343814
v = 9	−2.424464	−2.396624	−2.371529	−2.348861	−2.328348

	J = 41	J = 42	J = 43	J = 44	J = 45
v = 0	−2.488664	−2.451083	−2.418692	−2.390673	−2.366285
v = 1	−2.460481	−2.426891	−2.397676	−2.372165	−2.349766
v = 2	−2.435221	−2.404956	−2.378417	−2.355055	−2.334391
v = 3	−2.412384	−2.384927	−2.360674	−2.339176	−2.320042
v = 4	−2.391588	−2.366532	−2.344257	−2.324395	−2.306622
v = 5	−2.372538	−2.349558	−2.329014	−2.310600	−2.294045
v = 6	−2.355000	−2.333834	−2.314818	−2.297695	−2.282237
v = 7	−2.338788	−2.319220	−2.301563	−2.285599	−2.271136
v = 8	−2.323748	−2.305599	−2.289159	−2.274242	−2.260682
v = 9	−2.309753	−2.292873	−2.277529	−2.263561	−2.250826

	J = 46	J = 47	J = 48	J = 49	J = 50
v = 0	−2.344886	−2.325946	−2.309034	−2.293811	−2.280006
v = 1	−2.329966	−2.312336	−2.296520	−2.282230	−2.269236
v = 2	−2.316010	−2.299558	−2.284739	−2.271308	−2.259061
v = 3	−2.302930	−2.87546	−2.273638	−2.260996	−2.249441
v = 4	−2.290652	−2.276239	−2.263166	−2.251250	−2.240337

Table 1 (Continuation)

	J = 46	J = 47	J = 48	J = 49	J = 50
v = 5	−2.279109	−2.265581	−2.253276	−2.242032	−2.231713
v = 6	−2.268241	−2.255525	−2.243926	−2.233305	−2.223539
v = 7	−2.257997	−2.246025	−2.235079	−2.225035	−2.215782
v = 8	−2.248328	−2.237042	−2.226700	−2.217191	−2.208417
v = 9	−2.239192	−2.228539	−2.218757	−2.209746	−2.201418

Table 2. Energy levels E^{Jv} ($v = 0$—9) of $\bar{p}\,^4He^+$ system for $J = 31,..., 40$

	J = 31	J = 32	J = 33	J = 34	J = 35
v = 0	−3.506820	−3.353153	−3.215812	−3.093177	−2.983849
v = 1	−3.63873	−3.227111	−3.104987	−2.996078	−2.899136
v = 2	−3.237806	−3.116151	−3.007623	−2.910958	−2.825030
v = 3	−3.126711	−3.018536	−2.922125	−2.836337	−2.760145
v = 4	−3.028858	−2.932684	−2.847030	−2.770885	−2.703224
v = 5	−2.942677	−2.857151	−2.781005	−2.713289	−2.653134
v = 6	−2.866737	−2.790624	−2.722843	−2.662527	−2.608880
v = 7	−2.799745	−2.731916	−2.671465	−2.617599	−2.569594
v = 8	−2.749533	−2.679970	−2.625918	−2.577659	−2.534539
v = 9	−2.688063	−2.633852	−2.585372	−2.541980	−2.503091

	J = 36	J = 37	J = 38	J = 39	J = 40
v = 0	−2.886607	−2.800375	J = 38−2.724189	−2.657170	−2.598491
v = 1	−2.813061	−2.736859	−2.669628	−2.610523	−2.558743
v = 2	−2.748828	−2.6811430	−2.621982	−2.569679	−2.523761
v = 3	−2.692616	−2.632887	−2.580154	−2.533666	−2.492715
v = 4	−2.643262	−2.590172	−2.543207	−2.501676	−2.464938

Table 2 (Continuation)

	$J = 36$	$J = 37$	$J = 38$	$J = 39$	$J = 40$
$v = 5$	−2.599742	−2.552375	−2.510352	−2.473050	−2.439901
$v = 6$	−2.561169	−2.518726	−2.480939	−2.447255	−2.417180
$v = 7$	−2.526789	−2.488583	−2.454435	−2.423864	−2.396442
$v = 8$	−2.495969	−2.461417	−2.430411	−2.402533	−2.377417
$v = 9$	−2.468186	−2.436797	−2.408517	−2.382983	−2.359885

	$J = 41$	$J = 42$	$J = 43$	$J = 44$	$J = 45$
$v = 0$	−2.547355	−2.502973	−2.464554	−2.431309	−2.402474
$v = 1$	−2.513514	−2.474085	−2.439728	−2.409756	−2.383529
$v = 2$	−2.483500	−2.448210	−2.417251	−2.390035	−2.366034
$v = 3$	−2.456640	−2.424835	−2.396748	−2.371886	−2.349812
$v = 4$	−2.432410	−2.403564	−2.377933	−2.355105	−2.334717
$v = 5$	−2.410397	−2.384089	−2.360582	−2.339531	−2.320632
$v = 6$	−2.390279	−2.366168	−2.344515	−2.325029	−2.307457
$v = 7$	−2.371797	−2.349605	−2.329584	−2.311490	−2.295106
$v = 8$	−2.354745	−2.334242	−2.315669	−2.298818	−2.283507
$v = 9$	−2.338951	−2.319946	−2.302666	−2.286835	−2.272594

	$J = 46$	$J = 47$	$J = 48$	$J = 49$	$J = 50$
$v = 0$	−2.377342	−2.355284	−2.335770	−2.318361	−2.302707
$v = 1$	−2.360472	−2.340081	−2.321927	−2.305650	−2.290956
$v = 2$	−2.344780	−2.325862	−2.308928	−2.293679	−2.279864
$v = 3$	−2.330141	−2.312536	−2.296704	−2.282392	−2.269385
$v = 4$	−2.316451	−2.300024	−2.285192	−2.271737	−2.259475

Table 2. (Continuation)

	$J = 46$	$J = 47$	$J = 48$	$J = 49$	$J = 50$
$v = 5$	−2.303620	−2.288258	−2.274336	−2.261668	−2.250094
$v = 6$	−2.291573	−2.277176	−2.264087	−2.252144	−2.241206
$v = 7$	−2.280242	−2.266725	−2.254400	−2.243126	−2.232778
$v = 8$	−2.269569	−2.256857	−2.245234	−2.234578	−2.224778
$v = 9$	−2.259502	−2.247528	−2.236554	−2.226470	−2.217180

Acknowledgments

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