PHYSICAL REVIEW A **86**, 014502 (2012)

Borromean windows for H_2^+ with screened Coulomb potentials

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(Received 30 April 2012; published 5 July 2012)

We have carried out calculations to search Borromean windows for the bound F and G states of the H_2^+ system, where the nuclei and the electrons interact through a screened Coulomb (Yukawa-type) potential. The bound F and G state energies for different values of the screening parameters are obtained using correlated exponential wave functions in the framework of the Ritz variational principle. The critical values of the screening parameters for the bound F and G states are reported for which the H_2^+ system is stable, while all the possible fragments are unbound; that is, it shows windows for Borromean binding.

DOI: 10.1103/PhysRevA.86.014502 PACS number(s): 33.20.−t, 03.65.Ge

Search for Borromean states is an interesting topic of current research. A three-body system is called Borromean if it is bound while all the two-body subsystems are unbound [1,2]. The word "Borromean" has been proposed in nuclear physics to identify bound states in which all the possible subsystems are unbound [3]. It comes from the Borromean rings, which are interlaced in a subtle topological way such that if any one of them is removed, the two other become unlocked. For an N-body system, a bound state is called Borromean if there is no path to build it via a series of stable states by adding the constituents one by one. A connection between Borromean binding and two other fascinating phenomena, viz., the Efimov effects [4] and Thomas collapse [5], has been discussed in the articles by Richard [1,2]. The existence of Borromean binding in the ground states of different atomic and molecular systems has been discussed in a number of articles [6–16]. Borromean systems have also appeared in other areas such as nuclear physics [16], molecular physics [17], chemical physics [18], and DNA [19]. In the present work, we are mainly interested in investigating Borromean windows for F and G states of the hydrogen molecular ion H_2^+, one of the simplest molecules in nature. Recently we have reported the stability of S, P, and D states of H_2^+ with screened Coulomb potentials [9,15]. The stability of the bound F and G states of H_2^+ interacting with screened Coulomb (Yukawa) potentials has not been studied yet. In the free atomic case, several theoretical studies ([20–28], and references therein) and a few experimental investigations [29,30] have so far been performed for this system to investigate various properties of the H_2^+ molecular ion. With abundance of the H_2^+ ions in interstellar matter, with the recent experimental advancements in the experiments of H_2^+ using laser spectroscopy, and with wide applications of screened Coulomb potentials in different branches of physics and chemistry ([31,32], references therein), it is important to study various properties of this simplest three-body system in screening environments.

By applying the Rayleigh-Ritz variational principle and employing highly accurate exponential wave functions with a quasirandom process of nonlinear parameters, in the present work we have investigated the stability of the bound F and G states of the molecular H_2^+ ion in the field of screened Coulomb (Yukawa-type) potential of the form $\exp(-\mu r)/r$, where μ is the screening parameter. The existence of Borromean binding is established for the two lowest F states and two lowest G states of the molecular ion H_2^+. For the pure Coulomb cases, our results for the F and G states are comparable with the reported results [24,28]. Convergence of the calculations has been examined with the increasing number of terms in the wave functions. The atomic unit has been used throughout the work. The existence of Borromean bindings are found in F and G states of the H_2^+ molecular ion, and windows of Borromean bindings are also presented for such states.

The nonrelativistic screened Hamiltonian H_2^+ system can be written in the form

$$H = -\frac{1}{2m}\left[\nabla_1^2 + \nabla_2^2\right] - \frac{1}{2}\nabla_3^2 - \left[\frac{\exp(-\mu r_{31})}{r_{31}} + \frac{\exp(-\mu r_{32})}{r_{32}}\right] + \frac{\exp(-\mu r_{21})}{r_{21}}, \quad (1)$$

where 1, 2, and 3 denote the two nuclei and the electron respectively, $r_{ij} = |r_i - r_j| = r_{ji}$, and $m = 1836.152\,701$, where m denotes the nuclear mass in the units of electron mass. When the H_2^+ ion is placed in vacuum, we have $\mu = 0$. In plasma physics the parameter μ $(=1/\lambda_D$; λ_D is called Debye length) is known as the Debye screening parameter.

For triplet F and singlet G states of the hydrogen molecular ion, we consider the basis set of the form [15]

$$\left\{\exp(-\alpha_i r_{31} - \beta_i r_{32} - \gamma_i r_{21}) \mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_{31},\mathbf{r}_{32}) : i = 1,2,\ldots,N\right\}, \quad (2)$$

where the functions $\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_{31},\mathbf{r}_{32})$ are the bipolar harmonics, and α_i, β_i, γ_i are the nonlinear variation parameters. These nonlinear parameters in the basis set (2) are chosen by using a quasirandom process. The parameters α_i, β_i, and γ_i are chosen from the three positive intervals $[a_1, a_2]$, $[b_1, b_2]$, and $[d_1, d_2]$:

$$\begin{aligned}
\alpha_i &= \left\langle\!\left\langle \frac{1}{2} i(i+1)\sqrt{23} \right\rangle\!\right\rangle (a_2 - a_1) + a_1, \\
\beta_i &= \left\langle\!\left\langle \frac{1}{2} i(i+1)\sqrt{29} \right\rangle\!\right\rangle (b_2 - b_1) + b_1, \qquad (3)\\
\gamma_i &= \left\langle\!\left\langle \frac{1}{2} i(i+1)\sqrt{31} \right\rangle\!\right\rangle (d_2 - d_1) + d_1,
\end{aligned}$$

TABLE I. Bound F and G state energies of the hydrogen molecular ion for different screening parameters. The maximum uncertainty of the calculated energies is of the order of 10^{-6} a.u. for the $\nu = 0$ states. For the $\nu = 1$ states, we estimate the accuracy of our present calculations is about 1×10^{-4} a. u.

$1/\mu$	$^3F^o$ ($\nu = 0$, $J = 3$)	$^3F^o$ ($\nu = 1$, $J = 3$)	$^1G^e$ ($\nu = 0$, $J = 4$)	$^1G^e$ ($\nu = 1$, $J = 4$)	H($1s$ ^2S)[a]
∞	– 0.59 55 563	– 0.585 628	– 0.594 511	– 0.584 57	– 0.5 00 00 000
	– 0.59 55 558[b]	– 0.585 621[b]	– 0.594 509[b]	– 0.58 456[b]	
	– 0.59 55 549[c]	– 0.585 611[c]	– 0.594 507[c]	– 0.58 453[c]	
	– 0.59 55 576[d,e]	– 0.58 56 576[e]	– 0.594 517[d,e]	– 0.58 467[e]	
100	– 0.585 622	– 0.575 693	– 0.584 576	– 0.574 638	– 0.49 007 451
50	– 0.575 817	– 0.565 889	– 0.574 772	– 0.564 834	– 0.48 029 611
20	– 0.547 155	– 0.537 236	– 0.546 111	– 0.536 181	– 0.45 181 643
15	– 0.531 703	– 0.521 791	– 0.530 659	– 0.520 737	– 0.43 653 060
10	– 0.501 762	– 0.491 872	– 0.500 719	– 0.490 820	– 0.40 705 803
	– 0.501 760[c]	– 0.491 856[c]	– 0.500 715[c]	– 0.490 774[c]	
8	– 0.480 116	– 0.470 249	– 0.479 074	– 0.469 198	– 0.38 587 872
6	– 0.445 509	– 0.435 692	– 0.444 471	– 0.434 644	– 0.35 225 907
5	– 0.419 088	– 0.409 321	– 0.418 053	– 0.408 277	– 0.32 680 851
	– 0.419 088[b]	– 0.409 315[b]	– 0.418 049[b]	– 0.408 231[b]	
	– 0.419 087[c]	– 0.409 305[c]	– 0.418 049[c]	– 0.408 220[c]	
4	– 0.381 459	– 0.371 788	– 0.380 430	– 0.370 750	– 0.29 091 959
3	– 0.323 765	– 0.314 308	– 0.322 749	– 0.313 284	– 0.23 683 267
2.5	– 0.281 838	– 0.272 603	– 0.280 835	– 0.271 593	– 0.19 837 608
2	– 0.225 487	– 0.216 670	– 0.224 511	– 0.215 687	– 0.14 811 702
1.8	– 0.197 374	– 0.188 833	– 0.196 416	– 0.187 866	– 0.12 381 303
1.6	– 0.165 264	– 0.157 111	– 0.164 331	– 0.156 165	– 0.09 686 159
1.5	– 0.147 554	– 0.139 654	– 0.146 637	– 0.138 723	– 0.08 244 734
1.4	– 0.128 691	– 0.121 102	– 0.127 795	– 0.120 186	– 0.06 752 960
1.3	– 0.108 696	– 0.101 494	– 0.107 826	– 0.100 596	– 0.05 231 507
1.2	– 0.087 688	– 0.080 971	– 0.086 849	– 0.080 093	– 0.03 717 849
1.1	– 0.065 956	– 0.059 862	– 0.0065 156	– 0.058 999	– 0.02 278 129
1.0	– 0.044 123	– 0.038 845	– 0.043 397	– 0.038 104	– 0.01 028 579
0.88	– 0.019 632	– 0.015 754	– 0.018 808	– 0.014 091	– 0.000 815
0.86	– 0.015 990	– 0.012 398	– 0.015 093	– 0.010 428	– 0.000 213
0.85	– 0.014 242	– 0.0108 049	– 0.013 292	– 0.008 643	– 0.000 055
0.84	– 0.012 548	– 0.009 274	– 0.011 531	– 0.006 891	
0.82	– 0.00 935	– 0.00 641	– 0.00 876	– 0.00 569	
0.8	– 0.00 644	– 0.00 389	– 0.00 5876	– 0.00 312	
	– 0.00 642[c]				
		– 0.00 381[c]	– 0.00 5828[c]	– 0.00 296[c]	
0.78	– 0.00 388	– 0.00 175	– 0.003 308	– 0.00 091	
0.77	– 0.00 275	– 0.00 086	– 0.002 164		
0.765	– 0.00 223	– 0.00 045	– 0.001 638		
0.76	– 0.00 174		– 0.00 114		
0.75	– 0.00 084		– 0.00 022		
0.745	– 0.00 045				

[a] Reference [9].

[b] 1900-term basis function [Eq. (2)].

[c] 1800-term basis function [Eq. (2)].

[d] Reference [24].

[e] Reference [28].

where the symbol $\langle\langle \cdots \rangle\rangle$ designates the fractional part of a real number.

We first carry out calculations to obtain bound F and G state energies of the hydrogen molecular ion for different choices of screening parameters in the framework of the Rayleigh-Ritz variational principle using the basis functions (2). To designate molecular states it is convenient to use the rotational (J) and vibrational (ν) quantum numbers. It is known that the three-body states can also be classified as gerade or ungerade depending on the combined effect of the spin (S) and parity (π), $\pi(-1)^S$, with the resulting plus sign denoting gerade and

TABLE II. Windows for Borromean binding, $\mu_c^{\mathrm{H}} \leqslant \mu \leqslant \mu_c^{\mathrm{H}_2^+}$ for F and G states of H_2^+. The maximum uncertainty of the estimated parameters is of the order of 10^{-4} $(1/a_0)$.

System	μ_c^{H}	$\mu_c^{\mathrm{H}_2^+}$
$\mathrm{H}_2^+(^3F^o)$ ($\nu = 0$, $J = 3$)	1.1878	1.3532
$\mathrm{H}_2^+(^3F^o)$ ($\nu = 1$, $J = 3$)	1.1878	1.3178
$\mathrm{H}_2^+(^1G^e)$ ($\nu = 0$, $J = 4$)	1.1878	1.3362
$\mathrm{H}_2^+(^1G^e)$ ($\nu = 1$, $J = 4$)	1.1878	1.2991

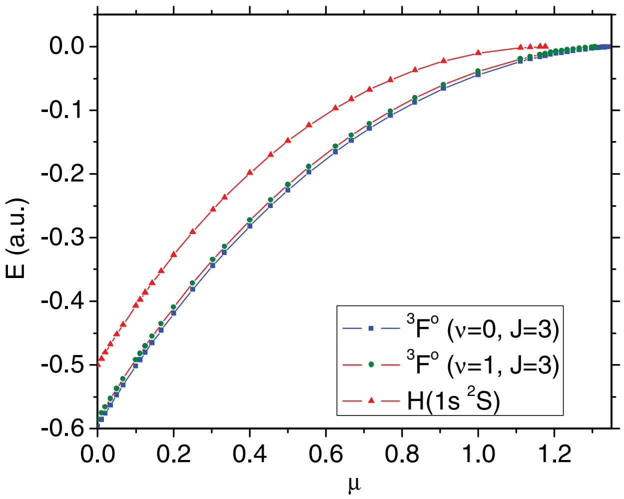

FIG. 1. (Color online) The bound $^3F^o$ ($\nu = 0$, $J = 3$) and $^3F^o$ ($\nu = 1$, $J = 3$) states of the molecular H_2^+ ion in terms of the screening parameters μ (units of a_0^{-1}) along with H($1s$ ^2S) threshold energies.

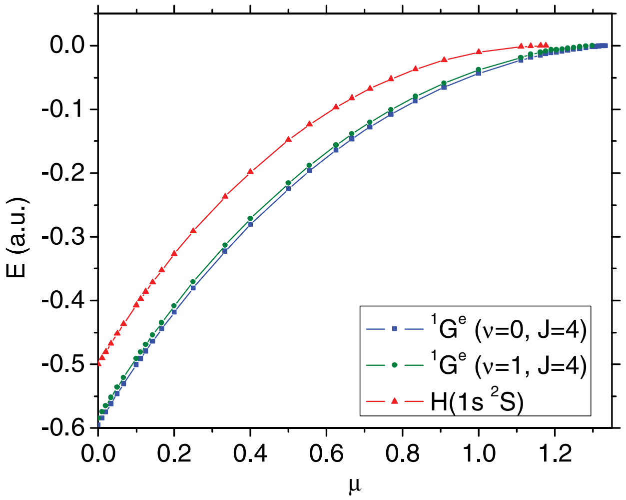

FIG. 2. (Color online) The bound $^1G^e$ ($\nu = 0$, $J = 4$) and $^1G^e$ ($\nu = 1$, $J = 4$) states of the molecular H_2^+ ion as functions of the screening parameters μ along with H ($1s$ ^2S) threshold energies.

the minus sign denoting ungerade. The atomic levels for the $J = 3$ and $J = 4$ gerade states are $^3F^o$ and $^1G^e$, respectively. In this work, we determine the bound $^3F^o$ ($\nu = 0$, $J = 3$), $^3F^o$ ($\nu = 1$, $J = 3$), $^1G^e$ ($\nu = 0$, $J = 4$), $^1G^e$ ($\nu = 1$, $J = 4$) state energies of the hydrogen molecular ion for different values of the screening parameters. In Table I and Figs. 1 and 2, we present the bound F and G state energies obtained from our present work. From Table I and Figs. 1 and 2, it is clear that the H_2^+ molecular ion is bound but the hydrogen atom is not bound for stronger screening for some screening parameters. This shows the existence of the Borromean binding for the H_2^+ molecular ion. Next, we fit the energy levels with a ninth degree polynomial to obtain the critical values of μ to estimate the window of Borromean binding for each of the F and G states. The critical values μ_c of μ obtained from the present work for different systems are presented in Table II. The range $\mu_c^{\mathrm{H}} \leqslant \mu \leqslant \mu_c^{\mathrm{H}_2^+}$ is commonly known as the Borromean window. Table II shows the range of the Borromean window for each of the bound F and G states of H_2^+. From these tables and figures, it is also clear that the energies of H_2^+ are lower than the energies of the corresponding H atom, and the critical parameter for H_2^+ is greater than that for H. For $\mu < \mu_c^{\mathrm{H}}$ the H-like atom is stable, and H plus H^+ would give the relevant threshold that implies the stability of H_2^+ against dissociation: $\mathrm{H}_2^+ \rightarrow \mathrm{H} + \mathrm{H}^+$. For $\mu > \mu_c^{\mathrm{H}}$, the hydrogenlike atom becomes unbound. But for $\mu_c^{\mathrm{H}} \leqslant \mu \leqslant \mu_c^{\mathrm{H}_2^+}$, the system is stable against the dissociation: $\mathrm{H}_2^+ \rightarrow \mathrm{H}^+ + \mathrm{H}^+ + e^-$, or into any other two-body subsystems, as in this range the H-like atom is not bound. In the unscreened cases, our calculated bound F and G state energies are accurate up to some part of 10^{-6} compared to the best reported results for the lowest states [24]. For the $\nu = 1$ states, we estimate the accuracy of our present calculations is about 1×10^{-4} a.u. compared to the best reported results [28]. The H($1s$ ^2S) energies are taken from our earlier work [9]. We have used a maximum of up to 2000-term wave functions for the F-state and G-state calculations. In Table I, we present convergence of our calculations with increasing number of terms in the basis functions. Since H_2^+ is stable even when H is not stable, H_2^+ can be considered as a prototype for the Borromean systems.

ACKNOWLEDGMENTS

S.K. wishes to thank the Natural Scientific Research Innovation Foundation in Harbin Institute of Technology for financial support. Y.K.H. is supported by NSC of Taiwan.

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