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Expansion of the H_2^+ ground state energy in inverse powers of the distance between the two protons

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Résumé. — L'énergie du fondamental de l'ion moléculaire H_2^+ a été développée en puissances de l'inverse de la distance entre les deux protons

$$E = \sum \frac{a_n}{R^n}.$$

Il est expliqué ici que les coefficients a_n se comportent pour n très grand selon la loi

$$a_n \simeq -\frac{2}{e^2} \frac{(n+1)!}{2^{n+1}}.$$

Abstract. — The ground state energy of the ionized hydrogen molecule H_2^+ has been expanded in inverse powers of the distance between the two protons

$$E = \sum \frac{a_n}{R^n}.$$

It is explained here that for n very large the coefficients a_n behave as

$$a_n \simeq -\frac{2}{e^2} \frac{(n+1)!}{2^{n+1}}.$$

In a recent article J. Morgan and B. Simon [1] have studied the expansion of the ground state energy of the ion H_2^+ in inverse powers of the distance between the two protons :

$$H = -\frac{1}{2} \Delta - \left(\frac{1}{r} + \frac{1}{|\mathbf{R} - \mathbf{r}|} \right) \quad (1)$$

$$E = \sum_{n=0}^{\infty} \frac{a_n}{R^n}. \quad (2)$$

It is shown in their study that the series (2) is asymptotic and presumably divergent and not Borel summable. This is conjectured on the basis of a numerical study by the same authors which indicates that the following asymptotic law for the coefficients a_n seems to hold :

$$a_n \underset{n \rightarrow \infty}{\sim} -C_0 \frac{(n+1)!}{2^{n+1}} \quad (3)$$

with C_0 a negative constant estimated to lie in the range (0.27-0.30).

As pointed out by these authors, it is not surprising that the series diverges in this way, since the expansion in powers of $1/R$ begins with a state localized around the origin. The expansion around this state is never able to reproduce the true wave function which is symmetric under the exchange $\mathbf{r} \leftrightarrow (\mathbf{R} - \mathbf{r})$ and thus peaked around the two centres. The situation is analogous to that of the simpler one-dimensional double well problem [2].

It is known [3] that one can relate the large order behaviour of this expansion to the splitting in energy of the two lowest lying states, symmetric and anti-symmetric under the exchange $\mathbf{r} \leftrightarrow (\mathbf{R} - \mathbf{r})$. The derivation relies on the fact that the large order estimates are related to well separated instanton-antiinstanton paths for which the action is twice the instanton action, and that the quantum fluctuations are the square of those around the single instanton

Table I.

$$\bar{a}_n = -a_n \frac{2^{n+1}}{(n+1)!} \text{ is taken from Ref. [1]}$$

$$b_n = n \bar{a}_n - (n-1) \bar{a}_{n-1}$$

$$c_n = \frac{1}{2} (b_n - (n-2) b_{n-1}).$$

$\bar{a}_n, b_n, c_n$ should approach the same limit with deviations of order $1/n, 1/n^2$ and $1/n^3$ respectively.

n	$\bar{a}_n$	b_n	c_n
20	0.281 988 43	0.291 723 5	0.270 749 3
21	0.282 318 98	0.288 930 0	0.262 391 9
22	0.282 529 96	0.286 960 5	0.267 266 1
23	0.282 640 16	0.285 064 6	0.265 156 8
24	0.282 683 16	0.283 672 2	0.268 355 8
25	0.282 668 47	0.282 315 9	0.266 719 0
26	0.282 616 03	0.281 305 0	0.269 174 5
27	0.282 530 70	0.280 312 1	0.267 900 7
28	0.282 424 40	0.279 554 3	0.269 702 6
29	0.282 299 60	0.278 805 2	0.268 692 4
30	0.282 163 59	0.278 219 3	0.270 016 7
31	0.282 017 64	0.277 639 1	0.269 226 8
32	0.281 866 32	0.277 175 4	0.270 219 3
33	0.281 710 21	0.276 714 7	0.269 573 7
34	0.281 552 26	0.276 339 9	0.270 343 4
35	0.281 392 70	0.275 967 7	0.269 825 5
36	0.281 233 42	0.275 658 6	0.270 404 9
37	0.281 107 443	0.275 350 8	0.269 963 8

path. We make the assumption that the same features hold for the more singular Coulomb problem.

This splitting has been calculated by Landau-Lifshitz [4] for large R :

$$\frac{1}{2} \Delta E \underset{R \text{ large}}{\simeq} \frac{2}{e} R e^{-R}. \quad (4)$$

The formula relating the asymptotic behaviour of the coefficients of the $1/R$ expansion to $\Delta E(R)$ is

$$a_n \underset{n \text{ large}}{\simeq} \int_0^\infty dR R^{n-1} \left(\frac{1}{2} \Delta E(R) \right)^2 \quad (5)$$

and thus for n large it requires an estimate of the large R behaviour of $\Delta E(R)$. Using the result (4) this leads to

$$a_n \simeq -C_0 \frac{(n+1)!}{2^{n+1}}, \quad (6)$$

with

$$C_0 = \frac{2}{e^2} = 0.270 670 57. \quad (7)$$

It is interesting to compare this result to the numbers given by Morgan and Simon [1]. The convergence of the sequence $\bar{a}_n = -\frac{2^{n+1} a_n}{(n+1)!}$ is not very rapid and we have used a Neville table [5]. A further numerical analysis suggests that

$$\bar{a}_n = \frac{2}{e^2} \left(1 + \frac{2}{n} + O\left(\frac{1}{n^2}\right) \right).$$

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