Corrigendum: The $\text{H}_2^+$ molecular ion: a solution

2011 J. Phys. B: At. Mol. Opt. Phys. 44 101002

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Received 22 April 2012
Published 18 May 2012
Online at stacks.iop.org/JPhysB/45/119501

Two unfortunate omissions occurred in the exponents of denominators in the central formula (14) in the published version of the paper. The correct form of equation (14) is as follows:

\[
\psi_{\mu,n,\Lambda}^{(\pm)} = \frac{(\xi^2 - 1)^{\Lambda/2} P_\mu(\xi)}{(\gamma + \xi)^{1+\mu+\Lambda-\frac{\epsilon}{2}}} \cdot \frac{(1 - \eta^2)^{\Lambda/2} Q_m(\eta^2)}{(1 + b_2\eta^2 + b_3\eta^4)^{1+\mu+\Lambda-\frac{\epsilon}{2}}} \times \left[ \frac{\cosh \left( \eta a_1 + p\eta^2 \right)}{\sinh \left( \frac{\eta}{1 + b_2\eta^2 + b_3\eta^4} \right)} \right] e^{i\Lambda\phi}.
\]

Also, in formulas (16) and (17) in potentials $V(\xi)$ and $W(\eta)$, respectively, the parameter $a$ should be replaced by $p$. The above omissions and typos did not influence any result presented in the published text.
FAST TRACK COMMUNICATION

The H$_2^+$ molecular ion: a solution

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Received 30 March 2011, in final form 11 April 2011
Published 10 May 2011
Online at stacks.iop.org/JPhysB/44/101002

Abstract
Combining the WKB expansion at large distances and perturbation theory at small distances a compact uniform approximation for eigenfunctions is constructed. For the lowest states 1s$_\sigma_g$ and 2p$_\sigma_u$, this approximation provides the relative accuracy $\lesssim 10^{-5}$ (5 s.d.) for any real $x$ in eigenfunctions and for total energy $E(R)$ it gives 10–11 s.d. for internuclear distances $R \in [0, 50]$. Corrections to proposed approximations are evaluated. Separation constants and the oscillator strength for the transition 1s$_\sigma_g$ $\rightarrow$ 2p$_\sigma_u$ are calculated and compared with existing data.

(Some figures in this article are in colour only in the electronic version)

1. Introduction
The H$_2^+$ molecular ion is the simplest molecular system which exists in nature. It was the first studied molecular system since the inception of the quantum mechanics which later appeared in all QM textbooks (see e.g. [1]). It is needless to say that this system plays a very important role in different physical sciences, in particular, in laser and plasma physics.

From the technical point of view, this is the unique molecular system which admits complete separation of variables (in elliptic coordinates). Definitely, this problem is non-solvable. Thus, the problem can be solved in an approximate way only. We introduce a natural definition of solvability of a non-solvable spectral problem: for any eigenfunction $\Psi_1$ we can indicate constructively a uniform approximation $\Psi_{1,app}$ such that

$$\left| \frac{\Psi_1(x) - \Psi_{1,app}(x)}{\Psi_1(x)} \right| \lesssim \delta,$$

in the coordinate space. It implies that any observable, matrix element can be found with an accuracy not less than $\delta$. A simple idea that we are going to employ is to combine a WKB expansion at large distances with perturbation theory at small distances near the extremum of the potential in one interpolation. Recently, this idea was realized for a quartic anharmonic oscillator [2] and a double-well potential [3]. In both cases, for the lowest states two-three parametric uniform approximations of the eigenfunction were constructed leading to 10 s.d. in energies and with $\delta \sim 10^{-5}$ for any value of the coupling constant and size of the barrier. The goal of this communication is to present such an approximation with $\delta \sim 10^{-5}$ for the two lowest (and the most important) states 1s$_\sigma_g$ and 2p$_\sigma_u$ of the H$_2^+$ molecular ion. It is worth mentioning that a study of the wavefunctions of the H$_2^+$ molecular ion in a form of expansion in some basis was initiated by Hylleraas [4] and successfully realized in the remarkable paper [5] (see also [6, 7]). Attempts to find bases leading to fast convergence are still continuing. At present, the pure exponential basis seems to be the fastest convergent (see e.g. [8] and references therein). It is worth noting that following the analysis of classical mechanics of the H$_2^+$ system and its subsequent semiclassical quantization some uniform approximations of the wavefunctions of low-lying electronic states were constructed [9]. Local accuracies of these approximations are unclear albeit eigenparameters are found with a few significant figures.

The Schrödinger equation, which describes the electron in the field of two centres of the charge $Z = 1$ at the distance $R$, is of the form

$$\left( -\Delta - \frac{2}{r_1} - \frac{2}{r_2} \right) \Psi = E' \Psi, \quad \Psi \in L^2(\mathbb{R}^3),$$

where $E' = (E - \frac{Z^2}{4})$ and the total energy $E$ is in Rydbergs; $r_{1,2}$ are the distances from electron to the first and second centres,
unambiguously continued in $/Psi_1$

and the azimuthal angle $\phi$. The Jacobian is $\propto (\xi^2 - \eta^2)$.

Equation (2) admits the separation of variables in (3). Since the
projection of the angular momentum to the molecular
axis $L_z$ commutes with the Hamiltonian$^2$, the eigenstate has
a definite magnetic quantum number $\Lambda$. The Hamiltonian
is permutationally symmetric $r_1 \leftrightarrow r_2$, or, equivalently,
$\eta \rightarrow -\eta$; hence, any eigenfunction is of a definite parity
($\pm$). As a result, it can be represented in a form

$$\Psi = X(\xi)(\xi^2 - \eta^2)^{\Lambda/2}Y(\eta)(1 - \eta^2)^{\Lambda/2}e^{i\pm A\phi},$$

$\Lambda = 0, 1, 2, \ldots$

(4)

where $Y(\eta)$ is of definite parity. After substitution of (4) into
(2) we arrive at the equations for $X(\xi)$ and $Y(\eta)$:

$$\partial_\xi[\xi(\xi^2 - 1)\partial_\xi X] + 2A\xi\partial_\xi X + \left[-p^2\xi^2 + 2RX + A\right]X = 0,$$

$X \in L^2(\xi \in [1, \infty]),$

(5)

$$\partial_\eta[(\eta^2 - 1)\partial_\eta Y] + 2A\eta\partial_\eta Y + \left[-p^2\eta^2 + A\right]Y = 0,$$

$Y \in L^2(\eta \in [-1, 1]),$

(6)

respectively, where following [5] we denote

$$p^2 = -\frac{E'R^2}{4},$$

(7)

and $A$ is a separation constant. Equations (5) and (6) define
a bispectral problem with $E, A$ spectral parameters. Both
spectral parameters $E, A$ depend on $R$. Square integrability
of the function $\Psi$ (4) implies non-singular behaviour of $X$ at
$\xi \rightarrow 1$ as well as non-singular behaviour of $Y$ at $\eta \rightarrow \pm 1$.
The latter condition implies certain behaviour of the solution
$Y$ at large arguments $\eta$. A non-singular solution $Y(\eta)$ can be
unambiguously continued in $\eta$ beyond the interval $[-1, 1]$: it
has to be growing (non-decaying) at $|\eta| \rightarrow \infty$. It
agrees in large-$\eta$ behaviour with the Hund–Mulliken
function (it mimics the incoherent interaction of electron with
charged centres) for both $1s\sigma_g$ (parity $+$) and $2p\sigma_u$ (parity $-$)
states:

$$\Psi_{10m}^{(\mp)} = e^{-2\alpha_3r_1} \pm e^{-2\alpha_3r_2} = 2e^{-\alpha_3R}$$

$$\left(\frac{\cosh(\alpha_3R\eta)}{\sinh(\alpha_3R\eta)}\right).$$

(8)

which describes large $R$ behaviour; similarly, for the
Guillemin–Zener function (it mimics the coherent interaction
of electron with charged centres),

$$\Psi_{GZ}^{(\pm)} = e^{-2\alpha_3r_1 - 2\alpha_3r_2} \pm e^{-2\alpha_3r_3 - 2\alpha_3r_4},$$

$$2e^{-\alpha_3r_\Lambda}R\left(\frac{\cosh((\alpha_3 - \alpha_4)R\eta)}{\sinh((\alpha_3 - \alpha_4)R\eta)}\right),$$

(9)

which has to correspond to small $R$ behaviour.

$^1$ From the 3D point of view they are prolate spheroidal.

$^2$ Due to the complete separation of variables one more integral in a form of
the second-order polynomial in momentum exists in [10]: it is closely related to
the Runge–Lenz vector [11] and commutes with $L_z$; hence, the $\mathrm{He}_2^+$ ion in the
adiabatic (Born–Oppenheimer) approximation is the completely integrable
system.

2. Asymptotics

If we put $X = e^{-\varphi}$, then at $\xi \rightarrow \infty$,

$$p^2 = -\frac{E'R^2}{4}$$

$$\left(\frac{\cosh(A + \frac{2}{p} - \Lambda - 1)(\frac{\xi}{p} + \Lambda)}{\frac{\xi}{p} - \Lambda - 1} - \frac{p}{2}\right)\frac{1}{2\xi^2} + \cdots,$$

(10)

which is nothing but a WKB expansion, and at $\xi \rightarrow 0$,

$$\varphi = -\frac{A}{2}\xi^2 - \frac{R}{3}\xi^3 + \left(\frac{p^2 + A^2 - A(2\Lambda + 3)}{12}\right)\xi^4 + \cdots.$$ (11)

Similar to $X$, we put $Y = e^{-\varphi}$; then at $\eta \rightarrow \infty$,

$$\varphi = -p\eta + (\Lambda + 1)\log \left(\frac{\Lambda + (\Lambda + 1)}{p} - 1\right)\frac{1}{2\eta^2} + \cdots,$$

(12)

and at $\eta \rightarrow 0$,

$$\varphi = -\frac{A}{2}\eta^2 + \left(\frac{p^2 + A^2 - A(2\Lambda + 3)}{12}\right)\eta^4 + \cdots.$$ (13)

The important property of expansions (10) and (12) is that the
coefficients in front of the growing terms at large distances
(linear and logarithmic) are found explicitly, since they do not
depend on the separation constant $A$.

3. Approximation

Making interpolation between the WKB expansion (10) and the perturbation
theory (11) for $X$, (12) and (13) for $Y$, correspondingly, and taking into account that the $Z_2$-symmetry
of $\Psi$: $\eta \rightarrow -\eta$ is realized through use of cosh(sinh)-function (cf (8) and (9)) we arrive at the following expression:

$$\Psi_{n,m,\Lambda}^{(\pm)} = \frac{(\xi^2 - 1)^{\Lambda/2}P_\Lambda(\xi)}{(\eta + \xi)^{1/2}\eta^{-2}}e^{-\frac{\varphi}{2\xi^2}}$$

$$\left(\frac{1 - \eta^2)^{\Lambda/2}Q_m(\eta^2)}{(1 + 2\eta^2 + 3\eta^4)^{1/2}}\right)e^{iA\phi},$$

(14)

for the eigenfunction of the state with the quantum numbers
$(n, m, \Lambda, \pm)$. Here, $\alpha, \gamma$ and $a_{1,2}$, $b_{2,3}$ are parameters (see below),
and $P_\Lambda(\xi)$ and $Q_m(\eta^2)$ are some polynomials of
degrees $n$ and $m$ with real coefficients with $n$ and $m$ real
roots in the intervals $[1, \infty)$ and $[0, 1]$, respectively. These
polynomials should be chosen in such a way as to ensure their
orthogonality.

4. Results

As an illustration we consider two lowest states—one of positive and one of negative parity, $1s\sigma_g (0, 0, 0, +)$
and $2p\sigma_u (0, 0, 0, -)$, respectively. The corresponding
approximations have the form

$$\Psi_{0,0,0}^{(\pm)} = \frac{1}{(\eta + \xi)^{1/2}\eta^{-2}}e^{-\frac{\varphi}{2\xi^2}}$$

$$\left(\frac{1 - \eta^2)^{\Lambda/2}Q_m(\eta^2)}{(1 + 2\eta^2 + 3\eta^4)^{1/2}}\right)e^{iA\phi},$$

(15)
of the form (cf (14)), and each of them depends on six parameters $\alpha, \gamma$ and $a_{1,2}, b_{2,3}$. The easiest way to find these parameters is to make a variational calculation taking (15) as a trial function for $R$ fixed and with $p$ as an extra variational parameter. The immediate striking result of the variational study is that for all $R \in [1.0, 1.997193]$ the optimal value of the parameter $p$ coincides with the exact value of $p$ (see (7)) with extremely high accuracy for both $1s_\sigma$ and $2p_\sigma$ states. It implies a very high quality of the trial function—the variational optimization wants to reproduce with very high accuracy a domain where the eigenfunction is exponentially small, hence the domain which gives a very small contribution to the energy functional. In Tables 1 and 2 the results for the total energy (as well as for sensitive $p$) versus $R$ of the $1s_\sigma$ and $2p_\sigma$ states are shown as well as their comparison with the ones obtained by Montgomery [6] in highly accurate realization of the approach by Bates et al [5], and also with the results we obtained in the Lagrange mesh method based on the Vincke–Baye approach [12] (details of calculations will be given elsewhere). For all of the studied values of $R$ for both $1s_\sigma$ and $2p_\sigma$ states our variational energy turns out to be in agreement with the level of 10 s.d. with these two alternative calculations. Variational parameters are smooth slow-changing functions of $R$, see tables 3–5. All calculations were implemented in double-precision arithmetics and checked in quadruple precision one.

Table 1. The total energy $E_t(R)$ for the $1s_\sigma$ state of the H$^+$-ion compared to [6] (rounded) and the Lagrange mesh method.

| $R$ (au) | $E_t$ (Ry) (present/[6]/mesh) | $p$   |
|---------|-------------------------------|------|
| 1.0     | $-0.903 572 626 76$           | 0.851 9936 |
| 1.997193 | $-1.205 269 238 21$           | 1.483 403 |
| 2.0     | $-1.205 268 428 99$           | 1.485 015 |
| 6.0     | $-1.023 938 0969$            | 3.495 06 |
| 10.0    | $-1.001 157 4579$             | 5.479 87 |
| 12.5    | $-1.000 261 1115$             | 6.732 21 |
| 30.0    | $-1.000 005 5815$             | 15.492 |
| 40.0    | $-1.000 001 7622$             | 20.4939 |
| 50.0    | $-1.000 000 7211$             | 25.495 11 |

Table 2. The total energy $E_t(R)$ for the $2p_\sigma$ state of the H$^+$-ion compared to [6] (rounded) and the Lagrange mesh method.

| $R$ (au) | $E_t$ (present/[6]/mesh) (Ry) | $p$   |
|---------|-------------------------------|------|
| 1.0     | 0.870 372 7499                | 0.531 4196 |
| 1.997 193 | $-0.333 280 0331$           | 1.153 6645 |
| 2.0     | $-0.335 068 7844$            | 1.155 452 |
| 4.0     | $-0.891 101 2787$            | 2.3589 |
| 10.0    | $-0.999 802 1372$             | 5.476 78 |
| 12.545 25  | $-1.000 121 5811$             | 6.754 34 |
| 20.0    | $-0.999 002 3953$             | 10.4882 |
| 30.0    | $-1.000 005 5815$             | 15.492 |
| 40.0    | $-1.000 001 7622$             | 20.4939 |

The difference between the original $V(\xi)$ and generated $V_0(\xi)$ is the perturbation, $V_1(\xi) = V(\xi) - V_0(\xi)$. For the sake of convenience we can insert a parameter $A$ in front of $V_1$ and develop the perturbation theory in powers of it:

$$ V_1(\xi) = A V_1(\xi) $$
Table 3. The parameters of the function (15) for the $1s\sigma_g$ state of the $\text{H}_2^+$-ion. The parameters $\alpha$, $\gamma$ and $a_{1,2}, b_{1,2}$ are found via minimization.

| $\alpha$  | $p$     | $\gamma$  | $a_1$  | $a_2$  | $b_2$  | $b_3$  |
|----------|---------|-----------|--------|--------|--------|--------|
| 1.48407  | 1.483403| 1.0299   | 0.9164 | 0.05344| 0.06   | 0.00011|
| 3.32381  | 3.49506 | 0.96357  | 2.59735| 0.53443| 0.58807| 0.00552|
| 10.0453  | 10.4882 | 0.95774  | 9.8775 | 6.8392 | 6.9016 | 1.352  |

Table 4. The parameters of the function (15) for the $2p\sigma_u$ state of the $\text{H}_2^+$-ion. The parameters $\alpha$, $\gamma$ and $a_{1,2}, b_{1,2}$ are found via minimization.

| $\alpha$  | $p$     | $\gamma$  | $a_1$  | $a_2$  | $b_2$  | $b_3$  |
|----------|---------|-----------|--------|--------|--------|--------|
| 3.24715  | 3.43971 | 0.95706  | 2.84566| 0.22098| 0.23611| -0.0027|
| 6.5275   | 6.75434 | 0.97045  | 6.075  | 1.46757| 1.5349 | 0.1675 |
| 10.7397  | 10.4882 | 1.0307   | 9.8077 | 2.3784 | 2.43705| 0.567  |

Table 5. Separation parameters $A_{1\xi}, A_{1\eta}$ for $1s\sigma_g$, $2p\sigma_u$ states of the $\text{H}_2^+$-ion compared to [14].

| $R$   | $A_{1\xi}$  | $A_{1\eta}$  | $A_{1\xi}$  | $A_{1\eta}$  |
|-------|--------------|--------------|--------------|--------------|
| 2.0   | 0.811729588  | 0.811729588  | 0.811729588  | 0.811729588  |
| 15.0  | 48.822353534 | 48.822353534| 48.822353534| 48.822353534|
| 20.0  | 90.052891187 | 90.052891187| 90.052891187| 90.052891187|
| 30.0  | 210.03459660 | 210.03459660| 210.03459660| 210.03459660|
Knowledge of wavefunctions with high local relative accuracy gives us a chance to calculate matrix elements with controlled relative accuracy \( \lesssim 10^{-5} \). As a demonstration we calculate the oscillator strength as a function of the interproton distance for the simplest radiative transition \( 2p_{\sigma_u} \rightarrow 1s_{\sigma_g} \) (see e.g. [7]):

\[
 f_{01}(R) = \frac{1}{2} (E_{2p_{\sigma_u}}(R) - E_{1s_{\sigma_g}}(R)) |Q(R)|^2 ,
\]

(29)

where \( Q(R) \) is the matrix element

\[
 Q(R) = \langle \Psi_{1s_{\sigma_g}}(R)|r|\Psi_{2p_{\sigma_u}}(R) \rangle ,
\]

where \( r \) is the vector of the electron position measured from the internuclear midpoint, and the wavefunctions \( \Psi_{1s_{\sigma_g}} \), \( \Psi_{2p_{\sigma_u}} \) are given by (15). It is assumed that this calculation should provide at least 5 s.d. correctly. In table 6 the results are presented. For all internuclear distances they coincide in 2 s.d. with those of Bishop et al [7], thus indicating that the third digit obtained in [7] is incorrect for \( R = 1, 2, 4 \) au, and in six figures with recent results [15] (with an exception at \( R=1 \) au where it deviates in one unit at the sixth digit) which increases up to eight figures for large \( R \). Modification of (15)
by adding the first corrections (28) and using it in (29) does not change our 6 s.d. in table 6.

Summarizing, we want to state that a simple uniform approximation of the eigenfunctions for the H$_2^+$ molecular ion is presented. It allows us to calculate any expectation value or matrix element with guaranteed accuracy. It manifests the approximate solution of the problem of spectra of the H$_2^+$ molecular ion. In a quite straightforward way similar approximations can be constructed for a general two-centre, one-electron system (Z$_a$, Z$_b$, e), in particular, for (HeH)$^{++}$. It will be done elsewhere.

The key element of the procedure is to construct an interpolation between the WKB expansion at large distances and perturbation series at small distances for the phase of the wavefunction, or, in other words, to find an approximate solution for the corresponding eikonal equation. Separation of variables allowed us to solve this problem. In the case of non-separability of variables the WKB expansion of a solution of the eikonal equation cannot be constructed in a unified
The representation realized in the action on polynomials in $\xi, \eta$ and $s \Theta$ of the hydrogen atom in a magnetic field and will be published elsewhere.

A curious fact that the problem (2) possesses the hidden algebra $sl(2) \oplus sl(2)$ is worth mentioning. It can be immediately seen—making the gauge rotation of the operators on the rhs of equations (5) and (6) with gauge factors $\exp{-p\xi}$ and $\exp{p\eta}$, respectively. We obtain the operators which are in the universal enveloping algebra of $sl(2)$ (see e.g. [16]). The dimensions of the representation are $-\Lambda$ and $-\Lambda + \frac{N}{2}$, respectively. For non-physical values of $\Lambda$ and the integer ratio $\frac{p}{p'}$ the algebras $sl(2)$ appear in the finite-dimensional representation realized in the action on polynomials in $\xi, \eta$. It explains a mystery sometimes observed of the existence of polynomial solutions for non-physical values of $\Lambda$ in the problem (2) (details will be given elsewhere).

Acknowledgments

The research is supported in part by DGAPA grant IN115709 and CONACyT grant 58942-F (Mexico). HOP is supported by CONACyT project for postdoctoral research. AVT thanks the University Program FENOMECE (UNAM, Mexico) for partial support.

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Table 6. Oscillator strength $f_{01}$ (29) for the transition $2p\sigma_u \rightarrow 1s\sigma_g$ versus $R$ compared to Bishop et al [7] and Tsogbayar et al [15] (rounded).

| $R$  | Present  | [7]  | [15] |
|------|----------|------|------|
| 1.0  | 0.538 675 | 0.538 | 0.538 6739 |
| 1.997 193 | 0.639 595 | — | — |
| 2.0  | 0.639 527 | 0.638 | 0.639 5268 |
| 4.0  | 0.469 200 | 0.476 | 0.469 2004 |
| 10.0 | 2.217 $\times 10^{-02}$ | 0.022 | 2.217 06 $\times 10^{-02}$ |
| 15.0 | 5.129 $\times 10^{-04}$ | — | 5.129 39 $\times 10^{-04}$ |
| 20.0 | 8.191 $\times 10^{-06}$ | — | 8.205 13 $\times 10^{-06}$ |
| 30.0 | 4.770 $\times 10^{-09}$ | — | — |
| 40.0 | 1.828 $\times 10^{-10}$ | — | — |