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Asymptotic behaviour of the equilibrium nuclear separation for the H_2^+ molecule in a strong magnetic field

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Abstract
We consider the hydrogen molecular ion H_2^+ in the fixed nuclear approximation, in the presence of a strong homogeneous magnetic field. We determine the leading asymptotic behaviour for the equilibrium distance between the nuclei of this molecule in the limit when the strength of the magnetic field goes to infinity.

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1. Introduction

One-dimensional Hamiltonians with delta function interactions have been used for a long time as toy models in atomic physics (see, e.g. [5], and references therein). However, with the study of matter in the presence of strong magnetic fields, these models have become more physically relevant.

It is now well established that atoms and molecules in the presence of a strong uniform magnetic field behave like systems in one dimension. In fact, a strong magnetic field confines the electrons to Landau orbitals which are orthogonal to the direction of the applied magnetic field. In this manner, only the behaviour of the electrons along the direction of the magnetic field is subject to the influence of their Coulomb interaction with the nuclei or to the interaction among themselves. Since one can extend the results of [4, section 9] to the present molecular case, this genuine molecular case reduces effectively to the one-dimensional ion model where Coulombic interactions between the electron and the nuclei are replaced by delta point interactions, see (1).

2. The asymptotic model

Our model consists of two nuclei, each one of nuclear charge Z, separated by a distance R. As we have discussed in the introduction, for large values of the magnetic field, the molecule we are considering is described by an asymptotic model defined by the following Hamiltonian:

$$H = L^2 Z^2 \left[\frac{p_z^2}{2} - \delta\left(z - \frac{RLZ}{2}\right) - \delta\left(z - \frac{RLZ}{2}\right)\right] + \frac{Z^2}{R}, \tag{1}$$

acting on $L^2(\mathbb{R})$ (see [1] for more details). The parameter L that appears in this Hamiltonian depends on the strength of the magnetic field and it is given explicitly by $L = 2W(\sqrt{B}/2)$, where W is the Lambert function [6]. If one considers the function $y(x) = x\exp(x)$, for $x \in [0, \infty)$, the Lambert function is its inverse, i.e., $x = W(y)$. It is elementary to derive the following asymptotics:

$$L = \log B - 2\log(\log B) + \mathcal{O}\left(\frac{\log(\log B)}{\log B}\right), \qquad B \to \infty.$$

The ground state energy of this system, which is a function of R, Z and L, can be computed in closed form in terms of the Lambert function, and it is given by

$$E(R, L, Z) = -L^2 Z^2 \frac{\alpha_0^2}{2} + \frac{Z^2}{R}, \tag{2}$$

where

$$\alpha_0 \equiv 1 + \frac{W(RLZ\,\mathrm{e}^{-RLZ})}{RLZ}.$$

The first term in (2) is the electronic energy, while the second term is just the Coulomb repulsion between the nuclei.

In this section we study the dependence of the ground state energy E, of the asymptotic model, on the nuclear separation R. In particular, we shall determine for which values of the parameters Z and L, the asymptotic model exhibits binding.

Let

$$F(x) \equiv \tfrac{1}{2}(x + W(x\,\mathrm{e}^{-x}))^2. \tag{3}$$

In terms of $F(x)$, the ground state energy of H can be written as

$$E(R, L, Z) = -\frac{F(RLZ)}{R^2} + \frac{Z^2}{R} = \frac{L^2 Z^2}{x}\left(\frac{Z}{L} - \frac{F(x)}{x}\right), \tag{4}$$

where $x = RLZ$. When the nuclei are infinitely apart, the ground state energy of H is given by

$$E_{\mathrm{at}} = -\frac{Z^2 L^2}{2}. \tag{5}$$

As usual, we define the *binding energy* of the molecule as the difference

$$E_B = \sup_R [E_{\mathrm{at}} - E(R, L, Z)]. \tag{6}$$

The molecule will exist (in the frame of this asymptotic model) if and only if $E_B > 0$, i.e., if $E_{\mathrm{at}} - E(R, L, Z) > 0$ for some $R \in (0, \infty)$. In case $E_B > 0$, we will denote R_{eq} the value of

R which maximizes $E_{at} - E(R, L, Z)$.R_{eq} is the actual separation between the nuclei of the molecule described by the asymptotic model.

In terms of $x = RLZ$ and the Lambert function, we can write

$$E_{at} - E(R, L, Z) = \frac{L^2 Z^2}{x}\left(J(x) - \frac{Z}{L}\right), \tag{7}$$

where

$$J(x) \equiv \frac{F(x)}{x} - \frac{x}{2} = \frac{(2x + W(x\,e^{-x}))W(x\,e^{-x})}{2x}. \tag{8}$$

Using (7), we see that there will be a molecule in the asymptotic model provided there is an x for which $J(x) > Z/L$. One can readily check that the function $J(x)$ is positive in $(0, \infty)$, $J(0) = 0$ and $\lim_{x\to\infty} J(x) = 0$. Moreover, $J(x)$ has only one maximum in $(0, \infty)$, located at $x_J \approx 0.84$ and $J(x_J) \approx 0.3205$, see lemma 1 in the appendix. Thus, if $(Z/L) < J(x_J)$, the molecule exists (in other words, there is a global minimum of $-E_{at} + E(R, L, Z))$ and therefore $E_B > 0$.

In case $Z/L > J(x_J)$, the molecule will not bind. However, there could still be a local minimum of $-E_{at} + E(R, L, Z)$ in $(0, \infty)$. If there is a local minimum, but $E_B \leqslant 0$, we will say that there is a *resonance*. To study local minima, we compute

$$\frac{\partial E}{\partial R}(R, L, Z). \tag{9}$$

Using (4) and the properties of the Lambert function we can express

$$\frac{\partial E}{\partial R}(R, L, Z) = \frac{LZ}{R^2}\left(G(x) - \frac{Z}{L}\right), \tag{10}$$

where, as before, $x = RLZ$ and

$$G(x) \equiv \frac{(x + W(x\,e^{-x}))^2 W(x\,e^{-x})}{x(1 + W(x\,e^{-x}))}. \tag{11}$$

Using the properties of the Lambert function, one can check that the function $G(x)$ is positive in $(0, \infty)$, $G(0) = 0$, $\lim_{x\to\infty} G(x) = 0$. Moreover, $G(x)$ has a unique maximum in this interval, attained at $x_G \approx 1.95$ and $G(x_G) \approx 0.4398$, see lemma 2 in the appendix. One can compare the functions J and G defined above. It turns out that $J(x) \geqslant G(x)$ if $0 \leqslant x \leqslant x_J$, whereas $J(x) \leqslant G(x)$ if $x_J \leqslant x < \infty$, hence $G(x_J) = J(x_J)$ (i.e., both functions agree at the maximum of J). From (10) and the properties of G we see that if $Z/L > G(x_G)$, $-E_{at} + E(R, L, Z)$ does not have a local minimum in $(0, \infty)$. On the other hand, if $J(x_J) < Z/L < G(x_G)$, $-E_{at} + E(R, L, Z)$ has a local minimum, i.e., we will have a *resonance*.

We can summarize our discussion above in the following theorem. See also figure 1.

Theorem 1. *For the system described by the Hamiltonian (1), the energy curve* $-E_{at} + E(R, L, Z)$

(a) has no local minimum if $G(x_G) \approx 0.44 < \frac{Z}{L}$,

(b) has a local minimum if $J(x_J) \approx 0.32 < \frac{Z}{L} < G(x_G) \approx 0.44$,

(c) has a global minimum (i.e, there is binding) if $\frac{Z}{L} < J(x_J) \approx 0.32$*; we denote by* R_{eq} *the position of this minimum.*

For fixed nuclear charge Z, Z/L can be made arbitrarily small by choosing the strength of the magnetic field sufficiently large, since $L = 2W(\sqrt{B}/2)$. Hence, for sufficiently large B,

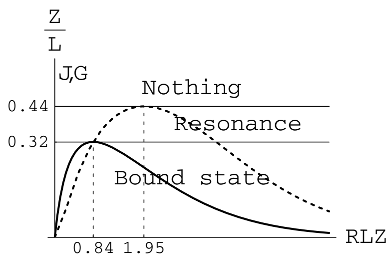

Figure 1. Graphs of J (thick solid curve), G (thick dashed curve), and Z/L (thin horizontal lines).

$-E_{\text{at}} + E(R, L, Z)$ will have a global minimum. In this case, it follows from (10) that the position of this minimum is given by

$$R_{\text{eq}} = \frac{1}{LZ} G^{-1}\left(\frac{Z}{L}\right). \tag{12}$$

If $Z/L \ll 1$, we get from (12) and (A.20) in the appendix that

$$R_{\text{eq}} = \frac{1}{2}\frac{1}{L^{3/2}Z^{1/2}} + \frac{5}{8}\frac{1}{L^2} + \frac{45}{64}\frac{Z^{1/2}}{L^{5/2}} + \frac{1}{L^2} O\left(\frac{Z}{L}\right). \tag{13}$$

For $Z/L \ll 1$, the minimum value of the energy, $E(R_{\text{eq}}, L, Z)$, can be obtained to leading order, using (4), (13) and (A.17) in the appendix. Thus we obtain,

$$E_{\min} \equiv E(R_{\text{eq}}, L, Z) = -2Z^2L^2\left(1 - 2\theta + \tfrac{5}{4}\theta^2 + O(\theta^3)\right), \tag{14}$$

where we have set $\theta = \sqrt{Z/L}$.

For our discussion below, it is convenient to give the asymptotic behaviour of the whole energy curve, $E(R, L, Z)$, for large values of the magnetic field (i.e., for large values of L). Using (4) and the asymptotic properties of $F(x)$, given in the appendix, see (A.17), we obtain

$$E(R, L, Z) = \frac{L^2Z^2}{x}\left(\frac{Z}{L} - 2x + 4x^2 - 10x^3 + O(x^4)\right), \tag{15}$$

with $x = RLZ$. This asymptotic behaviour is valid for values of R such that $R \ll \frac{1}{LZ}$.

3. The leading behaviour of the nuclear separation of the H_2^+ molecule in the presence of a strong magnetic field

With the help of the calculations on the asymptotic model of Section 2, we will compute the leading behaviour of the equilibrium nuclear separation of the H_2^+ molecule, in the limit when the strength of the magnetic field goes to infinity. Since we are interested in the H_2^+ molecule, we set $Z = 1$ throughout this section. Denote by r_{eq} the equilibrium distance between the nuclei of the H_2^+ molecule in the presence of a strong magnetic field. Here we will prove the following estimate for r_{eq}.

Theorem 2.

$$r_{\text{eq}} = \frac{1}{2L^{3/2}} + \mathcal{O}\left(L^{-\frac{7}{4}}\right), \qquad \textit{as} \quad B \to \infty \tag{16}$$

where $L = 2W(\sqrt{B}/2)$ *and* W *is the Lambert function ([6]).*

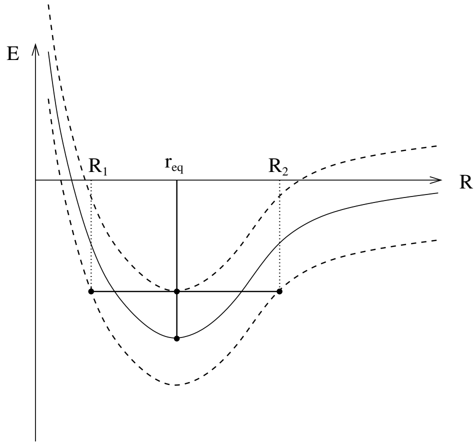

Figure 2. A sketch of the curves $R \to E(R, L, Z)$ and $R \to E(R, L, Z) \pm \alpha_\pm$ with the points $R_{1,2}$ and r_{eq}.

In [1], we have said that the ground state energy of the H_2^+ molecule can be estimated in terms of the ground state energy of the asymptotic model, using the norm-resolvent convergence method developed by Brummelhuis and Duclos in [4]. We will denote by $E(R, L, 1)$ the ground state energy of the asymptotic model studied in section 2, for $Z = 1$ and by $e(R, L, 1)$ the ground state energy of the asymptotic model. As said in [1], for B large enough one has

$$E(R, L, 1) - \alpha_- \leqslant e(R, L, 1) \leqslant E(R, L, 1) + \alpha_+, \tag{17}$$

where $\alpha_\pm$ are positive constants that only depend on L. Moreover,

$$\alpha_+ + \alpha_- = cL, \tag{18}$$

where c is a constant, independent of L and R. These above two equations can be derived with the method of [4]; see in particular theorem 1.5 and section 9 there.

In section 2, we have computed the equilibrium distance, R_{eq} (13), and the minimum energy, E_{min} (14), for the asymptotic delta model. Given these values and the error estimates embodied in (17) and (18), we can estimate the actual separation of the nuclei of the H_2^+ molecule in the presence of a strong magnetic field. In figure 2, we have pictured the energy curve for the asymptotic model, $E(R, L, 1)$, as well as the curves $E(R, L, 1) \pm \alpha_\pm$. Recall that we denote by r_{eq} the equilibrium distance of the nuclei of the real molecule in the presence of a strong magnetic field; it follows from the figure that

$$R_1 < r_{eq} < R_2, \tag{19}$$

where R_1 and R_2 are the solutions of the equation

$$E_{min} + \alpha_+ = E(R, L, 1) - \alpha_-,$$

i.e.,

$$E_{min} + cL = E(R, L, 1); \tag{20}$$

one can see easily that they both go to 0 as $L \to \infty$, see the end of the appendix. Replacing the asymptotic behaviour (14) for E_{min} (with $Z = 1$) and (15) for $E(R_i, L, 1)$ in (20), we get

$$-2L^2\left(1 - 2L^{-1/2} + \frac{5}{4}L^{-1} + O(L^{-3/2})\right) + cL = \frac{L^2}{x}\left(\frac{1}{L} - 2x + 4x^2 - 10x^3 + O(x^4)\right), \tag{21}$$

where $x = R_i L$ (since $Z = 1$). It follows that

$$\left(1 - 2L^{\frac{1}{2}}x\right)^2 = \left(c - \tfrac{5}{2}\right)x + 10x^3 L + \mathcal{O}(x^4 L) + \mathcal{O}\left(L^{-\frac{1}{2}}x\right). \tag{22}$$

Assume now that $L^{\frac{1}{2}}x$ is not bounded, this would mean that there exists a subsequence of L values so that $L^{\frac{1}{2}}x \to \infty$. Substituting this sequence in (22) gives

$$4Lx^2 \sim \left(c - \tfrac{5}{2}\right)x + 10x^3 L \sim 10x^3 L$$

since $x^2 L \to \infty$; however, this is a contradiction. Using in (22) that $R_i L^{\frac{3}{2}} = xL^{\frac{1}{2}}$ is bounded gives

$$R_i = \frac{1}{2L^{\frac{3}{2}}} + \mathcal{O}\left(L^{-\frac{7}{4}}\right),$$

which proves the theorem.

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Appendix A

Definition 1. *We define the function* $J(x)$ *as*

$$J(x) \equiv W(y) + \frac{W(y)^2}{2x}, \tag{A.1}$$

for all $0 \leqslant x < \infty$, *where* $y = x\exp(-x)$, *and* W *denotes the Lambert function, as defined in section 2. Since in the following* W *as well as its derivative is always evaluated at* $y = x\exp(-x)$, *we shall sometimes omit this argument.*

In our next lemma, we prove some properties of $J(x)$ needed in the main body of the manuscript.

Lemma 1. *The function* $J(x)$ *is positive in* $(0, \infty)$, *it is real analytic, it has a unique maximum, with value* $\max J \sim 0.32$ *taken at* $x_J \sim 0.84$.

Proof. That J is positive in $(0, \infty)$ follows immediately from (A.1) and the definition of W. The Lambert function is real analytic. Moreover, for small values of its argument, $W(y) = y + \mathcal{O}(y)$, thus $W(y)^2/2x$ will also be real analytic in $(0, \infty)$. Hence, we need only prove that J has a unique critical point (a maximum) in $(0, \infty)$. Taking the derivative of (A.1) with respect to x, we get

$$\frac{\mathrm{d}J}{\mathrm{d}x} = \frac{\mathrm{d}W}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x} + W\frac{\mathrm{d}W}{\mathrm{d}y}\frac{\mathrm{d}y}{\mathrm{d}x}\frac{1}{x} - \frac{W(y)^2}{2x^2}. \tag{A.2}$$

From the definition of the Lambert function, it follows that

$$\frac{\mathrm{d}W}{\mathrm{d}y} = \frac{W(y)}{y(1 + W(y))}, \tag{A.3}$$

and from the definition of $y = x\exp(-x)$ we have

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \frac{y}{x}(1-x). \tag{A.4}$$

Using (A.2), (A.3) and (A.4) we get

$$\frac{\mathrm{d}J}{\mathrm{d}x} = \frac{W(y)}{2(1+W(y))x^2} j(x), \tag{A.5}$$

where we have set

$$j(x) = 2x(1-x) + 2W(y)(1-x) - W(y)(1+W(y)). \tag{A.6}$$

Since W is positive in $(0,\infty)$, the sign of $j(x)$ determines the sign of $\mathrm{d}J/\mathrm{d}x$. The function $j(x)$ is clearly negative for $x > 1$. On the other hand, we can rewrite

$$j(x) = x(1-2x) + x(1-2W(y)) + W(y)(1-W(y)). \tag{A.7}$$

Since $W(y) \leqslant y$ and $y = x\,\mathrm{e}^{-x} < x \leqslant 1/2$, if $0 \leqslant x \leqslant 1/2$, it follows from (A.7) that $j(x) > 0$ for all $x \in (0, 1/2)$. Using (A.3) and (A.4), we can compute

$$x(1+W(y))j'(x) = x(1+W)[2(1-2x) - 2W] + (1-x)W[(1-2x) - 2W]. \tag{A.8}$$

In the interval $(1/2, 1)$ each of the terms on the right-hand side of (A.8) is negative. Hence, $j(x)$ decreases in $(1/2, 1)$. In summary, $j(x) > 0$ in $(0, 1/2)$, $j(x)$ strictly decreases in $(1/2, 1)$ and $j(x) < 0$ in $(1, \infty)$. From here it follows that $j(x)$ has a unique zero in $(0,\infty)$. If we denote x_J by this zero, it follows from the proof that $1/2 < x_J < 1$. Numerically, $x_J \approx 0, 84$. □

Definition 2. *We define the function $G(x)$ as*

$$G(x) \equiv \frac{W(y)(x+W(y))^2}{x(1+W(y))}, \tag{A.9}$$

for all $0 \leqslant x < \infty$ where, as before, $y = x\exp(-x)$, and W denotes the Lambert function. Concerning the function $G(x)$, in our next lemma, we prove some properties needed in the main body of the manuscript.

Lemma 2. *The function $G(x)$ is positive in $(0,\infty)$, it is real analytic, it has a unique maximum $\max G \sim 0.44$ taken at $x_G \sim 1.95$. Moreover, the functions $J(x)$ and $G(x)$ intersect at a unique point in $(0,\infty)$ precisely at $x = x_J$.*

Proof. Let us begin by proving that G and J only cross at x_J, i.e., at the maximum point of $J(x)$. From (A.1) and (A.9), we see that the equation $G(x) = J(x)$ can be simplified to read

$$2x - 2x^2 - 2xW = W^2 - W,$$

which is precisely the condition $j(x) = 0$ (see equation (A.7)), which has only one solution which we have denoted by x_J. □

Now, using (A.9), (A.3) and (A.4), after some simplifications we can write

$$\frac{\mathrm{d}G}{\mathrm{d}x} = \frac{(W+x)W}{x^2(1+W)^2} g(x), \tag{A.10}$$

where we have set

$$g(x) \equiv 2W(y)(1-x) + (x - W(y))(1+W(y)) + \frac{1}{1+W(y)}(W+x)(1-x). \tag{A.11}$$

If $x < 1$, the first and the last term of (A.11) are positive. On the other hand, $y < x$ and $W(y) < y$ imply that the second term is also positive. Thus, $g(x) > 0$ if $0 < x < 1$. Moreover, we can regroup terms in (A.11) to write

$$(1 + W(y))g(x) = (2 - x)(W(y) + x) - xW(y)^2 - W(y)^3. \tag{A.12}$$

From (A.12) it follows that $g(x) < 0$ if $x > 2$. Finally, we can compute

$$\phi(x) \equiv x(1 + W(y))[(1 + W)g]', \tag{A.13}$$

using as before (A.3) and (A.4). After several simplifications, we get

$$\phi(x) = 2W(1 - x) + 2xW^2(x - 2) + 2(1 - x)x + 2W^3(x - 2) - (x^2 - W^2)W. \tag{A.14}$$

If $1 < x < 2$, the first four terms of (A.14) are negative. The last term is also negative, since $W < x$. In summary, $(1 + W)g(x) > 0$ in $(0, 1)$, $(1 + W)g(x)$ is strictly decreasing in $(1, 2)$ and $(1 + W)g(x) < 0$ in $(2, \infty)$. From here it follows that $g(x)$ has a unique zero in $(0, \infty)$. If we denote x_G by this zero, it follows from the proof that $1 < x_G < 2$. Numerically, $x_G \approx 1,95$.

We continue this appendix by giving the leading behaviour of several special functions that are used in this manuscript. We begin with the leading behaviour of the Lambert function. From the definition of W we have

$$W(x) = x - x^2 + \tfrac{3}{2}x^3 - \tfrac{8}{3}x^4 + O(x^5). \tag{A.15}$$

In fact, $W(x) = \sum_{n=1}^{\infty} x^n(-n)^{n-1}/n!$. From (A.15) it follows that

$$W(x\,\mathrm{e}^{-x}) = x - 2x^2 + 4x^3 - \tfrac{28}{3}x^4 + O(x^5). \tag{A.16}$$

For the function $F(x)$, defined by (3) we have

$$F(x) = 2x^2[1 - 2x + 5x^2 + O(x^3)]. \tag{A.17}$$

Hence, for $J(x)$ defined by (8) we obtain

$$J(x) = \tfrac{3}{2}x - 4x^2 + 10x^3 + O(x^4), \tag{A.18}$$

whereas for the function $G(x)$, defined by (11) we get

$$G(x) = 4x^2[1 - 5x + 20x^2 + O(x^3)]. \tag{A.19}$$

From (A.19) we obtain the leading behaviour of $G^{-1}(x)$, which is given by

$$G^{-1}(x) = \tfrac{1}{2}x^{1/2} + \tfrac{5}{8}x + \tfrac{45}{64}x^{3/2} + O(x^{5/2}). \tag{A.20}$$

We end this appendix by proving that both roots R_1 and R_2 of the equation $E_{\min} + \alpha_+ = E(R, L, 1) - \alpha_-$ tend to 0 as $L \to \infty$, see the proof of theorem 2. This is clear for R_1 since it is bounded by R_{eq}. Then one has, thanks to (14),

$$E(R_2, L, 1) = cL + E_{\min} \sim -2L^2. \tag{A.21}$$

Assume first that R_2L is bounded below at least for a subsequence of values L which tends to ∞. Then on this subsequence one has

$$E(R_2, L, 1) \sim -L^2\frac{F(R_2L)}{(R_2L)^2},$$

since $F(x)/x$ is bounded below by a positive constant on $[x_0, \infty[$, $x_0 > 0$. Using that $F(x)/x^2 < 2$ on all intervals $[x_0, \infty[$, $x_0 > 0$ this contradicts (A.21). Thus one has $R_2L \to 0$ as $L \to \infty$.

References

[1] Benguria R D, Brummelhuis R, Duclos P and Pérez–Oyarzún S 2004 H_2^+ in a strong magnetic field described via a solvable model *J. Phys. B: At. Mol. Opt. Phys.* **37** 2311–20

[2] Brummelhuis R and Duclos P 2001 On the one–dimensional behaviour of atoms in intense homogeneous magnetic fields *Partial Differential Equations and Spectral Theory* ed M Demuth and B-W Schulze (Basel: Birkhäuser) (*Operator Theory, Advances and Applications* vol 126) pp 25–35

[3] Brummelhuis R and Duclos P 2002 Effective Hamiltonians for atoms in very strong magnetic fields *Few–Body Syst.* **31** 1–6

[4] Brummelhuis R and Duclos P 2006 Effective Hamiltonians for atoms in very strong magnetic fields *J. Math. Phys.* **47** 032103

[5] Rosenthal C M 1971 Solution of the delta function model for heliumlike ions *J. Chem. Phys.* **55** 2474–83

[6] Corless R M, Gonnet G H, Hare D E, Jeffrey D J and Knuth D E 1996 *Adv. Comput. Math.* **5** 329