

1           Integral forms for the quantum He Hamiltonian  
2 approximation of chemical bonds in RNA and protein  
3           scaling comparisons.

4           *A numerical proof of concept*

5                           Han Geurdes<sup>1</sup>

6                           *GDS Applied Mathematics BV*  
7                           *CvdLinstraat 164 2593NN Den Haag Netherlands*  
8                           *han.geurdes@gmail.com*

---

9   **Abstract**

In the paper a mathematical method, originated from studies of nonlinear partial differential equations, is applied to the He approximation of outer electron chemical bonds. The results can be used in the study of large molecules like RNA and proteins. We follow a pairwise atom by atom coordinates approximation. Coordinates can be obtained from crystallography or electron microscopy. The present paper solely presents the proof of concept of the existence of an algorithm. It is expected that such algorithm can be employed in studies of larger molecules.

**Keywords:** He Hamiltonian approximation outer electrons;proof of concept numerics; method preparation for *in silico* RNA-RNA and protein-RNA studies

---

10 **Introduction**

11       In a bi-atomic chemical bond as part of a larger molecule, one can try to use  
12 the He Schrödinger equation to incorporate the quantum mechanical behaviour  
13 of the two electrons. It can make sense to consider the two atoms as a kind of  
14 "super" Helium nucleus when looking at the two outer electrons. The author  
15 is aware that other quantum chemical methods do exist [1]. The presented  
16 method attempts to look at large molecules. Moreover we believe that the  
17 mathematics can add to our understanding of the atomic physics of the light  
18 elements. Accepting that the He approach can be allowed, then still there is  
19 this problem that the He Schrödinger equation has no exact solution.

20       In the present paper we will try to come with an "in principle" exact solution  
21 form where the energy eigen value must be approximated in iterative steps of  
22 an algorithm. The "in principle solution" form is based on spectral integration  
23 theory. Previously, the present author applied a certain aspect of the theory with

---

<sup>1</sup>The author wishes to thank Ad Popper Director Xilion BV.  
*Preprint CONFIDENTIAL ...*

24 integrals with quadratic dispersion, to a nonlinear partial differential equation  
 25 [2]. The algorithm that we present here derives from concepts of linear integral  
 26 equations. It is a proof of concept and changes to it must be made in order to  
 27 study large molecules effectively.

## 28 Method

### 29 1. Math of He Hamiltonian integral patching

30 Let us start with the following two partial wave functions with dependence  
 31 on the two electron coordinates  $\mathbf{x}_1 = (x_{1,1}, x_{2,1}, x_{3,1})$  and  $\mathbf{x}_2 = (x_{1,2}, x_{2,2}, x_{3,2})$ .  
 32 The He Schrödinger equation in  $\hbar = c = 1$  and  $m_e = 1$  equals  $H\varphi = E\varphi$  with

$$33 \quad H = -\frac{1}{2}(\Delta_1 + \Delta_2) + \frac{1}{r_{1,2}} - \left( \frac{2}{r_1} + \frac{2}{r_2} \right) \quad (1)$$

34 and  $E$  the energy eigenvalue [1]. Here,  $r_{1,2} = \sqrt{(\mathbf{x}_1 - \mathbf{x}_2)^T \cdot (\mathbf{x}_1 - \mathbf{x}_2)}$  and  
 35 upper index  $T$  denotes the transposed. The  $r_{1,2}$  represents the Euclidean distance  
 36 between electron 1 and electron 2. Furthermore,  $r_1 = \sqrt{\mathbf{x}_1^T \cdot \mathbf{x}_1}$  and  $r_2 =$   
 37  $\sqrt{\mathbf{x}_2^T \cdot \mathbf{x}_2}$  together with  $\Delta_1 = \frac{\partial^2}{\partial x_{1,1}^2} + \frac{\partial^2}{\partial x_{2,1}^2} + \frac{\partial^2}{\partial x_{3,1}^2}$ . Similar  $\Delta_2 = \frac{\partial^2}{\partial x_{1,2}^2} + \frac{\partial^2}{\partial x_{2,2}^2} +$   
 38  $\frac{\partial^2}{\partial x_{3,2}^2}$ .

### 39 1.1. Partial wavefunctions

40 In this section we will try to find ways to approximately solve the He equation  
 41 starting from two primitive functions

$$42 \quad \psi_{0,k} = f_k \exp[\alpha_k r_{1,2}] \quad (2)$$

$$43 \quad \psi_{1,k} = g_k \exp[-2\beta_k(r_1 + r_2)]$$

44 The  $k$  index is an auxiliary variable that can enter into auxiliary integration.  
 45 For completeness of the argument let us look at

$$46 \quad \frac{\partial}{\partial x_{1,1}} \psi_{0,k} = \alpha_k \left( \frac{x_{1,1} - x_{1,2}}{r_{1,2}} \right) \psi_{0,k} \quad (3)$$

47 And therefore,

$$48 \quad \frac{\partial^2}{\partial x_{1,1}^2} \psi_{0,k} = \frac{\alpha_k}{r_{1,2}^2} \left( r_{1,2} - (x_{1,1} - x_{1,2}) \left( \frac{x_{1,1} - x_{1,2}}{r_{1,1}} \right) \right) \psi_{0,k} + \quad (4)$$

$$49 \quad \alpha_k^2 \left( \frac{x_{1,1} - x_{1,2}}{r_{1,2}} \right)^2 \psi_{0,k}$$

50 Similarly,

$$51 \quad \frac{\partial^2}{\partial x_{1,2}^2} \psi_{0,k} = \frac{\alpha_k}{r_{1,2}^2} \left( r_{1,2} - (x_{1,2} - x_{1,1}) \left( \frac{x_{1,2} - x_{1,1}}{r_{1,1}} \right) \right) \psi_{0,k} + \quad (5)$$

$$52 \quad \alpha_k^2 \left( \frac{x_{1,2} - x_{1,1}}{r_{1,2}} \right)^2 \psi_{0,k}$$

53 In addition,

$$54 \quad \frac{\partial}{\partial x_{1,1}} \psi_{1,k} = \frac{-2\beta_k x_{1,1}}{r_1} \psi_{1,k} \quad (6)$$

55 Therefore,

$$56 \quad \frac{\partial^2}{\partial x_{1,1}^2} \psi_{1,k} = \frac{-2\beta_k}{r_1^2} \left( r_1 - \frac{x_{1,1}^2}{r_1} \right) \psi_{1,k} + 4\beta_k^2 \left( \frac{x_{1,1}}{r_1} \right)^2 \psi_{1,k} \quad (7)$$

57 and similar

$$58 \quad \frac{\partial^2}{\partial x_{1,2}^2} \psi_{1,k} = \frac{-2\beta_k}{r_2^2} \left( r_2 - \frac{x_{1,2}^2}{r_2} \right) \psi_{1,k} + 4\beta_k^2 \left( \frac{x_{1,2}}{r_2} \right)^2 \psi_{1,k} \quad (8)$$

59 From which the following can be derived.

### 60 1.2. Preliminaries

61 Let us define  $H_0 = -\frac{1}{2}(\Delta_1 + \Delta_2)$ , then we may write

$$62 \quad H_0 \psi_{0,k} = -\frac{2\alpha_k}{r_{1,2}} \psi_{0,k} - \alpha_k^2 \psi_{0,k} \quad (9)$$

63 and

$$64 \quad H_0 \psi_{1,k} = 2\beta_k \left( \frac{1}{r_1} + \frac{1}{r_2} \right) \psi_{1,k} - 4\beta_k^2 \psi_{1,k} \quad (10)$$

65 Let us define the wave function  $\varphi$

$$66 \quad \varphi = \int_C d\lambda_k \psi_{0,k} + \int_D d\mu_k \psi_{1,k} \quad (11)$$

67 with very generally defined integrations over  $k$ . Looking at (9) and (10) we find

$$68 \quad H_0 \varphi = - \int_C d\lambda_k \left\{ \frac{2\alpha_k}{r_{1,2}} + \alpha_k^2 \right\} \psi_{0,k} + \int_D d\mu_k \left\{ 2\beta_k \left( \frac{1}{r_1} + \frac{1}{r_2} \right) - 4\beta_k^2 \right\} \psi_{1,k} \quad (12)$$

69 Furthermore, in order to obtain the He Schrödinger equation

$$70 \quad \varphi = 2 \int_C d\lambda_k \alpha_k \psi_{0,k} = \int_D d\mu_k \beta_k \psi_{1,k} \quad (13)$$

71 and

$$72 \quad E\varphi = - \int_C d\lambda_k \alpha_k^2 \psi_{0,k} - 4 \int_D d\mu_k \beta_k^2 \psi_{1,k} \quad (14)$$

73 Hence,

$$74 \quad H\varphi \equiv H_0 \varphi + \frac{1}{r_{1,2}} \varphi - \left( \frac{2}{r_1} + \frac{2}{r_2} \right) \varphi = E\varphi \quad (15)$$

75 *2. Essential equations*

76 In the first place let us combine (11) with (13). This gives

$$\begin{aligned}
 77 \quad \int_C d\lambda_k (1 - 2\alpha_k) \psi_{0,k} &= - \int_D d\mu_k \psi_{1,k} & (16) \\
 78 \quad \int_D d\mu_k (1 - \beta_k) \psi_{1,k} &= - \int_C d\lambda_k \psi_{0,k}
 \end{aligned}$$

79 Secondly we combine (11) and (14) this gives

$$80 \quad \int_C d\lambda_k E \psi_{0,k} + \int_D d\mu_k E \psi_{1,k} = - \int_C d\lambda_k \alpha_k^2 \psi_{0,k} - 4 \int_D d\mu_k \beta_k^2 \psi_{1,k} \quad (17)$$

81 Thirdly, (13) and (14)

$$\begin{aligned}
 82 \quad 2 \int_C d\lambda_k E \alpha_k \psi_{0,k} &= \int_D d\mu_k E \beta_k \psi_{1,k} = & (18) \\
 83 \quad - \int_C d\lambda_k \alpha_k^2 \psi_{0,k} - 4 \int_D d\mu_k \beta_k^2 \psi_{1,k}
 \end{aligned}$$

84 this latter equation can be rewritten in two equations

$$\begin{aligned}
 85 \quad \int_C d\lambda_k (2E\alpha_k + \alpha_k^2) \psi_{0,k} &= -4 \int_D d\mu_k \beta_k^2 \psi_{1,k} & (19) \\
 86 \quad \int_D d\mu_k (E\beta_k + 4\beta_k^2) \psi_{1,k} &= - \int_C d\lambda_k \alpha_k^2 \psi_{0,k}
 \end{aligned}$$

87 *3. Lagrangian*

88 Suppose  $f_k = \exp[-\alpha_k \rho_{1,2}]$  and  $g_k = \exp[\beta_k(\rho_1 + \rho_2)]$ . The  $\rho_{1,2}, \rho_1$  and  
 89  $\rho_2$  must be consistent with  $\mathbf{x}_1$  and  $\mathbf{x}_2$  because  $r_{1,2}, r_1$  and  $r_2$  are in a "close  
 90 neighbourhood" of  $\rho_{1,2}, \rho_1$  and  $\rho_2$ . The Lagrangian, with explicit (2), together  
 91 with conditions derived from (13), weighted by  $\kappa$  and (16) weighted by  $\kappa'$

$$\begin{aligned}
 92 \quad \mathcal{L} &= \int_C d\lambda_k (\alpha_k^2 + 2E\alpha_k - E) e^{\alpha_k(r_{1,2} - \rho_{1,2})} + & (20) \\
 93 \quad &\int_D d\mu_k (4\beta_k^2 + E\beta_k - E) e^{-2\beta_k((r_1 - \rho_1) + (r_2 - \rho_2))} + \\
 94 \quad &\kappa \left( 2 \int_C d\lambda_k \alpha_k e^{\alpha_k(r_{1,2} - \rho_{1,2})} - \int_D d\mu_k \beta_k e^{-2\beta_k((r_1 - \rho_1) + (r_2 - \rho_2))} \right) + \\
 95 \quad &\kappa' \left( 2 \int_C d\lambda_k (1 - \alpha_k) e^{\alpha_k(r_{1,2} - \rho_{1,2})} + \int_D d\mu_k (2 - \beta_k) e^{-2\beta_k((r_1 - \rho_1) + (r_2 - \rho_2))} \right)
 \end{aligned}$$

96 With  $\mathcal{L} = \mathcal{L}(\rho_{1,2}, \rho_1, \rho_2)$ . Because of the two separate  $\alpha_k$  and  $\beta_k$ , may write  
 97  $\mathcal{L} = \mathcal{L}_a + \mathcal{L}_b$ . To study the zero-pont of the Lagrangian we will look at the  
 98 derivatives to  $\alpha_k$  and  $\beta_k$  because they can indicate the minimum.

99 *3.1. Derivative to  $\alpha_k$*

100 Let us define  $\mathcal{L}_a$  as

$$101 \quad \mathcal{L}_a = \int_C d\lambda_k e^{\alpha_k(r_{1,2}-\rho_{1,2})} \{ \alpha_k^2 + 2(E + \kappa - \kappa')\alpha_k + (2\kappa' - E) \} \quad (21)$$

102 This is the  $\alpha_k$  dependent part of (20). Hence,  $\frac{\partial \mathcal{L}_a}{\partial \alpha_k} = \frac{\partial \mathcal{L}}{\partial \alpha_k}$ . Therefore we may  
103 write

$$104 \quad \frac{\partial \mathcal{L}}{\partial \alpha_k} = (r_{1,2} - \rho_{1,2}) \int_C d\lambda_k e^{\alpha_k(r_{1,2}-\rho_{1,2})} (\alpha_k^2 + 2(E + \kappa - \kappa')\alpha_k + (2\kappa' - E)) \quad (22)$$

$$105 \quad + \int_C d\lambda_k e^{\alpha_k(r_{1,2}-\rho_{1,2})} (2\alpha_k + 2(E + \kappa - \kappa'))$$

106 The  $k$  integrands premultiplied by  $r_{1,2} - \rho_{1,2}$  can be assembled to give the  
107 following quadratic equation

$$108 \quad u(\alpha_k) = \alpha_k^2 + 2(E + \kappa - \kappa')\alpha_k + (2\kappa' - E) \quad (23)$$

109 Hence, if we are looking for  $\frac{\partial \mathcal{L}}{\partial \alpha_k} = 0$  then because  $u(\alpha_{\pm}) = 0$

$$110 \quad \alpha_{\pm} = -(E + \kappa - \kappa') \pm \frac{1}{2}\sqrt{D} \quad (24)$$

111 and  $D \equiv 4(E + \kappa - \kappa')^2 - 4(2\kappa' - E) > 0$ . Suppose now that  $\alpha_{k_1} = \alpha_-$  and  
112  $\alpha_{k_2} = \alpha_+$  and that the operation  $\int_C d\lambda_k$  is

$$113 \quad \int_C d\lambda_k \equiv \int_{-\infty}^{+\infty} dk (\delta(k - k_1) + \delta(k - k_2)) \quad (25)$$

114 where  $\delta(x)$  represents the Dirac delta function. This implies that in (21)  $\mathcal{L}_a = 0$   
115 and that the first term weighed by  $(r_{1,2} - \rho_{1,2})$  in (22) can vanish. The second  
116 term in (22 now reads

$$117 \quad (2\alpha_- + 2(E + \kappa - \kappa')) \exp[\alpha_-(r_{1,2} - \rho_{1,2})] + \quad (26)$$

$$118 \quad (2\alpha_+ + 2(E + \kappa - \kappa')) \exp[\alpha_+(r_{1,2} - \rho_{1,2})] \approx 0$$

119 because,  $\exp[\alpha_-(r_{1,2} - \rho_{1,2})] \approx \exp[\alpha_+(r_{1,2} - \rho_{1,2})] \approx 1$  with  $r_{1,2}$  in a close  
120 neighbourhood of  $\rho_{1,2}$ .  $\alpha_{\pm}$  not extremely large. Note from(24),  $(2\alpha_- + 2(E +$   
121  $\kappa - \kappa')) = -\sqrt{D}$  combined with  $(2\alpha_+ + 2(E + \kappa - \kappa')) = \sqrt{D}$ . Hence, it follows  
122 that with (25) we have  $\mathcal{L}_a = 0$  together with  $\frac{\partial \mathcal{L}}{\partial \alpha_k} \approx 0$ .

123 *3.2. Derivative to  $\beta_k$*

124 Subsequently, let us define  $\mathcal{L}_b$  as

$$125 \quad \mathcal{L}_b = \int_D d\mu_k e^{-2\beta_k((r_1-\rho_1)+(r_2-\rho_2))} \{ 4\beta_k^2 + (E - \kappa - \kappa')\beta_k + (2\kappa' - E) \} \quad (27)$$

126 Let us have  $c \equiv 2(r_1 + r_2 - \rho_1 - \rho_2)$  This is the  $\beta_k$  dependent part of (20). It  
 127 follows that,  $\frac{\partial \mathcal{L}_b}{\partial \beta_k} = \frac{\partial \mathcal{L}}{\partial \beta_k}$ . Therefore we may write

$$128 \quad \frac{\partial \mathcal{L}}{\partial \beta_k} = -c \int_D d\mu_k e^{-c\beta_k} (4\beta_k^2 + (E - \kappa - \kappa')\beta_k + (2\kappa' - E)) \quad (28)$$

$$129 \quad + \int_D d\mu_k e^{-c\beta_k} (8\beta_k + E - \kappa - \kappa')$$

130 The  $k$  integrands premultiplied by  $(r_1 - \rho_1 + r_2 - \rho_2)$  give the following quadratic  
 131 equation

$$132 \quad v(\beta_k) = 4\beta_k^2 + (E - \kappa - \kappa')\beta_k + (2\kappa' - E) \quad (29)$$

133 Hence, if we are looking for  $\frac{\partial \mathcal{L}}{\partial \beta_k} = 0$  then with  $v(\beta_{\pm}) = 0$

$$134 \quad \beta_{\pm} = -\frac{1}{8}(E - \kappa - \kappa') \pm \frac{1}{8}\sqrt{D'} \quad (30)$$

135 and  $D' \equiv (E - \kappa - \kappa')^2 - 16(2\kappa' - E) > 0$ . Suppose now that  $\beta_{k_3} = \beta_-$  and  
 136  $\beta_{k_4} = \beta_+$  and that the operation  $\int_D d\mu_k$  can be written like

$$137 \quad \int_D d\mu_k \equiv \int_{-\infty}^{+\infty} dk (\delta(k - k_3) + \delta(k - k_4)) \quad (31)$$

138 where, such as was stated previously,  $\delta(x)$  is the Dirac delta function. This  
 139 implies that in (27)  $\mathcal{L}_b = 0$ . The second term in (28) now reads

$$140 \quad (8\beta_- + E - \kappa - \kappa') \exp[\beta_-(r_1 - \rho_1 + r_2 - \rho_2)] + \quad (32)$$

$$141 \quad (8\beta_+ + E - \kappa - \kappa') \exp[\beta_+(r_1 - \rho_1 + r_2 - \rho_2)] \approx 0$$

142 because,  $\exp[\beta_-(r_1 - \rho_1 + r_2 - \rho_2)] \approx \exp[\beta_+(r_1 - \rho_1 + r_2 - \rho_2)] \approx 1$  with  $r_1$   
 143 in a close neighbourhood of  $\rho_1$  and  $r_2$  in a close neighbourhood of  $\rho_2$ .  $\beta_{\pm}$  not  
 144 extremely large. Note from(30),  $(8\beta_- + E - \kappa - \kappa') = -\sqrt{D'}$  combined with  
 145  $(8\beta_+ + E - \kappa - \kappa') = \sqrt{D'}$ . Hence, it follows that with (31) we have  $\mathcal{L}_b = 0$   
 146 together with  $\frac{\partial \mathcal{L}}{\partial \beta_k} \approx 0$ .

#### 147 4. Meaning of $\mathcal{L} = 0$

148 After the detour concerning the Lagrangian, we may rightfully ask what it  
 149 means that for the integrals selected in (25) and (31) we may conclude  $\mathcal{L} =$   
 150  $\mathcal{L}(\rho_{1,2}, \rho_1, \rho_2) = 0$  close to the extremum  $\frac{\partial \mathcal{L}}{\partial \alpha_k} \approx 0$  and  $\frac{\partial \mathcal{L}}{\partial \beta_k} \approx 0$ . It means  
 151 that under this particular selection of the  $\lambda_k$  integral and the  $\mu_k$  integral the  
 152  $\varphi = \int_C d\lambda_k \psi_{0,k} + \int_D d\mu_k \psi_{1,k}$  in (11) equals the one in (13) and the one

$$153 \quad \varphi = \frac{-1}{E} \left( \int_C d\lambda_k \alpha_k^2 \psi_{0,k} + 4 \int_D d\mu_k \beta_k^2 \psi_{1,k} \right) \quad (33)$$

154 in (14). The  $\psi$ 's are given in (2).

155 Therefore, with still unknown energy eigenvalue  $E \neq 0$ , we have construed  
 156 a "solution form" for the Helium problem based on primitive initial functions  
 157 (2) and a proper selection of patching them together with integral procedures  
 158 over a parameter independent of coordinates  $\mathbf{x}_1$  and  $\mathbf{x}_2$ . The restriction is  
 159 in the extremum requirement where only in a "close neighbourhood" of pres-  
 160 elected constants  $\rho_{1,2}$ ,  $\rho_1$  and  $\rho_2$  we have the  $\mathcal{L} = 0$  of the He form is close  
 161 to the extrema. Note that  $\rho_{1,2}$ ,  $\rho_1$  and  $\rho_2$  can be freely selected but must be  
 162 possible/plausible with  $\mathbf{x}_1$  and  $\mathbf{x}_2$ .

#### 163 4.1. Proof of minimum

164 Here it is demonstrated that with the selection of integral forms, (25) and  
 165 (31), we approximate a minimum value with  $\mathcal{L} = 0$ . Looking at (22) the second  
 166 derivative of  $\mathcal{L}$  to  $\alpha_k$  is, for  $a \equiv r_{1,2} - \rho_{1,2}$

$$167 \quad \frac{\partial^2 \mathcal{L}}{\partial \alpha_k^2} = a^2 \int_C d\lambda_k e^{a\alpha_k} (\alpha_k^2 + 2(E + \kappa - \kappa')\alpha_k + (2\kappa' - E)) \quad (34)$$

$$168 \quad + 2a \int_C d\lambda_k e^{a\alpha_k} (2\alpha_k + 2(E + \kappa - \kappa')) + 2 \int_C d\lambda_k e^{a\alpha_k}$$

169 Therefore, with (24) and (25) and  $\int_C d\lambda_k e^{\alpha_k(r_{1,2} - \rho_{1,2})} > 0$ . This warrants the  
 170 conclusion that  $\frac{\partial^2 \mathcal{L}}{\partial \alpha_k^2} > 0$ . Similarly, we can conclude that  $\frac{\partial^2 \mathcal{L}}{\partial \beta_k^2} > 0$ . For, let us  
 171 write,  $c \equiv r_1 - \rho_1 + r_2 - \rho_2$ . Then from (28)

$$172 \quad \frac{\partial^2 \mathcal{L}}{\partial \beta_k^2} = c^2 \int_D d\mu_k e^{-c\beta_k} (4\beta_k^2 + (E - \kappa - \kappa')\beta_k + (2\kappa' - E)) \quad (35)$$

$$173 \quad - 2c \int_D d\mu_k e^{-c\beta_k} (8\beta_k + E - \kappa - \kappa') + 8 \int_D d\mu_k e^{-c\beta_k}$$

174 The conclusion is that  $\mathcal{L} = 0$  is, close to a minimum because:  $\frac{\partial \mathcal{L}}{\partial \alpha_k} \approx 0$  and  
 175  $\frac{\partial \mathcal{L}}{\partial \beta_k} \approx 0$  and  $\frac{\partial^2 \mathcal{L}}{\partial \alpha_k^2} > 0$  together with  $\frac{\partial^2 \mathcal{L}}{\partial \beta_k^2} > 0$  for  $\alpha_{\pm}$  and  $\beta_{\pm}$ .

#### 176 4.2. Numerical proof of concept

177 Obviously, when abstract mathematics provides a "solution form", the ques-  
 178 tion arises; will it be numerical practicable and can its principles be recovered  
 179 in an algorithm. We are especially interested in RNA crystallographic or elec-  
 180 tron microscope coordinate data. Here in this test we use 6XRZ cryo-electron-  
 181 microscopic coordinate data [rcsb.org/structure/6XRZ](https://rcsb.org/structure/6XRZ), doi:10.2210/pdb6XRZ/pdb  
 182 of K. Zhang et al [3] 10.1101/2020.07.18.209270. In this section let us look at  
 183 G coordinates C5' and C4'

```
184 h<-0.02707993
185 xAtom1<-c(76.96, 77.639, 55.436)
186 xAtom2<-c(78.265, 78.358, 55.199)
187 xMean<-(xAtom1+xAtom2)/2
188 x1<-xMean+h*c(1,1,1)*0.747
189 x2<-xMean-h*c(1,2,1)*1.08
```

190 The  $x_1$  and  $x_2$  vectors indicate possible positions of two electrons. Here,  $r_{1,2} =$   
191  $0.08569327$  with  $r_1 = 123.191$  and  $r_2 = 123.1063$ . Moreover,  $\rho_{1,2} = rh =$   
192  $0.06005371$  and  $\rho_1 + \rho_2 = rk = 246.3337$  and fixed them in this computation.  
193 Subsequently, the  $\alpha$ 's and  $\beta$ 's were computed like in (24) and (30) with the use  
194 of  $\kappa = 1.179449$  and  $\kappa' = -104.971$ . The iteration started here in  $E = -104.971$   
195 and with  $dE = 1 \times 10^{-3}$  approached  $E \leftarrow E + dE$  zero in a number of steps.  
196 The discriminants were computed like

```
197 b<-2*(E+k-k1)
198 b1<-E-k-k1
199 D<-b^2+(4*(-(2*k1)+E))
200 D1<-b1^2+(16*(-(2*k1)+E))
```

201 The requirement was  $D > 0$  and  $D1 > 0$ . The  $\alpha$ 's and  $\beta$ 's followed

```
202 aPlus<--0.5*b+(0.5*sqrt(D))
203 bPlus<--(1/8)*b1+((1/8)*sqrt(D1))
204 aMin<--0.5*b-(0.5*sqrt(D))
205 bMin<--(1/8)*b1-((1/8)*sqrt(D1))
```

206 The two primitive wave functions were computed in two functional expressions

```
207 funPsi0<-function(alph,r12,rh){
208   y<-exp(alph*(r12-rh))
209   return(y)
210 }
211 funPsi1<-function(bet,x1,x2,rk){
212   r1<-sqrt(t(x1)%*%x1)
213   r2<-sqrt(t(x2)%*%x2)
214   y<-exp(-2*bet*((r1+r2)-rk))
215   return(y)
216 }
```

217 Then the three  $\varphi$  forms are computed referring to (11), (13) and the form in  
218 (33). Hence

```
219 phi1<-funPsi0(aMin,r,rh)+funPsi1(bMin,x1,x2,rk)
220 phi1<-phi1+(funPsi0(aPlus,r,rh)+funPsi1(bPlus,x1,x2,rk))
221 phi2a<-(aMin*funPsi0(aMin,r,rh))+(aPlus*funPsi0(aPlus,r,rh))
222 phi2a<-2*phi2a
223 phi2b<-(bMin*funPsi1(bMin,x1,x2,rk))+(bPlus*funPsi1(bPlus,x1,x2,rk))
224 phi2<-(phi2a+phi2b)/2
225 phi3<-((aMin^2)*funPsi0(aMin,r,rh))+((aPlus^2)*funPsi0(aPlus,r,rh))
226 phi3<-phi3+((4*(bMin^2)*funPsi1(bMin,x1,x2,rk))+(4*(bPlus^2)*funPsi1(bPlus,x1,x2,rk)))
227 phi3<-phi3/abs(E)
228 dPhi<-(abs(phi1-phi2)+abs(phi2-phi3)+abs(phi1-phi3))/3
```

229 The  $\phi_2/2$  form is used also in the condition weighed by  $\kappa'$  in (20). The  
230  $(\phi_3a+\phi_3b)/2$  refers to one entity, (33). The differences in a loop of max  
231 10000 iterations is computed as

232  $d\Phi \leftarrow (\text{abs}(\phi_1 - \phi_2) + \text{abs}(\phi_2 - \phi_3) + \text{abs}(\phi_1 - \phi_3)) / 3$

233 The result of computations under these conditions and with those parametriza-  
234 tion was  $d\Phi = 3.366759 \times 10^{-4}$  after  $N = 490$  iterations and

235  $\text{print}(c(\phi_1, \phi_2, \phi_3)) = c(4.139733, 4.140239, 4.139738)$

236 We note that  $\phi_{2a} = 4.13982$  (lefthand integral (13)) while  $\phi_{2b} = 4.14066$  (right-  
237 hand integral (13)). The obtained approximated energy eigenvalue in this equa-  
238 tion is:  $E = -104.482$ .

## 239 Results

240 The error margin is reasonably low but there are quite a number of iteration  
241 steps necessary to get there. The computations don't need much computer  
242 power. The approximation of the left and right hand side equality of (13) can  
243 still be improved but the difference of  $\approx 0.00084$  look reasonable.

244 The, fig 1,  $err_n = d\Phi$  goes upwards again beyond  $N=490$  with start value  
245  $E = -104.971$  and  $dE = 1 \times 10^{-3}$  and  $\kappa$  and  $\kappa'$ , together with  $\rho_{1,2}$ ,  $\rho_1$  and  $\rho_2$ ,  
246 selected in the algorithm (viz. §4.2). However, it is also noted that an initial  
247 declining trend is demonstrated in figure 1. Therefore the principal solution is  
248 demonstrated here. Most likely the efficiency of the program can be improved  
249 and finally can be employed to better approximate the quantum electron density  
250 from the crystallographic coordinates of RNA.

## 251 Conclusion

252 In the present paper a mathematical scheme is employed to solve iteratively  
253 the He approximation for two binding electrons. Its importance is that the He  
254 approximation can be applied to pairs of atoms in larger molecules and can  
255 be a part of multidimensional scaling comparison of RNA-RNA. The affinity  
256 of protein for RNA in RNA-protein complexes can be studied as well with the  
257 quantum He approximation.

258 If  $\varphi$  is defined as in (11) and is found approximately equal to the forms in (13)  
259 and (33) then the He Schrödinger equation has been solved in approximation.  
260 Hence the formal mathematics allows approximative but quantum chemistry  
261 based computations of large molecules. A computation that can be extended  
262 to large molecules like RNA and protein whose coordinate data are obtained  
263 from crystallography and cryo-electron-microscopy. The method is considered  
264 an improvement. It supplements earlier studies [4] and enables multidimensional  
265 scaling (MDS) statistics with less qualitative data in the MDS-based comparison  
266 geometry.

267 **References**

- 268 [1] Piela, L., *Ideas of quantum chemistry*, Elsevier, Amsterdam, Boston, 2007.
- 269 [2] Geurdes, H., A nonlinear second-order partial differential equation derived  
270 from a linear type-II integral equation with quadratic dispersion, *J Phys*  
271 *A:Math Gen*, 1990, 23:2315.
- 272 [3] Zhang, K., Zheludev, I., Hagey, R. et al, *Cryo-electron Microscopy and Ex-*  
273 *ploratory Antisense Targeting of 20kDa Frameshift Stimulation Element from*  
274 *the SARS-CoV-2 RNA genome*, 2020, [biorXiv 10.1101\2020.07.18.209270](https://doi.org/10.1101/2020.07.18.209270).
- 275 [4] Geurdes, H., Approximative He Hamiltonian in descriptive multidimen-  
276 sional scaling statistics of RNA contained information with application  
277 to SARS-CoV-2 Spike mRNA and 7SLRNA, RN7SL2 and RN7SL3, 2021,  
278 [ssrn.com/abstract=3772670](https://ssrn.com/abstract=3772670)

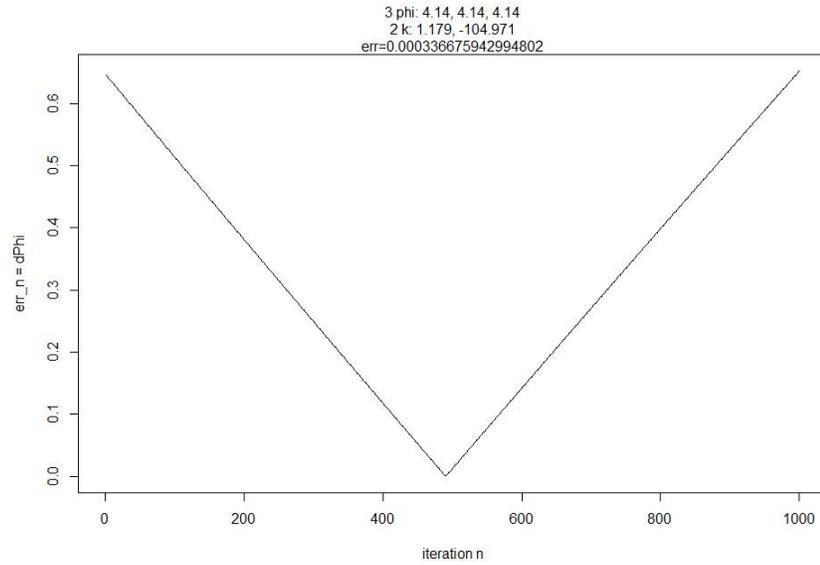


Figure 1: Representation of dPhi error in n iterations. There appears a linear steady decline. However, at point N=490, ( $err_n \approx 3.366759 \times 10^{-4}$ ) the  $err_n = dPhi$  does no longer substantially change and further downstream goes up.