Integral forms for the quantum He Hamiltonian approximation of chemical bonds in RNA and protein scaling comparisons.
A numerical proof of concept

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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

Introduction

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

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

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

Method

1. Math of He Hamiltonian integral patching

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

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

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 upper index T denotes the transposed The $r_{1,2}$ represents the Euclidean distance between electron 1 and electron 2. Furthermore, $r_1 = \sqrt{\mathbf{x}_1^T \cdot \mathbf{x}_1}$ and $r_2 = \sqrt{\mathbf{x}_2^T \cdot \mathbf{x}_2}$ 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 $\Delta_2 = \frac{\partial^2}{\partial x_{1,2}^2} + \frac{\partial^2}{\partial x_{2,2}^2} + \frac{\partial^2}{\partial x_{3,2}^2}$.

1.1. Partial wavefunctions

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

$$\psi_{0,k} = f_k \exp\left[\alpha_k r_{1,2}\right] \tag{2}$$

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

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

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

And therefore,

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

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

Similarly,

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

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

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From which the following can be derived.

1.2. Preliminaries

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

$$H_0\psi_{0,k} = -\frac{2\alpha_k}{r_{1,2}}\psi_{0,k} - \alpha_k^2\psi_{0,k} \tag{6}$$

and

$$H_0\psi_{1,k} = 2\beta_k\left(\frac{1}{r_1} + \frac{1}{r_2}\right)\psi_{1,k} - \beta_k^2\psi_{1,k} \tag{7}$$

Let us define the wave function φ

$$\varphi = \int_C d\lambda_k\psi_{0,k} + \int_D d\mu_k\psi_{1,k} \tag{8}$$

with very generally defined integrations over k. Looking at (6) and (7) we find

$$H_0\varphi = -\int_C d\lambda_k\left\{\frac{2\alpha_k}{r_{1,2}} + \alpha_k^2\right\}\psi_{0,k} + \int_D d\mu_k\left\{2\beta_k\left(\frac{1}{r_1} + \frac{1}{r_2}\right) - \beta_k^2\right\}\psi_{1,k} \tag{9}$$

Furthermore, in order to obtain the He Schrödinger equation

$$\varphi = 2\int_C d\lambda_k\alpha_k\psi_{0,k} = 2\int_D d\mu_k\beta_k\psi_{1,k} \tag{10}$$

and

$$E\varphi = -\int_C d\lambda_k\alpha_k^2\psi_{0,k} - \int_D d\mu_k\beta_k^2\psi_{1,k} \tag{11}$$

Hence,

$$H\varphi \equiv H_0\varphi + \frac{1}{r_{1,2}}\varphi - \left(\frac{1}{r_1} + \frac{1}{r_2}\right)\varphi = E\varphi \tag{12}$$

2. Essential equations

In the first place let us combine (8) with (10). This gives

$$\int_C d\lambda_k(1 - 2\alpha_k)\psi_{0,k} = -\int_D d\mu_k\psi_{1,k} \tag{13}$$

$$\int_D d\mu_k(1 - 2\beta_k)\psi_{1,k} = -\int_C d\lambda_k\psi_{0,k}$$

Secondly we combine (8) and (11) this gives

$$\int_C d\lambda_k E\psi_{0,k} + \int_D d\mu_k E\psi_{1,k} = -\int_C d\lambda_k\alpha_k^2\psi_{0,k} - \int_D d\mu_k\beta_k^2\psi_{1,k} \tag{14}$$

Thirdly, (10) and (11)

$$\int_C d\lambda_k (2E)\alpha_k \psi_{0,k} = \int_D d\mu_k (2E)\beta_k \psi_{1,k} = \tag{15}$$

$$-\int_C d\lambda_k \alpha_k^2 \psi_{0,k} - \int_D d\mu_k \beta_k^2 \psi_{1,k}$$

this latter equation can be rewritten in two equations

$$\int_C d\lambda_k (2E\alpha_k + \alpha_k^2)\psi_{0,k} = -\int_D d\mu_k \beta_k^2 \psi_{1,k} \tag{16}$$

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

3. Lagrangian

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 ρ_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 neighbourhood" of $\rho_{1,2}, \rho_1$ and ρ_2. The Lagrangian, with explicit (2), together with conditions derived from (10), weighted by κ and (13) weighted by κ'

$$\mathcal{L} = \int_C d\lambda_k \left(\alpha_k^2 + 2E\alpha_k - E \right) \, e^{\alpha_k(r_{1,2}-\rho_{1,2})} \; + \tag{17}$$

$$\int_D d\mu_k \left(\beta_k^2 + 2E\beta_k - E \right) \, e^{-\beta_k((r_1-\rho_1)+(r_2-\rho_2))} \; +$$

$$\kappa \left(\int_C d\lambda_k \alpha_k \, e^{\alpha_k(r_{1,2}-\rho_{1,2})} \; - \int_D d\mu_k \beta_k \, e^{-\beta_k((r_1-\rho_1)+(r_2-\rho_2))} \right) +$$

$$\kappa' \left(\int_C d\lambda_k (1 - \alpha_k) \, e^{\alpha_k(r_{1,2}-\rho_{1,2})} \; + \int_D d\mu_k (1 - \beta_k) \, e^{-\beta_k((r_1-\rho_1)+(r_2-\rho_2))} \right)$$

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

3.1. Derivative to α_k

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

$$\mathcal{L}_a = \int_C d\lambda_k \, e^{\alpha_k(r_{1,2}-\rho_{1,2})} \, \{\alpha_k^2 + (2E + \kappa - \kappa')\alpha_k + (\kappa' - E)\} \tag{18}$$

This is the α_k dependent part of (17). Hence, $\frac{\partial \mathcal{L}_a}{\partial \alpha_k} = \frac{\partial \mathcal{L}}{\partial \alpha_k}$. Therefore we may write

$$\frac{\partial \mathcal{L}}{\partial \alpha_k} = (r_{1,2} - \rho_{1,2}) \int_C d\lambda_k \, e^{\alpha_k(r_{1,2}-\rho_{1,2})} \, \left(\alpha_k^2 + (2E + \kappa - \kappa')\alpha_k + (\kappa' - E) \right) \tag{19}$$

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

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

$$u(\alpha_k) = \alpha_k^2 + (2E + \kappa - \kappa')\alpha_k + (\kappa' - E) \tag{20}$$

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

$$\alpha_\pm = -\frac{1}{2}(2E + \kappa - \kappa') \pm \frac{1}{2}\sqrt{D} \tag{21}$$

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

$$\int_C d\lambda_k \equiv \int_{-\infty}^{+\infty} dk \, (\delta(k - k_1) + \delta(k - k_2)) \tag{22}$$

where $\delta(x)$ represents the Dirac delta function. This implies that in (18) $\mathcal{L}_a = 0$ and that the first term weighed by $(r_{1,2} - \rho_{1,2})$ in (19) can vanish. The second term in (19 now reads

$$(2\alpha_- + 2E + \kappa - \kappa') \exp[\alpha_-(r_{1,2} - \rho_{1,2})] + \tag{23}$$
$$(2\alpha_+ + 2E + \kappa - \kappa') \exp[\alpha_+(r_{1,2} - \rho_{1,2})] \approx 0$$

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 neighbourhood of $\rho_{1,2}$. $\alpha_\pm$ not extremely large. Note from(21), $(2\alpha_- + 2E + \kappa - \kappa') = -\sqrt{D}$ combined with $(2\alpha_+ + 2E + \kappa - \kappa') = \sqrt{D}$. Hence, it follows that with (22) we have $\mathcal{L}_a = 0$ together with $\frac{\partial \mathcal{L}}{\partial \alpha_k} \approx 0$.

3.2. Derivative to β_k

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

$$\mathcal{L}_b = \int_D d\mu_k \, e^{-\beta_k((r_1 - \rho_1) + (r_2 - \rho_2))} \left\{ \beta_k^2 + (2E - \kappa - \kappa')\beta_k + (\kappa' - E) \right\} \tag{24}$$

This is the β_k dependent part of (17). It follows that, $\frac{\partial \mathcal{L}_b}{\partial \beta_k} = \frac{\partial \mathcal{L}}{\partial \beta_k}$. Therefore we may write

$$\frac{\partial \mathcal{L}}{\partial \beta_k} = -(r_1 - \rho_1 + r_2 - \rho_2) \int_D d\mu_k \, e^{-\beta_k((r_1 - \rho_1) + (r_2 - \rho_2))} \tag{25}$$
$$\times \left(\beta_k^2 + (2E - \kappa - \kappa')\beta_k + (\kappa' - E) \right)$$
$$+ \int_D d\mu_k \, e^{\alpha_k(r_{1,2} - \rho_{1,2})} \left(2\beta_k + 2E - \kappa - \kappa' \right)$$

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

$$v(\beta_k) = \beta_k^2 + (2E - \kappa - \kappa')\beta_k + (\kappa' - E) \tag{26}$$

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

$$\beta_\pm = -\frac{1}{2}(2E - \kappa - \kappa') \pm \frac{1}{2}\sqrt{D'} \tag{27}$$

and $D' \equiv (2E - \kappa - \kappa')^2 - 4(\kappa' - E) > 0$. Suppose now that $\beta_{k_3} = \beta_-$ and $\beta_{k_4} = \beta_+$ and that the operation $\int_D d\mu_k$ can be written like

$$\int_D d\mu_k \equiv \int_{-\infty}^{+\infty} dk \left(\delta(k - k_3) + \delta(k - k_4)\right) \tag{28}$$

where, such as was stated previously, $\delta(x)$ is the Dirac delta function. This implies that in (24) $\mathcal{L}_b = 0$. The second term in (25) now reads

$$(2\beta_- + 2E - \kappa - \kappa') \exp[\beta_-(r_1 - \rho_1 + r_2 - \rho_2)] + \tag{29}$$
$$(2\beta_+ + 2E - \kappa - \kappa') \exp[\beta_+(r_1 - \rho_1 + r_2 - \rho_2)] \approx 0$$

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 in a close neighbourhood of ρ_1 and r_2 in a close neighbourhood of ρ_2. $\beta_\pm$ not extremely large. Note from (27), $(2\beta_- + 2E - \kappa - \kappa') = -\sqrt{D'}$ combined with $(2\beta_+ + 2E - \kappa - \kappa') = \sqrt{D'}$. Hence, it follows that with (28) we have $\mathcal{L}_b = 0$ together with $\frac{\partial \mathcal{L}}{\partial \beta_k} \approx 0$.

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

After the detour concerning the Lagrangian, we may rightfully ask what it means that for the integrals selected in (22) and (28) we may conclude $\mathcal{L} = \mathcal{L}(\rho_{1,2}, \rho_1, \rho_2) = 0$ 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 that under this particular selection of the λ_k integral and the μ_k integral the $\varphi = \int_C d\lambda_k \psi_{0,k} + \int_D d\mu_k \psi_{1,k}$ in (8) equals the one in (10) and the one

$$\varphi = \frac{-1}{E} \left(\int_C d\lambda_k \alpha_k^2 \psi_{0,k} + \int_D d\mu_k \beta_k^2 \psi_{1,k} \right) \tag{30}$$

in (11). The ψ's are given in (2).

Therefore, with still unknown energy eigenvalue $E \neq 0$, we have construed a "solution form" for the Helium problem based on primitive initial functions (2) and a proper selection of patching them together with integral procedures over a parameter independent of coordinates $\mathbf{x}_1$ and $\mathbf{x}_2$. The restriction is in the extremum requirement where only in a "close neighbourhood" of pres-elected constants $\rho_{1,2}$, ρ_1 and ρ_2 we have the $\mathcal{L} = 0$ of the He form is close to the extrema. Note that $\rho_{1,2}$, ρ_1 and ρ_2 can be freely selected but must be possible/plausible with $\mathbf{x}_1$ and $\mathbf{x}_2$.

4.1. Proof of minimum

Here it is demonstrated that with the selection of integral forms, (22) and (28), we approximate a minimum value with $\mathcal{L} = 0$. Looking at (19) the second

derivative of $\mathcal{L}$ to α_k is, for $a \equiv r_{1,2} - \rho_{1,2}$

$$\frac{\partial^2 \mathcal{L}}{\partial \alpha_k^2} = a^2 \int_C d\lambda_k \ e^{a\alpha_k} \ \left(\alpha_k^2 + (2E + \kappa - \kappa')\alpha_k + (\kappa' - E) \right) \tag{31}$$

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

Therefore, with (21) and (22) and $\int_C d\lambda_k \ e^{\alpha_k(r_{1,2} - \rho_{1,2})} > 0$. This warrants the 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 write, $c \equiv r_1 - \rho_1 + r_2 - \rho_2$. Then from (25)

$$\frac{\partial^2 \mathcal{L}}{\partial \beta_k^2} = c^2 \int_D d\mu_k \ e^{-c\beta_k} \ \left(\beta_k^2 + (2E - \kappa - \kappa')\beta_k + (\kappa' - E) \right) \tag{32}$$

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

The conclusion is that $\mathcal{L} = 0$ is, close to a minimum because: $\frac{\partial \mathcal{L}}{\partial \alpha_k} \approx 0$ and $\frac{\partial \mathcal{L}}{\partial \beta_k} \approx 0$ 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 $\beta_\pm$.

4.2. Numerical proof of concept

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

```
h<-0.02707993
xAtom1<-c(76.96,  77.639,  55.436)
xAtom2<-c(78.265,  78.358  , 55.199)
xMean<-(xAtom1+xAtom2)/2
x1<-xMean+h*c(1,1,1)
x2<-xMean-h*c(1,2,1)
```

The $x1$ and $x2$ vectors indicate possible positions of two electrons. Here, $r_{1,2} = 0.09380763$ with $r_1 = 123.2028$ and $r_2 = 123.1100$. Moreover, $\rho_{1,2} = rh = 0.06005371$ and $\rho_1 + \rho_2 = rk = 246.3337$ and fixed them in this computation. Subsequently, the α's and β's were computed like in (21) and (27) with the use of $\kappa = 0.02342234$ and $\kappa' = -1.990899$. The iteration started here in $E = -1.990899$ and with $dE = 1 \times 10^{-5}$ approached $E \leftarrow E + dE$ zero in a number of steps. The discriminants were computed like

```
D<-((2*E+k-k1)^2)+(4*(-k1+E))
D1<-((2*E-k-k1)^2)+(4*(-k1+E))
```

The requirement was $D > 0$ and $D1 > 0$. The α's and β's followed

```
195  aPlus<--0.5*(2*E+k-k1)+(0.5*sqrt(D))
196  bPlus<--0.5*(2*E-k-k1)+(0.5*sqrt(D1))
197  aMin<--0.5*(2*E+k-k1)-(0.5*sqrt(D))
198  bMin<--0.5*(2*E-k-k1)-(0.5*sqrt(D1))
```

The two primitive wave functions were computed in two functional expressions

```
200  funPsi0<-function(alph,r12,rh){
201    y<-exp(alph*(r12-rh))
202    return(y)
203  }
204  funPsi1<-function(bet,x1,x2,rk){
205    r1<-sqrt(t(x1)%*%x1)
206    r2<-sqrt(t(x2)%*%x2)
207    y<-exp(-bet*((r1+r2)-rk))
208    return(y)
209  }
```

Then the three φ forms are computed referring to (8), (10) and the form in (30). Hence

```
212  phi1<-funPsi0(aMin,r,rh)+funPsi1(bMin,x1,x2,rk)
213  phi1<-phi1+(funPsi0(aPlus,r,rh)+funPsi1(bPlus,x1,x2,rk))
214  phi2a<-(2*aMin*funPsi0(aMin,r,rh))+(2*aPlus*funPsi0(aPlus,r,rh))
215  phi2b<-(2*bMin*funPsi1(bMin,x1,x2,rk))+(2*bPlus*funPsi1(bPlus,x1,x2,rk))
216  phi2<-(phi2a+phi2b)/2
217  phi3a<-((aMin^2)*funPsi0(aMin,r,rh))+((aPlus^2)*funPsi0(aPlus,r,rh))
218  phi3b<-((bMin^2)*funPsi1(bMin,x1,x2,rk))+((bPlus^2)*funPsi1(bPlus,x1,x2,rk))
219  phi3<-(phi3a+phi3b)/abs(E)
```

The phi2/2 form is used also in the condition weighed by κ' in (17). The (phi3a+phi3b)/2 refers to one entity, (30). The differences in a loop of max 10000 iterations is computed as

```
223  dPhi<-(abs(phi1-phi2)+abs(phi2-phi3)+abs(phi1-phi3))/3
```

The result of computations under these conditions and with those parametrization was dPhi=4.172812×10^{-6} after $N = 2511$ iterations and

```
226  print(c(phi1,phi2,phi3))=c(4.179276, 4.179270, 4.179270)
```

We note that phi2a=4.17928 (lefthand integral (10)) while phi2b=4.17926 (righthand integral (10)). The obtained approximated energy eigenvalue in this equation is: $E = -1.965799$.

Results

The error margin is reasonably low but there are quite a number of iteration steps necessary to get there. The computations don't need much computer

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power. The approximation of the left and right hand side equality of (10) can still be improved but the difference of 2.4963×10^{-5} look reasonable.

The, fig 1, $err_n = $ dPhi goes upwards again beyond N=2511 with start value E=-1.990899 and dE=1×10^{-5} and κ and κ', together with $\rho_{1,2}$, ρ_1 and ρ_2, selected in the algorithm (viz. §4.2). However, it is also noted that an initial declining trend is demonstrated in figure 1. Therefore the principal solution is demonstrated here. Most likely the efficiency of the program can be improved and finally can be employed to better approximate the quantum electron density from the crystallographic coordinates of RNA.

Conclusion

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

If φ is defined as in (8) and is found approximately equal to the forms in (10) and (30) then the He Schrödinger equation has been solved in approximation. Hence the formal mathematics allows approximative but quantum chemistry based computations of large molecules. A computation that can be extended to large molecues like RNA and protein whose coordinate data are obtained from crystallography and cryo-electron-microscopy. The method is considered an improvement. It supplements earlier studies [4] and enables multidimensional scaling (MDS) statistics with less qualitative data in the MDS-based comparison geometry.

References

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3 phi: 4.179, 4.179, 4.179
2 k: 0.023, -2.018
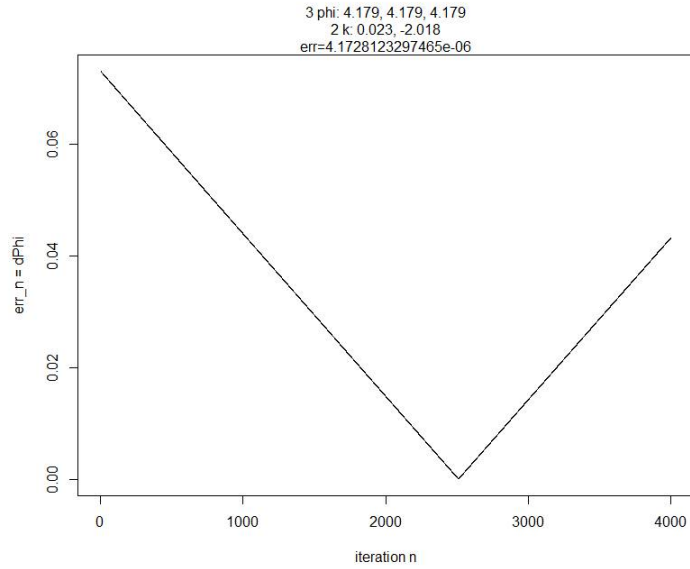err=4.1728123297465e-06

Figure 1: Representation of dPhi error in n iterations. There appears a linear steady de-
cline. However, at point N=2511, ($err_n \approx 4.172812 \times 10^{-6}$) the err_n = dPhi does no longer
substantially change and further downstream goes up.

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