

Disproof of Self Consistent Field theory

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Abstract

Numerical computation of a ground state of a one-dimensional two-body system was done to obtain a best numerical solution. Since the degree of the self-relative error has become the order of 10^{-14} power, this numerical solution may be called quasi-correct solution. From this quasi-correct wave function one can calculate one-body density distribution function. The square root function of this one-body density function may be regarded as a one-body wave function. In the conventional Self Consistent Field theory scheme, such a one-body wave function is assumed to satisfy the associated set of integro-differential equations in which one-body wave function satisfies a Schroedinger-like equation that involves an average potential, that is, the self consistent potential term. The afore mentioned semi-rigorous numerical solution can be used to compute both of such an average potential and an absolutely correct one-body potential. Doing these computations, one must notice a significant difference between the theoretical self consistent field and the numerically correct real average field. Based on this case study, one cannot help but deny the backbone that is running through the conventional Self Consistent Field theory.

Model system

As a model system for which the ground state seeking computation is done, the author chose a one-dimensional two particle system. These two particles are repelling with each other, but both of them are contained in a mother potential well. This may be rather called a three body problem. But since the mother well potential is fixed in space, the author named this case study a two-body problem. In practical research, computation on three-dimensional problem may rather be preferred for it is more realistically depicting the real quantum mechanical objects like an atom. The real electrons are repelling each other by inverse squared force, and are attracted by the nucleus by the same but negative inverse squared force. In the real space, the electron can pass by the nucleus and other electrons because there is literally a passable side space near the nucleus. In one-dimensional case, if the inter-particle force obeys the squared inverse law, then a particle cannot pass by another particle since there exists a singularity where the coordinates of both particles coincide. In addition to this difficulty, the nuclear potential is also problematic similarly if it produces the inverse potential because it causes singularity when the distance between the nucleus and an electron becomes zero.

In order to avoid such singularity difficulty, the model system is designed to have a negative attractive Gaussian mother potential well and a positive Gaussian repulsive inter-particle potential. In mathematical notation, these assumptions may be written like,

$$V_n(x) = -A_n \exp\{-x^2/\sigma^2\} \quad A_n > 0 \quad (1)$$

$$V_{ee}(x_1, x_2) = +A_{ee} \exp\{-(x_1 - x_2)^2/\sigma^2\} \quad A_{ee} > 0 \quad (2)$$

With these crude approximations for real Coulomb interaction, and using a unit system in which electron mass is unity and the Dirac constant is also unity, one can write the Hamiltonian as follows.

$$H = -\frac{1}{2} \frac{\partial^2}{\partial x_1^2} - \frac{1}{2} \frac{\partial^2}{\partial x_2^2} + V_{ee}(x_1, x_2) + V_n(x_1) + V_n(x_2) \quad (3)$$

From this Hamiltonian, we will compute the ground state wave function numerically first.

Computational method

There may be various ways for computing the ground state wave function. The author applied the Kimball-Shortley method[1], [2] to this two-body system. It is one kind of repetitive computation, but in principle, it can approach the truly exact numerical solution. Many may regard it as a kind of variation method, but the truth is not. Usual variation method is restricted and hindered to approach the true solution by artificially imposed assumption or assumptions. The Kimball-Shortley method has no assumption, will approach the true numerical solution infinitely. In the initial trial of the Kimball-Shortley method done in the past, only one-dimensional case was investigated by the inventors. So it was uncertain if this method can be expanded to many-dimensional case or many-body system. Does the numerical solution converge to a sound solution? To confirm it, only executing it actually was necessary.

Briefing the method is plain. It just discretizes and rewrites the original Schroedinger equation. The reason why the author takes the trouble to introduce the procedure is to reinforce and endorse the rightness of the resultant wave function. One may reach the same solution even if one uses other method.

First, every spatial variable is discretized.

$$x_1 = x_i \quad i = 1 \cdots N \quad (4)$$

$$x_2 = x_j \quad j = 1 \cdots N \quad (5)$$

$$\Psi(x_1, x_2) = \Psi_{i,j} \quad (6)$$

$$V_n(x_1) = V_i \quad (7)$$

$$V_n(x_2) = V_j \quad (8)$$

$$V_{ee}(x_1, x_2) = v_{i,j} \quad (9)$$

where N is the number of lattice points. Then the original Schroedinger equation may be written as,

$$-\frac{1}{2} \frac{\Psi_{i+1,j} - 2\Psi_{i,j} + \Psi_{i-1,j}}{a^2} - \frac{1}{2} \frac{\Psi_{i,j+1} - 2\Psi_{i,j} + \Psi_{i,j-1}}{a^2} + (V_i + V_j + v_{i,j})\Psi_{i,j} = E\Psi_{i,j} \quad (10)$$

where a is the lattice constant. If one solves the $\Psi_{i,j}$ from the above equation, then one will obtain the following equation.

$$\Psi_{i,j} = \frac{\Psi_{i+1,j} + \Psi_{i-1,j} + \Psi_{i,j+1} + \Psi_{i,j-1}}{4 + 2a^2(V_i + V_j + v_{i,j} - E)} \quad (11)$$

In the Kimball-Schortley scheme, the left hand side is regarded as the renewed wave value calculated from the old wave function values on the four neighboring lattice points $(i+1, j), (i-1, j), (i, j+1), (i, j-1)$ in the numerator of the right hand side. In a more explicit notation,

$$\Psi_{i,j}^{NEW} = \frac{\Psi_{i+1,j}^{OLD} + \Psi_{i-1,j}^{OLD} + \Psi_{i,j+1}^{OLD} + \Psi_{i,j-1}^{OLD}}{4 + 2a^2(V_i + V_j + v_{i,j} - E)} \quad (12)$$

The energy representing variable E is defined as the energy expectation value in the Kimball-Schortley method. It can be easily calculated.

$$E \equiv a^2 \sum_i \sum_j \left[-\frac{\Psi_{i,j}^{OLD}}{2} \frac{(\Psi_{i+1,j}^{OLD} - 2\Psi_{i,j}^{OLD} + \Psi_{i-1,j}^{OLD})}{a^2} - \frac{\Psi_{i,j}^{OLD}}{2} \frac{(\Psi_{i,j+1}^{OLD} - 2\Psi_{i,j}^{OLD} + \Psi_{i,j-1}^{OLD})}{a^2} \right] + a^2 \sum_i \sum_j \Psi_{i,j}^{OLD^2} (V_i + V_j + v_{i,j}) \quad (13)$$

But before calculating the equation (13), one needs to normalize the wave function.

$$Norm = \sqrt{a^2 \sum_i \sum_j \Psi_{i,j}^{OLD^2}} \quad (14)$$

$$\Psi_{i,j}^{OLD} \leftarrow \frac{\Psi_{i,j}^{OLD}}{Norm} \quad (15)$$

Like the usual bounded wave function, boundary conditioning is also necessary.

$$\Psi_{1,j}^{OLD} = 0 \quad \text{for } j = 1 \cdots N \quad (16)$$

$$\Psi_{N,j}^{OLD} = 0 \quad \text{for } j = 1 \cdots N \quad (17)$$

$$\Psi_{i,1}^{OLD} = 0 \quad \text{for } i = 1 \cdots N \quad (18)$$

$$\Psi_{i,N}^{OLD} = 0 \quad \text{for } i = 1 \cdots N \quad (19)$$

The final procedure is to replace the old wave function with the new wave function.

$$\Psi_{i,j}^{OLD} \leftarrow \Psi_{i,j}^{NEW} \quad (20)$$

For the last explanation of the Kimball-Shortley method, it must be added that as the initial wave function to start, one should employ a smoothly varying, variable exchangeable function.

$$\Psi_{i,j}^{OLD} = f(x_i, x_j) + f(x_j, x_i) \quad (21)$$

To sum up, the whole procedure of the Kimball-Shortley method comprises

1. Definition of initial wave function given by the equation (21).
2. Boundary conditioning defined by the equations (16) through (19).
3. Normalization of the wave function defined by the equations (14) and (15).
4. Energy expectation calculation given by the equation (13).
5. Wave function renewal given by the equation (12).
6. Replacement of old wave function with the renewed wave function (20).
7. Return to 2 and repeat the cycle as many times as one wants.

Then, how much times of repetition is sufficient? In order to answer this question, one can measure the degree of error that the wave function $\Psi_{i,j}$ makes when it is substituted into the original discretized Schroedinger equation (10). The energy eigenvalue E in the right hand side of the equation (10) becomes space-independent constant only if the wave function becomes the true exact eigen function. That is, in actual, the parameter E remains a function of space, that is, depends on the indices i, j until the wave function $\Psi_{i,j}$ reaches the true solution. So, a quantity can be defined to measure the degree of the local energy deviation.

$$\delta_{i,j} = \frac{|E_{i,j} - E|}{|E|} \quad (22)$$

where E is calculated by the equation (13) and local energy $E_{i,j}$ is calculated by

$$E_{i,j} = -\frac{1}{2} \frac{\Psi_{i+1,j}^{OLD} - 2\Psi_{i,j}^{OLD} + \Psi_{i-1,j}^{OLD}}{a^2 \Psi_{i,j}^{OLD}} - \frac{1}{2} \frac{\Psi_{i,j+1}^{OLD} - 2\Psi_{i,j}^{OLD} + \Psi_{i,j-1}^{OLD}}{a^2 \Psi_{i,j}^{OLD}} + (V_i + V_j + v_{i,j}) \quad (23)$$

By scanning the indices i, j , one can detect the maximum deviation index δ_{MAX} .

$$\delta_{MAX} = \max\{\delta_{i,j} | i = 1 \cdots N, j = 1 \cdots N\} \quad (24)$$

This error measure can be of course plotted as a function of cycle k .

$$\delta_{MAX}(k) \quad (25)$$

Though all of cases is not investigated yet, there are cases that show well behavior of $\delta_{MAX}(k)$. For some cases $\delta_{MAX}(k)$ goes down to a minimum and then soars up. For some other cases, it goes down to a minimum and then goes up a little, and then shows horizontal slight constant oscillation, that is, it becomes the so called metastable state. The result of the case study presented in this article showed just the metastable feature.

Conditions and result of the case study

The entire feature of the system is summarized in the three parameters which appeared in the equations (1) and (2) that define the potentials. Arbitrarily, the following numbers were assigned for each.

$$\begin{aligned}
 A_n &= 16 \\
 A_{ee} &= 16 \\
 \sigma &= 2 \\
 N &= 101 \\
 a &= 0.12 \\
 x_1 &= -6 \\
 x_{101} &= +6
 \end{aligned} \tag{26}$$

For the initial starting function, the following equation was used.

$$f(x_1, x_2) = \exp\left\{-\frac{(x_1 - 1.5)^2}{\sigma}\right\} \exp\left\{-\frac{(x_2 + 1.5)^2}{\sigma}\right\} \tag{27}$$

That is, the initial wave function is,

$$\begin{aligned}
 \Psi_{i,j}^{OLD} &= \exp\left\{-\frac{(x_i - 1.5)^2}{\sigma}\right\} \exp\left\{-\frac{(x_j + 1.5)^2}{\sigma}\right\} \\
 &+ \exp\left\{-\frac{(x_i + 1.5)^2}{\sigma}\right\} \exp\left\{-\frac{(x_j - 1.5)^2}{\sigma}\right\}
 \end{aligned} \tag{28}$$

Using these conditions and repeating the cycle about 3000 times, the following results have been obtained. The characters of the effect of the repetition of cycle can be seen in Fig. 1 through Fig. 4. Looking at the Fig.1, the energy expectation curve is seen to decrease and converge in well manner. The Fig. 2 shows the extremely magnified portion of the horizontal part of the Fig. 1. The Fig. 2 says that the energy minimum in a strict meaning occurs at the 1,873'th time of cycles. But energy expectation only is not an absolute measure that assures the correctness of the wave function. Rather the maximum deviation index $\delta_{MAX}(k)$ is much more reliable.

Fig. 3 shows the curve of the maximum deviation index $\delta_{MAX}(k)$. It decreases

sharply and stays almost zero after cycle 600. However, when magnified as shown in Fig 4, it shows microscopic fluctuation, and attains a minimum value at a cycle 2581. After cycle around 2700, it shows apparently a metastable state. Thus, the author adopted the 2581'th wave function as the most correct wave function. To emphasize the point, at 2581'th cycle, the maximum deviation index δ_{MAX} took the lowest value of order 10^{-14} . This result almost completely justifies the correctness of the numerical wave function $\Psi_{i,j}^{2581}$

In Fig. 5, the very wave function $\Psi_{i,j}^{2581}$ is depicted by three contour lines. It is like a dumbbell-shaped island. Fig.6 shows the square of the wave function $\Psi_{i,j}^{2581}$, that is, the density distribution function $\rho_2(x_1, x_2) = |\Psi_{i,j}^{2581}|^2 = \rho_{i,j}$. This figure indicates that the two particles have tendency to exist at opposite coordinates since the density islands are seen to locate in the second and in the fourth quadrants. For we assumed the repulsive potential between two particle and a fixed common potential well for them, these results are physically consistent with the assumed conditions

The main issue

The numerical solution thus far pursued and obtained in the foregoing sections may be obtained by other methods for solving eigenvalue equation. The objective of the foregoing sections was to present the fundamental proof of the correctness of the resultant ground state wave function $\Psi_{i,j}^{2581}$. This wave function $\Psi_{i,j}^{2581}$ is never an approximation, rather it may even be said it is a correct solution. Here begins the main issue of the present article.

By the following summation, one can calculate the one-body density distribution function.

$$\rho_1(x_i) \equiv a \sum_j |\Psi_{i,j}^{2581}|^2 = a \sum_j \rho_{i,j} = \rho_i \quad (29)$$

This curve is shown in Fig. 7.

The currently prevailing methods for solving many-body problem take anyway some method to decompose the entire wave function into an assembly of component function of one-body equation. In such a scheme, a virtual concept of average field that acts on one particle from other particle is often assumed. Such a concept may be conceivable if we know that the average potential can be calculated using the quantum mechanically behaving wave functions of the other particles[3]. At a first glance, such a strategy might seem to be correct. If such a many-body problem to one-body problem reduction were to be valid, then the square root of the above function (29) may be considered to represent one-body wave function that should satisfy a Self Consistent Field scheme.

$$\phi(x) \equiv \sqrt{\rho_1(x)} \quad (30)$$

$$-\frac{1}{2} \frac{\partial^2}{\partial x^2} \phi(x_1) + V_{SCF}(x_1) \phi(x_1) = E' \phi(x_1) \quad (31)$$

In the present study, two identical particle are considered, so that if one particle can be in a state that is expressed by a function $\phi(x_1)$, then the other must be in the same state $\phi(x_2)$. For convenience, let us change the mathematical notation from summation to usual integration. By aforementioned definition, the self consistent potential $V_{SCF}(x_1)$ that appears in the second term in the left hand side of equation (31) should be an averaged integration of the interaction potential $v(x_1, x_2)$ plus the common potential well V_n .

$$V_{SCF}(x_1) = \int v(x_1, x_2) \rho_1(x_2) dx_2 + V_n(x_1) = a \sum_j v_{i,j} \rho_1(x_j) + V_i \quad (32)$$

Furthermore, there is another way for us to know the self consistent potential. That is, since we are aware of the one-body wave function $\phi(x_1)$ already, we can calculate the assumed self consistent potential by solving the equation (31) reversely. The result is

simply the following potential function named V_{SCD} .

$$V_{SCD}(x_1) = E' + \frac{\frac{1}{2} \frac{\partial^2}{\partial x_1^2} \phi(x_1)}{\phi(x_1)} = E' + \frac{\frac{1}{2} \frac{\phi(x_{i+1}) - 2\phi(x_i) + \phi(x_{i-1}))}{a^2}}{\phi(x_i)} \quad (33)$$

Both of the equation (32) and (33) is calculable separately. The actual results are depicted as curves in the Fig. 8. The ultimate doctrine of the prevailing Self Consistent Field method demands that they should coincide with each other. Seeing the Fig. 8 in which $V_{SCF}(x_1)$ is drawn by red curve and $V_{SCD}(x_1)$ is drawn by blue curve, they are definitely different.

Therefore the fundamental base of the theory of the Self Consistent Field method is wrong, and at least in this article, there has been found one exceptional case that the self consistency of the reduced one-body potential does not hold.

Summary

Two-body problem was solved by numerical method. The degree of the accuracy was measured and ascertained to be good enough to call the numerical solution as a correct solution. From the numerical solution thus obtained, one-body reduced problem was examined if the self consistent field method really holds or not. The result showed us that it does not hold at least for the case study presented in this article.

Conclusion

One-dimensional two-body problem is relatively easy to solve numerically and consumes little time. And the correctness of the numerical solution can also be measured and ascertained easily. Further it is possible to calculate accurate various functions from the resulted entire wave function. There is no doubt about

the correctness of the functions thus calculated from the entire numerical wave function. The concept of one-body problem assumes the existence of the one-body reduced self consistent potential function that is calculable by some way. Two ways for calculating such function, that is, a self consistent potential function, were raised in this article to find they do not coincide.

Therefore, somewhere in the system of the theory of Self Consistent Field, there is a mistake. Perhaps, it may be not possible to replace many-body problem with a one-body problem, and this in turn means that for a n -body d -dimensional problem, one cannot but solve the nd -variables partial differential equation anyway.

References

- [1] G. E. Kimball and G. H. Shortley. Phys. Rev. 45,815 (1934)
- [2] Pauling, L;Bright Wilson, E. Introduction of Quantum Mechanics; McGraw-Hill: NewYork,1935,page202-204
- [3] Slaton, J. C. Quantum Theory of Matter; McGraw-Hill: New York, 1951

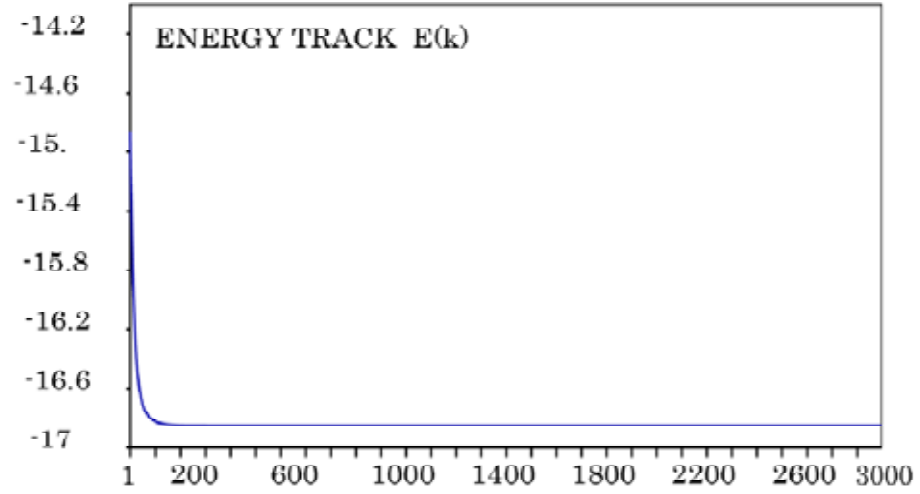


Fig. 1. The abscissa is Kimball cycle. For executing 3000 times of computation, it consumed about 15 minutes. In the figure, the blue energy track curve decreases very fast at first. After about 200 cycle, it show no appearent decreases that can be noticed by naked eye. For we have no definite proof yet that the Kimball-Shortley method can give an accurate solution for many body-system, it was lucky to be able to observe the monotonically decreasing track of the energy.

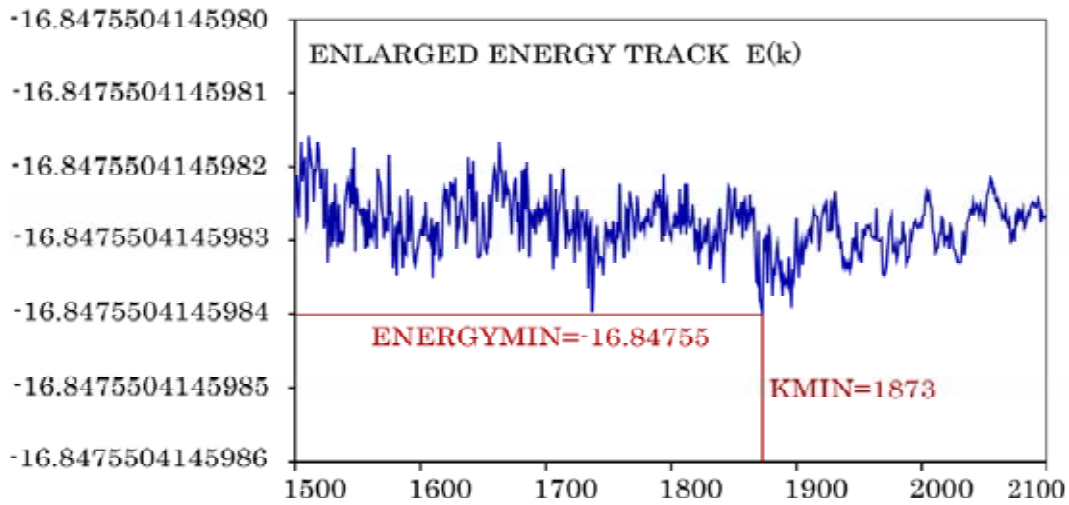


Fig. 2. Magnified energy track, magnified by by a factor of 10 to the power of +13 to show the location of the energy minimum at cycle 1873. Although the computer is treating and calculating the very small decimal, the usual computer does not display figures to the very deep decimal places on the screen. As can be seen in this figure, the microscopic fluctuation is of the order of 10 to the power of -13. The cause of this microscopic fluctuation is not clear whether it is due to the machine error itself or due to a character of the Kimball Shortley method.

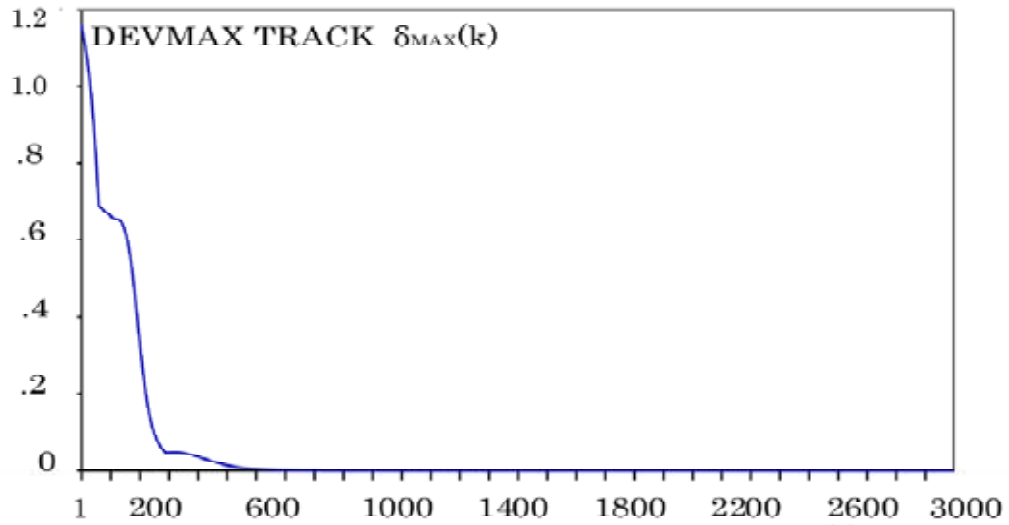


Fig. 3. The abscissa is Kimball cycle. This error measure $\delta_{\text{MAX}}(k)$ lowers as the cycle proceeds, though the initial two step behavior seems unnatural. After about 600 cycle, one cannot discern a variation of the track by one's naked eye.

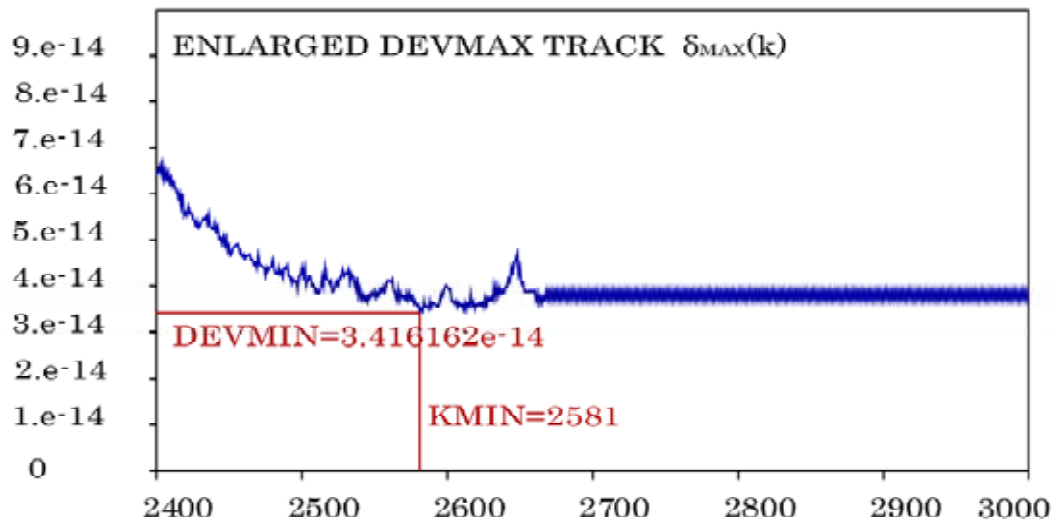


Fig. 4. Magnified track of $\delta_{\text{MAX}}(k)$, magnified by a factor 10 to the power of +14. Since the similar behavior are detected for other case, this track suggests the soundness of the Kimball process. After around 2670 cycle, the curve changes to a regularly and constantly oscillating curve, i.e., it becomes metastable state. Though the energy expectation track reaches minimum at cycle 1873 as shown in Fig. 2, mathematically speaking, to refer to the $\delta_{\text{MAX}}(k)$ minimum at cycle 2581 is better for defining the best solution of the wave function.

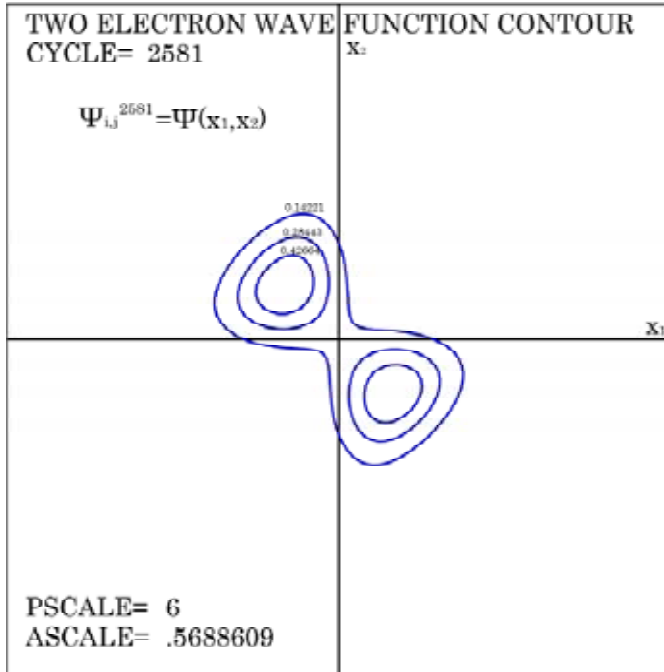


Fig. 5. Normalized contour line map of the resultant ground state wave function Ψ_{ij}^{2581} . The word “normalized” is meant here that the contour lines are sections of the wave function mountain cut by three horizontal planes which are separated by 1/4 of the mountain peak height $ASCALE = 0.5688609$. The contour map can be likened to twin islands connected by a low sandbar. The model system comprises finite intensity potentials. If the potential were to possess singularity, then this sandbar must disappear certainly. That is, the two particle will repel each other completely and the two islands must become independent ones that have oblique narrow shapes.

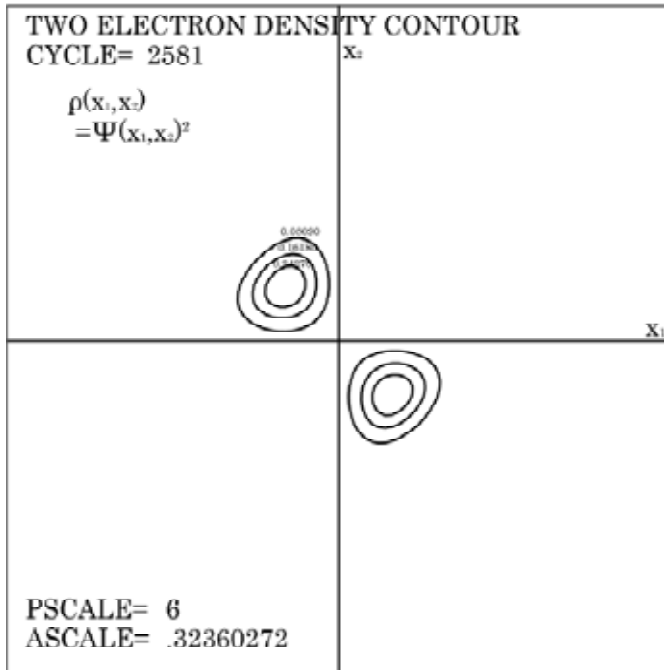


Fig. 6. Contour map of squared function of the above function Ψ_{ij}^{2581} in the figure 5. In the figure, PSCALE means plane scale, that is, the half length of the coordinate axis, and ASCALE means the altitude scale, that is, the maximum height of the mountain of the island. If we compare the radius of virtual circle in which the density function takes significant value, which may be about two, with the full space $R=6$, then one can be relieved to be confident to know or anticipate that at the peripheral region, the density function decreases enough to continue on smoothly to the boundary conditions. If the problem were to be expanded to n-particle 1-dimensional problem, then there will be n! islands in n-dimensional space.

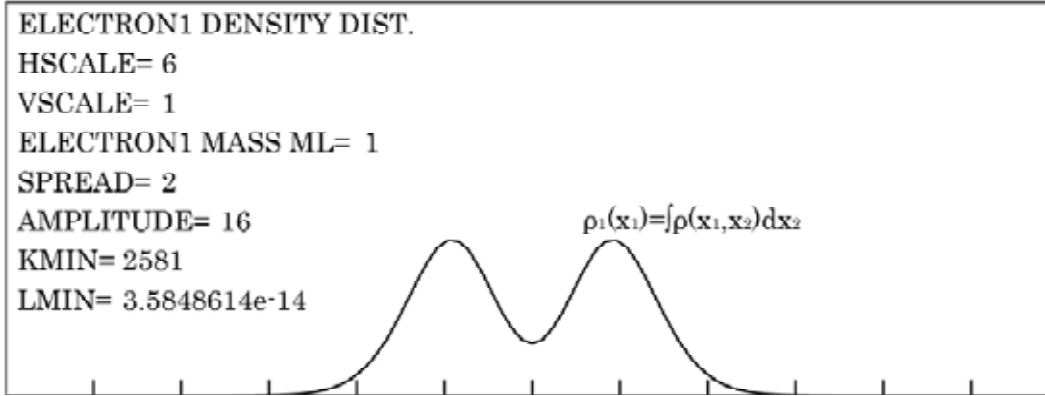


Fig. 7. Supposed one-body density function curve. One may imagine this curve as a projection of the two-dimensional topography of Fig. 6 onto a x_1 - z plane where the z axis is defined as an axis perpendicular to the sheet. The two humped-camel-like feature is logically probable. This is a mild expression that if one particle happens to be in the one side mountain, either right or left, then the other particle left behind with which the first particle repels, would exist in the other left hump region. Even as this figure seems comprehensive, the accurate and detailed physical contents are still contained in the original contour map of Fig. 5 or Fig. 6.

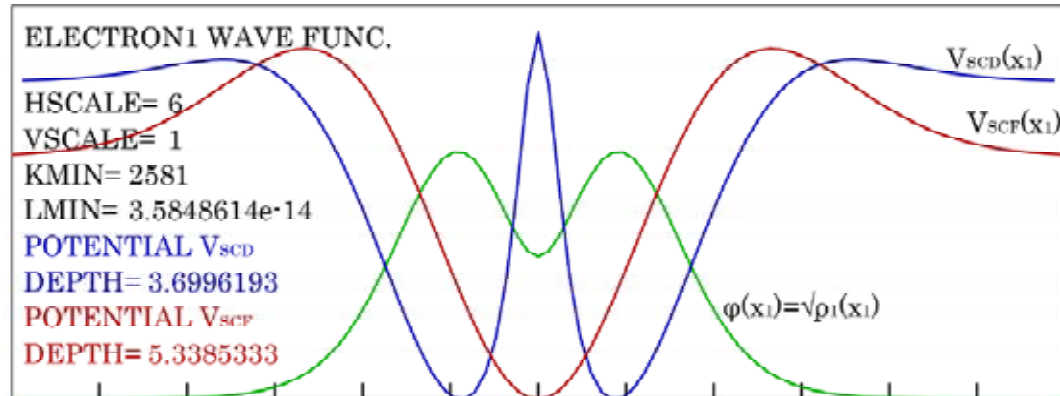


Fig. 8. Ultimate curves that the present article would like to emphasize to the readers. The green curve is a square root function of the one-body density distribution function shown in Fig. 7, and is deemed to be a one-body wave function assumed to be in the Self Consistent Field theory scheme. If one assumes that a Schrodinger-like equation for numerically known function $\phi(x_1)$ should hold, then the actually effecting one-body potential V_{SCD} can be calculated at once. On the other hand, the main assumption of the Self Consistent Field theory requests an existence of averaged field V_{SCF} that can be assumed to be possible to be calculated from averaging integration of the function of interparticle potential times the density distribution function of the other particle plus the mother potential well, i.e., $V_{SCF} = \int v(x_1, x_2) \rho_1(x_2) dx_2 + V_n(x_1)$. The doctrine of the Self Consistent theory demands that the V_{SCD} and V_{SCF} coincide with each other. But in actual practice, seeing the blue curve V_{SCD} and red curve V_{SCF} , they were found not to coincide.