Stochastic Variational Method as a Machine Learning Approach to Large-Scale Few-Body System Calculations

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Abstract. Stochastic variational method as a machine learning approach to large-scale few-body system calculations is performed with Gaussian expansion method. As a basic research to far beyond the three-body systems, the methodology is confirmed in three-body system called ^{4}He trimer. When the number of particles is large, it becomes impossible to perform the calculations at around seven-body system even with a massively parallel computer such as Fugaku supercomputer, mainly due to memory capacity limitations, but this limitation can be significantly alleviated by reducing the number of necessary basis functions. Therefore, a machine learning approach that searches for basis functions with as few basis functions as possible is expected. In the present calculation with a machine learning approach based on SVM, the calculated minimum energ with 625 basis functions, which is a standard number in GEM, is reproduced with learned significantly less 54 basis functions.

Keywords: few-body system · machine learning · massive parallel computing

1 Introduction

In the research field of quantum few-body systems, several method are proposed and applied to solve few-body problems. One of standard and powerful methods has been known as Gaussian Expansion Method (GEM) [1–8]. Currently, the cutting edge of many methods for few-body system calculations is around five-body systems although there have been successful cases of more than six-body

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systems through simplification and ingenuity of the problems. On the other hand, in the region with a large number of particles, other methods such as density functional theory are used, but there are not practical methods for the region of about 10-body systems, and there is no direct relationship between few-body calculations and model calculations for many bodies. When large-scale few-body system calculations more than 10-body is possible, there is possibility to gives a strong foundation for model calculations.

In GEM, the relative wave function is expanded in Gaussians basis functions with the order of 10. When the number of particles is increased by one, the number of basis functions in GEM describing that degree of freedom takes effect as a product of those for the previous degrees of freedom. That is 10 times larger at least when the number of particles increases by one. Therefore, the computing time for matrix elements and computer memories are required 100 times the amount compared to the case where there is one less particle. Furthermore, since it is known that the computational time of the diagonalization is $\mathcal{O}(N^3)$, reducing the number of basis functions N is important. Actually, the limitation of GEM using cutting-edge massively parallel computers like Fugaku is 7-body or 8-body systems even with optimistic estimates.

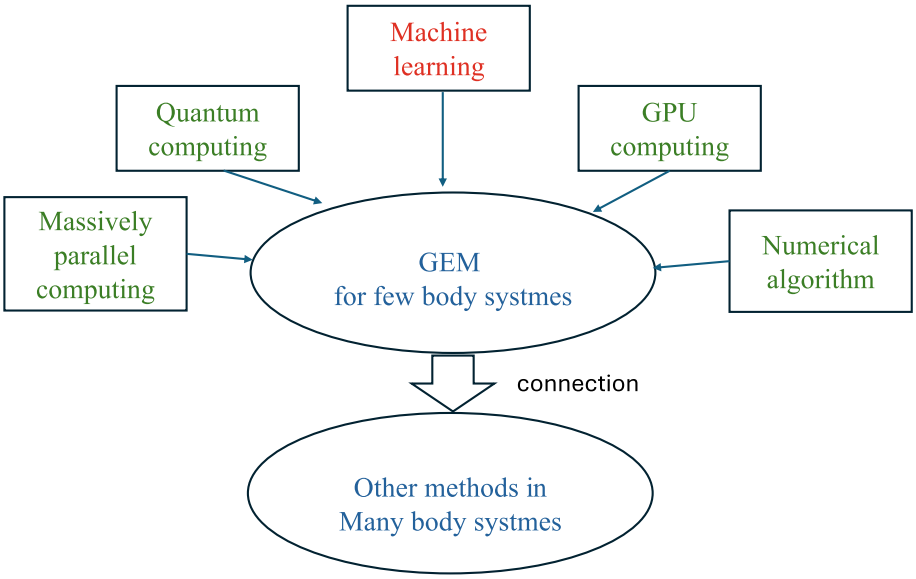

Fig. 1. Schematic diagram of GEM's development and expansion.

We have a plan revising and expanding the GEM calculation code with the aim of applying it to up to 10-body systems and connecting to many-body system calculations (Fig. 1). However, if we want to expand it to beyond 10-body systems, the calculation code needs to be revised as two points:

i) accelerating calculation of individual matrix elements,
ii) reducing the number of basis functions for the diagonalization.

First one (i) would be achieved by the so called hybrid computing with parallel computer+GPU and/or parallel computer+quantum computer, and revisions of numerical algorithms. The calculation of GEM matrix elements involves extensive use of algebraic and matrix operations, so it is also expected that GPU programming will speed up the process. Energy variation problems are expected to be a representative application of quantum computers, and GEM is a method for solving typical energy variation problems. Second one (ii) would be achieved by the machine learning. In GEM, as the number of basis functions increases, non-important basis functions are searched for to reduce the computation time with like craftsmanship approach. Or the stochastic variational method (SVM) [9–13] has been used to find automatically unimportant basis functions. The purpose of this research is investigate the availability of of SVM as a first example of a machine learning approach. The machine learning approach is expected to be powerful in other point of views. Since N-body system is a sub-system of more than N+1-body systems, the learned important basis functions would be also important in more than N+1-body systems.

In Sect. 2, GEM and SVM as a machine learning approach are explained. In Sect. 3, the calculation results and discussions for them are given. Finally, summary and conclusions are given.

2 Method

2.1 Gaussian Expansion Method

Here, we briefly explain GEM for three body bosonic system with Jacobi coordinate. The detail is given in review papers [3,14]. In GEM, the wave function Ψ_{JM} (J is the total angular momentum and M is its z-component) of the Schrödinger equation,

$$(H - E)\Psi_{JM} = 0, \tag{1}$$

is obtained by diagonalizing the Hamiltonian in a space spanned by basis functions which are constructed on Jacobi coordinates. ^{4}He-^{4}He potential in the Hamiltonian used in this research is B2+B2, which is two range (attractive and repulsive) Gaussian potential [15]. In Fig. 2, the Jacobi coordinate for three body system is displayed. $\boldsymbol{R_i}$ is i-th Jacobi coordinate, L_i is angler momentum, b_i is a range parameter of Gaussian type basis functions.

The total wave function Ψ_{JM} is written as

$$\Psi_{JM} = \sum_{i=1}^{i_{\max}} c_i \mathcal{S}\Phi_i \left(\boldsymbol{R_1}, \boldsymbol{R_2}\right). \tag{2}$$

where $\mathcal{S}$ is symmetrization operator to the bosonic systems and Φ_i is three-body basis functions. In a three-body bosonic system with the same mass, the

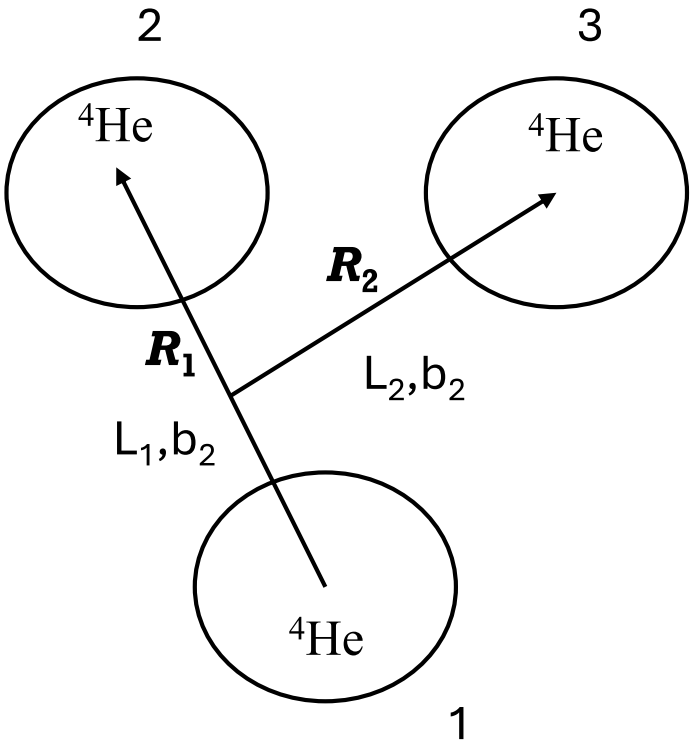

Fig. 2. Jacobi coordinate for three body system.

symmetrization for the wave function is equivalent to rearranging the Jacobi coordinates [3,14].

The three body basis functions are taken as

$$\Phi_i\left(\boldsymbol{R_1}, \boldsymbol{R_2}\right) = \phi_{n_1 L_1}\left(R_1\right)\phi_{n_2 L_2}\left(R_2\right)\left[Y_{L_1}\left(\widehat{R}_1\right)Y_{L_2}\left(\widehat{R}_2\right)\right]_{JM}, \tag{3}$$

$$i \equiv \left\{n_1 L_1, n_2, L_2\right\}. \tag{4}$$

R_i is i-th Jacobi coordinate, L_i is angler momentum of the spherical harmonic function Y_L, n_i is the basis number. Radial dependence of the basis functions $\phi_{nl}(r)$ is taken as Gaussians multiplied by r^L with ranges in geometric progression [3,14],

$$\phi_{nL}(r) = N_{nL} r^L \mathrm{e}^{-a_n r^2}, \tag{5}$$

$$a_n = 1/b_n^2, \tag{6}$$

$$b_n = b_{min}\gamma^{n-1} \quad (n = 1, \ldots, n_{\max}), \tag{7}$$

b_i is a range parameter and N_{nL} is a normalization constant.

2.2 Stochastic Variational Method

Here, SVM is explained in brief. In the next subsection, its extension are explained from the perspective of machine learning approach to solving few-body problems.

As a prerequisite, suppose that we have i-1 basis functions $\{\Phi_1, \ldots, \Phi_{i-1}\}$ and know the lowest energy $\mathcal{E}^{i-1}$ with them by diagonalizing the Hamiltonian matrix. This can be achieved by following the steps below from the single basis function. The basis function would be selected as follows:

(i) the i-th basis function Φ_i is generated randomly,
(ii) determine the corresponding lowest energy $\mathcal{E}^i$ with $\{\Phi_1, \ldots, \Phi_i\}$,
(iii) when the calculated energy difference $\mathcal{E}^{i-1} - \mathcal{E}^i$ is larger than a standard energy (for example, we employ $0.0001K$ for the ^{4}He trimer calculation in this paper), we employ the basis function as the i-th basis function and increase the dimension to i, return to i) until the calculated energy converges. The larger calculated energy difference, $\mathcal{E}^{i-1} - \mathcal{E}^i$, means that the calculated energy is closer to the true energy. In other words, the h in the regression equation of Eq.(8) in the next subsection is better.

Thus, the SVM automatically selects the important basis function through steps (i)→(iii). The advantage of this algorithm is that relatively small number of matrix elements (i-th row or column) need to be calculated for each step and the unimportant basis functions because of non-orthogonal basis function is automatically removed.

2.3 SVM as a Machine Learning Approach

Regression is known as a typical machine learning technique. Concept of SVM is very related to a regression using function expansions. As one of regression expressions, we can describe,

$$\Delta E = |E_{min} - h(N, b_1, b_2, \ldots, b_N)|, \tag{8}$$

$$\rightarrow 0. \tag{9}$$

E_{min} is the minimum energy for the given Hamiltonian, h is a lowest energy function, b's correspond to the range parameters in the Gaussian expansion,

$$\phi(r) = \sum_{j=1}^{N} c_j \exp(-\frac{r^2}{b_j^2}), \tag{10}$$

the angler momentum part is dropped for simplicity. The problem to be solved in regression is to find $N, b_1, b_2, \ldots, b_N$ so that ΔE is as close to 0 as possible. The algorithm of (i)-(iii) in subsection 2.2 is a practical method to determine $N, b_1, b_2, \ldots, b_N$. The energy variation principle dictates that the energy will always go down when good basis functions are adopted, so we can choose the

variation parameter $b's$ to get closer and closer to E_{min}. However, it is easy to imagine that the energy minimum state is not realized by stochastically selecting bad basis functions only. Also, there is no guarantee that the number of basis functions will be extremely smaller than the standards calculations using ranges in geometric progression. In that sense, there is some room for improvement in SVM that are currently used.

In this paper, we propose and investigate an additional procedure called SVM+:
iv)many SVM calculations of (i)-(iii) is performed at the same time,
v)by using the basis functions used for the wave functions that give the lower energies, the SVM calculation of the procedure of (i)-(iii) is performed again. Adding iv) and v) is easy and the computational time is also not so much different at present thanks to the development of the parallel computer unlike when it was first proposed a quarter century ago. In other words, the calcurational time for 1000 times SVM calculation (as performed in the present paper) is essentially takes the same for just one time SVM calculation if we use 1000 cores. When SVM was first proposed (1977) and the methodology subsequently developed in late 90's, supercomputers were not equipped with the capabilities to anticipate an algorithm that could run 1,000 or 10,000 times SVM calculations simultaneously. The practical application of iv) and v) is shown later in the next section.

3 Results

Figure 3 shows the convergence of the ground state energy for ^{4}He trimer when SVM is performed. The solid line represents the calculated energy with SVM and the dashed line represents the calculated energy with GEM. ^{4}He-^{4}He potential is 2B+2B (Gaussian type) [15], which reproduce the scattering length, and the ground and excited state energies. The horizontal axis represents the number of trials and the vertical axis represents the calculated energy. Note that the horizontal axis is the number of diagonalization attempts, not the dimension of the matrix that is being diagonalized. For example, the dimension of a matrix diagonalized at 100 on the horizontal axis is 69.

In this calculation, the trial basis functions are selected from the same ones as those for GEM. In Table 1 to compare the energy calculated by GEM. L_1, L_2, L are orbital angular momentum. b^i_{min} and b^i_{max} are minimum and maximum range parameters for Gaussian basis functions. i represents the Jacobi coordinate. N^i is a number of basis function superpositions for the i-th Jacobian coordinate. So the total number of basis functions is 625 (400=20×20 for channel1 and 225 = 15×15 for channel2. Since typical number of basis function in GEM for three body system is around 1,000–2,000 which is depend on systems of course, 625 basis functions would be reasonable to the present purpose. In GEM, the energy is calculated with all (625) basis functions considered. The calculated energy for the 625 basis functions is E= −0.125 K. Hereafter, the main question is whether this energy can be reproduced with fewer than 625 basis functions.

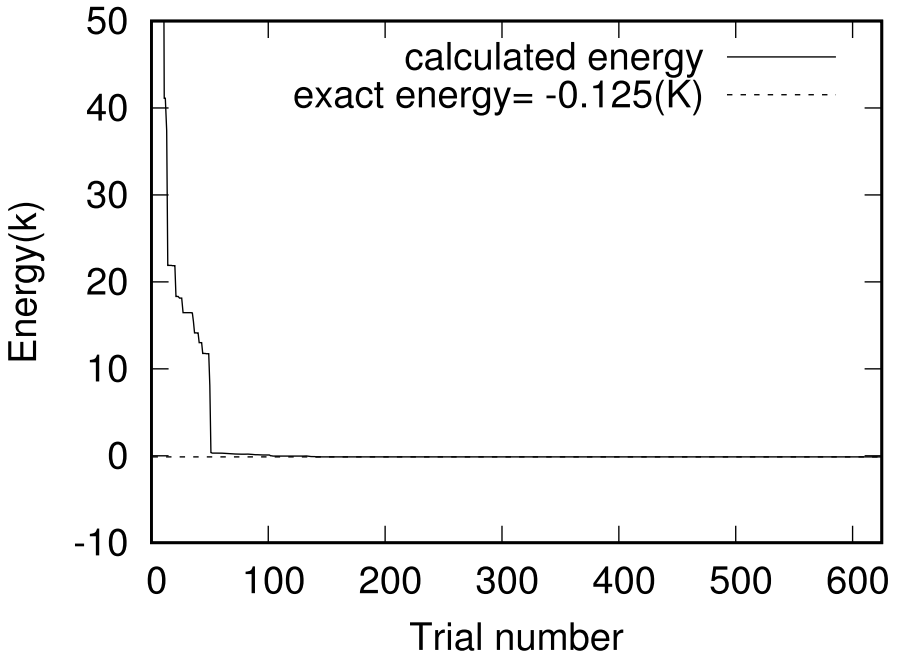

Fig. 3. Convergence of energy for ^{4}He trimer with increasing trial basis function. The horizontal axis represents the number of trials. The solid line represents the calculated energy with SVM. The dashed line represents the exact energy.

Table 1. Basis functions of GEM for ^{4}He trimer

Channel	L_1	L_2	J	$b^1_{min.}$(Å)	$b^1_{max.}$(Å)	N_1	$b^2_{min.}$(Å)	$b^2_{max.}$(Å)	N_2
1	0	0	0	0.2	30	20	0.2	30	20
2	2	2	0	0.2	15	20	0.2	30	15

In Fig. 3, the calculated energy with (solid line) approaches to that of GEM with three-digit accuracy with at 460 trial. The number of basis function is 129 smaller than 625. In other words, of the 625 basis functions employed in conventional GEM, approximately 500 are redundant to make the wave function with three-degit accurate energy. The main reason why the number of basis functions can be small is that the basis functions are overcomplete in two respects. One respect is that Gaussian basis functions are not orthogonal. Another is that the channel with rearranged Jacobi coordinates represents overcomplete basis functions before the original Jacobichannel.

In Fig. 4, the convergences of energy for ^{4}He trimer are displayed when SVM is performed. The difference in the line colors represents five trials (try1, try2, try3, try4, try5). In these trials, the 625 basis functions are same but the order in which the basis functions are selected from 625 ones is different. As seen from

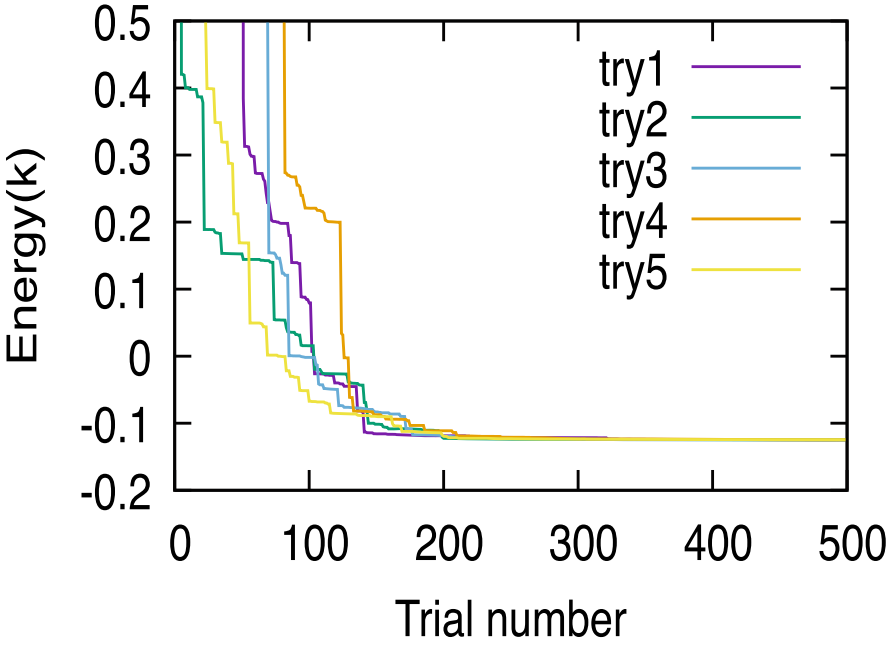

Fig. 4. Convergence of energy for ^{4}He trimer with increasing trial basis function. The horizontal axis represents the number of trials. The difference in the line colors represents five trials.

Fig. 4, the calculated energies converge the same energy ($E = -0.125$K) even if the order of the selection is different. We can not distinguish the difference from the figure at around 200–300 trials where about 100 basis functions are employed.

In Table 2, number of try and number of basis function employed to obtain convergent energy for ^{4}He trimer. The second column represents number of trial to reproduce the exact energy E=−0.125 K. The third column represents number of basis functions to reproduce the exact energy. About 100 basis functions (instead of 625) are enough to reproduce the exact energy. The least number of basis functions is 90 for try 2(green line).

Furthermore, we search the smallest number of basis functions among 1000 trial (step (iv)). The motivation for this research is how to reduce the number of basis functions. Thanks to the progress of parallel computing such as MPI over the last quarter century, it is now possible to use SVM algorithms that were not possible when originally proposed. Since each SVM try is completely independent, the calculation time can essentially be the same for 1,000 trials as for one trial when we have enough cores and memory. In Fig. 5, we show the tendency of number of the employed basis functions. The horizontal axis represents trials and the vertical represents the number of the employed basis functions. The all calculated energies are $E = -0.125$K (or -0.124K as a rare case) for

Table 2. Number of trial and number of basis function employed to obtain convergent energy for ^{4}He trimer. Different combinations of trial basis functions are used in Tyr1-Try5.

Basis function set	Number of try	Number of basis functions employed	Energy(k)
try1	460	129	−0.125
try2	410	90	−0.125
try3	337	126	−0.125
try4	443	138	−0.125
try5	485	110	−0.125

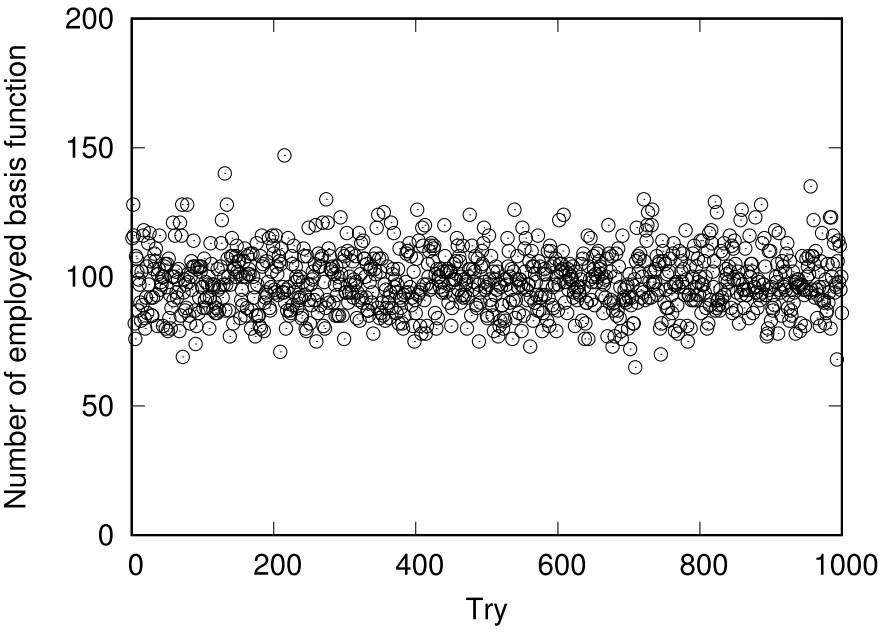

Fig. 5. The tendency of number of the employed basis functions.

the standard energy $\delta E = 0.0001$K and there were no failed trials. The smallest number of the employed basis function is 68 and the largest number is 146. It is found that about 90% of the basis functions are redundant to describe the wave function with the energy minimum.

We compare the employed basis functions between the smallest number of basis functions and the second smallest number of basis functions to check whether the selected basis function is almost the same. Although 18 basis function are consistent, the selected basis functions are not essencially the same. This is expected to be originating from non-orthogonal property for the Gaussian type basis function, a basis function is almost replaced by the superposition of other

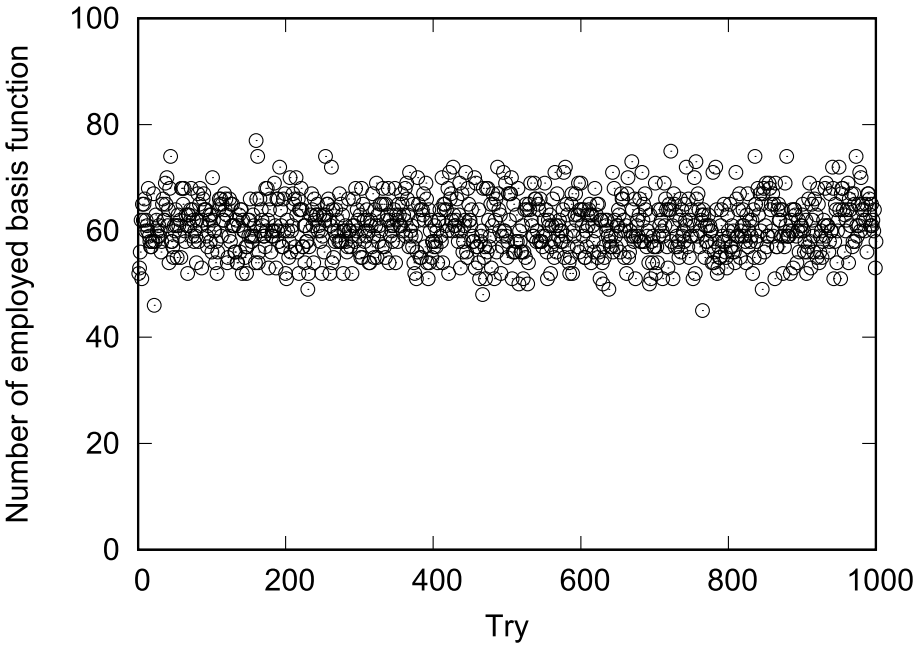

Fig. 6. The tendency of number of the employed basis functions from 119 basis functions. The 119 basis functions are the smallest number of basis functions and the second smallest number of basis functions employed from the first 625 basis functions.

basis functions. This is a good property because the energy minimum state is obtained independently of the basis functions initially chosen.

To verify the above procedure, the important 119 basis functions, which are used in the energy minimum state with the smallest number of 68 basis functions and the second smallest number of 69 basis function. Since 18 basis functions are same, the total number is 119 = 68+69-18.

In Fig. 6, the tendency of number of the employed basis functions from 119 basis functions is displayed. The lowest number of basis functions are 46, but the calculated energy is $E = -0.123$(K). This is considered to be some important basis functions are not employed for diagonalization steps, although it may be recovered adding other remained (625–119) basis functions. However, many energy minimum states of $E = -0.125$(K) are also obtained. The lowest number of basis functions are 54 for the energy minimum state. Thus, by adding the procedure (iv) and (v), the lowest number of basis functions becomes 54 from 68. Thus, the important 54 basis functions are learned from 625 basis functions. As mentioned before, three body system is a sub system of more than four body system, the corresponding part of basis functions is replaced with the learned basis functions in three body system, we can expect to be reduced the number of basis function for more than 7-body systems.

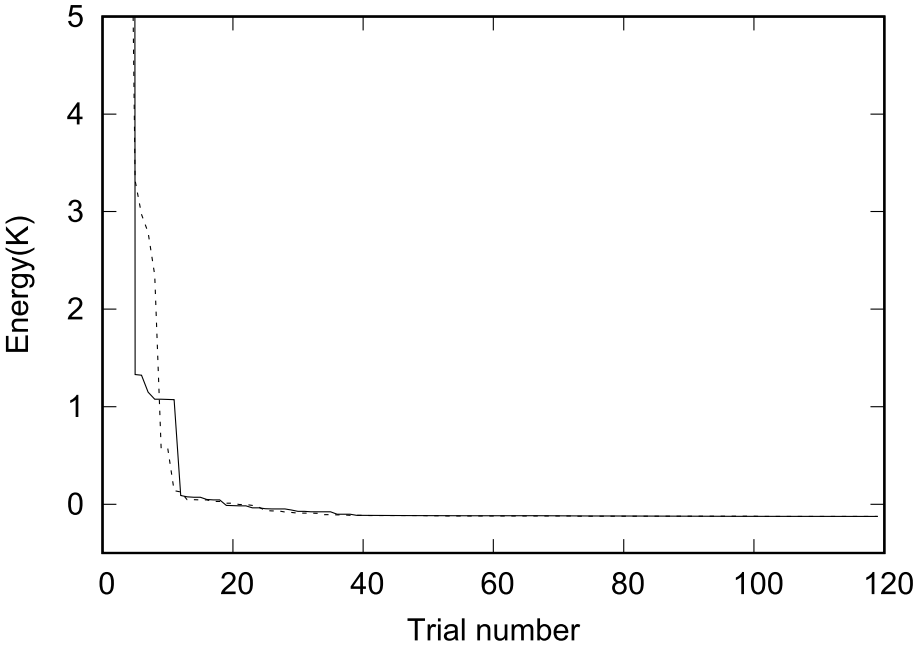

Fig. 7. Convergence of energy for ^{4}He trimer with increasing trial basis functions for the smallest 54 basis number employed.

In Fig. 7, we display convergence of energy for ^{4}He trimer with increasing trial basis functions for the smallest 54 basis number employed. There are two cases for the smallest 54 basis number employed. We can easily see quick convergence for both cases.

4 Summary and Conclusion

In this paper, we calculate ^{4}He trimer using SVM as a machine learning approach with GEM. When we proceed to more few-body systems, the reduction of the number of the basis functions becomes important. By using the present procedure which is employed in this paper, the number of basis functions for the energy minimum states of ^{4}He trimer reduced significantly. That is 54 instead of a standard number 625.

We conclude the present added procedures iv) and v) are very reasonable to learn the energy minimum wave function with a smaller basis numbers. Therefore, starting from three-body system to larger body systems, the limits are being pushed even further large body systems.

In the near future, we apply this method to the larger body systems and investigate its applicability.

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