Precise Calculations for Few-Body Atomic Systems using the Gaussian Expansion Method and Applications to Cold Atoms

Project Representative
Emiko Hiyama RIKEN Nishina Center for Accelerator-Based Science

Authors
Emiko Hiyama*1, Hiroya Suno*2, 1, Masayasu Kamimura*1
*1 RIKEN Nishina Center for Accelerator-Based Science
*2 RIKEN Advanced Institute for Computational Science

The Gaussian Expansion Method (GEM) for ab initio variational calculations of few-body systems, proposed in 1988, has been extensively used for a variety of systems involving nuclei, hypernuclei, quarks, and exotic atoms, in the fields of nuclear physics as well as exotic atomic and molecular physics, in order to obtain bound state and scattering properties. The aim of our project is to study cold few-body atomic systems using the sophisticated numerical technique through the Gaussian Expansion Method. So far, three-, four- and five-body codes are available to treat problems in nuclear physics, but thorough optimization is necessary to apply to weakly-bound cold atomic systems on the Earth Simulator 2 (ES2) supercomputer.

We are interested in treating three-, four-, and five-body systems of cold atoms. Few-body systems involving helium are of great interest, since some of them are characterized as "weakly-bound systems", showing a wave function of very diffused nature, and therefore presenting a challenge in numerical calculations. We have studied the three-body ^{4}He molecule and its isotopic species ^{4}He$_2$^{3}He, as well as the ^{4}He$_2$^{7}Li molecule. We have also carried out optimization of the four-body and five-body codes in order to run them on ES2.

Keywords: cold atoms, weakly bound molecules, variational calculation

1. Introduction

There are many examples of precision numerical calculations which have contributed to examining fundamental laws of physics and interactions in physical systems. One recent example is the determination of the upper limit of the difference between the masses of proton and antiproton, m_p and $m_{\bar{p}}$, respectively. The first recommended upper limit of $|m_p\text{-}m_{\bar{p}}|/m_p$ by the Particle Data Group listed in Particle Listings 2000 was 5×10^{-7}, while could be used for a test of *CPT* invariance. This number was extracted from a high-resolution laser experiment involving metastable states of antiprotonic helium atom ($He^{2+}+e^-+\bar{p}$) through a theoretical analysis of the Coulomb three-body system using Gaussian Expansion Method (GEM) of calculation developed for few-body systems. The ration was improved to $|m_p\text{-}m_{\bar{p}}|/m_p \leq 6\times10^{-8}$ as listed in the Particle Listings 2002, by a later more extensive experiment and an additional calculation.

Many important problems in physics can be addressed by solving the Schrödinger equation with high precision for three- and four-body systems. It is therefore of particular importance to develop methods for precision calculations for such problems. In the calculation of three-body systems such as the one mentioned above, the interaction is precisely known. In newly developing fields of physics, however, there are cases in which interactions are not well known. Studies of such subjects with precision (few-body) calculations are also meaningful and important. In order to extract reliable new information and constrain the ambiguity in the interaction being examined, the calculation must be sufficiently rigorous. The Gaussian Expansion Method was proposed by Kamimura [1] in 1988 to carry out non-adiabatic three-body calculations of muonic molecules and muon-atomic collisions, and since then has been applied to a variety of few-body systems involving nuclei, hypernuclei, quarks, and exotic atoms, in the fields of nuclear physics and exotic atomic and molecular physics [2]. The aim of our project is here to apply Gaussian Expansion Method to three-, four- and five- body systems of cold atoms.

2. Gaussian Expansion Method

2.1. Three-body wave function

We take all three sets of Jacobi coordinates, $\vec{x}_1=\vec{r}_2-\vec{r}_3$, and $\vec{y}_1=\vec{r}_1-(m_2\vec{r}_2+m_3\vec{r}_3)/(m_2+m_3)$ and cyclically for ($\vec{x}_2$, $\vec{y}_2$) and

($\vec{x}_3$, $\vec{y}_3$), $\vec{r}_i$ being the position vector of the ith particle. The Hamiltonian of the system is expressed as

$$H = -\frac{\hbar^2}{2\mu_x}\nabla_x^2 - \frac{\hbar^2}{2\mu_y}\nabla_y^2 + \sum_{1=i<j}^{3} V(r_{ij}), \quad (1)$$

where $\mu_x=m_1m_2/(m_1+m_2)$ and $\mu_y=(m_1+m_2)\ m_3/m_1+m_2+m_3)$, m_i being the mass of atom i. $V(r_{ij})$ is the two-body potential as a function of the interatomic distance $r_{ij}=|\vec{r}_j-\vec{r}_i|$.

We calculate the three-body bound-state wave function Ψ_3, which satisfies the Schrödinger equation

$$(H-E)\Psi_3 = 0. \quad (2)$$

In this work, we consider three spinless atoms and the three-body wave function is described as a sum of amplitudes of three arrangement channels c=1,2,3:

$$\Psi_3 = \Phi^{(c=1)}(\vec{x}_1,\vec{y}_1) + \Phi^{(c=2)}(\vec{x}_2,\vec{y}_2) + \Phi^{(c=3)}(\vec{x}_3,\vec{y}_3). \quad (3)$$

Each amplitude is expanded in terms of the Gaussian basis functions written in Jacobi coordinates $\vec{x}_c$ and $\vec{y}_c$:

$$\Phi^{(c)}(\vec{x}_c,\vec{y}_c) = \sum_{n_x,l_x,n_y,l_y} A^{(c)}_{n_x,l_x,n_y,l_y}\left[\phi_{n_x,l_x}(\vec{x}_c)\psi_{,n_y,l_y}(\vec{y}_c)\right]_{JM} \equiv \sum_\alpha A_\alpha \Phi_\alpha, \quad (4)$$

where

$$\phi_{nlm}(\vec{r}) = N_{nl} r^l e^{-\nu_n r^2} Y_{lm}(\hat{r}), \quad (5)$$

$$\psi_{NLM}(\vec{r}) = N_{NL} r^L e^{-\lambda_N r^2} Y_{LM}(\hat{r}). \quad (6)$$

Here, N_{nl} and N_{NL} are the normalization constants and the Gaussian ranges are given by

$$\nu_n = \frac{1}{x_n^2}, x_n = x_1 a^{n-1}, \lambda_N = \frac{1}{y_N^2}, y_N = y_1 A^{N-1}.$$

The eigenenergies E and amplitudes $A_\alpha \equiv A^{(c)}_{nx,lx,ny,ly}$ of the ground and excited states are determined by the Rayleigh-Ritz variational principle:

$$\langle \Psi_3 | H - E | \Psi_3 \rangle = 0, \quad (7)$$

which results in a generalized eigenvalue problem:

$$\sum_\alpha [H_{\alpha\alpha'} - E N_{\alpha\alpha'}] A_{\alpha'} = 0. \quad (8)$$

The matrix elements are written as

$$H_{\alpha\alpha'} = \langle \Phi_\alpha | H | \Phi_{\alpha'} \rangle, N_{\alpha\alpha'} = \langle \Phi_\alpha | 1 | \Phi_{\alpha'} \rangle.$$

2.2 Four-body wave function

We take two types of Jacobi coordinate sets, K type and H type. For the K type, $\vec{x}_1=\vec{r}_2-\vec{r}_1$, $\vec{y}_1=\vec{r}_3-(m_1\vec{r}_1+m_2\vec{r}_2)/(m_1+m_2)$, and $\vec{z}_1=\vec{r}_4-(m_1\vec{r}_1+m_2\vec{r}_2+m_3\vec{r}_3)/(m_1+m_2+m_3)$ and cyclically for $\{\vec{x}_i,\vec{y}_i,\vec{z}_i;\ i=2,\ldots,12\}$. For the H type, $\vec{x}_{13}=\vec{r}_2-\vec{r}_1$, $\vec{y}_{13}=\vec{r}_4-\vec{r}_3$, and $\vec{z}_{13}=\frac{(m_3\vec{r}_3+m_4\vec{r}_4)}{(m_3+m_4)}-\frac{(m_1\vec{r}_1+m_2\vec{r}_2)}{(m_1+m_2)}$, and cyclically $\{\vec{x}_i,\vec{y}_i,\vec{z}_i;\ i=14,\ldots,18\}$. The total four-body wave function Ψ_4 is obtained by solving the Schrödinger equation

$$(H-E)\Psi_4 = 0$$

with the Hamiltonian

$$H = -\frac{\hbar^2}{2\mu_x}\nabla_x^2 - \frac{\hbar^2}{2\mu_y}\nabla_y^2 - \frac{\hbar^2}{2\mu_z}\nabla_z^2 + \sum_{1=i<j}^{4} V(r_{ij}),$$

where μ_x,μ_y, and μ_z can be calculated in the same way as in the three-body case. Specifically, in the case of four identical atoms of mass m, we have $\mu_x=\frac{1}{2}m$, $\mu_y=\frac{2}{3}m$, and $\mu_z=\frac{3}{4}m$ on the K-type coordinates, and $\mu_x=\mu_y=\frac{1}{2}m$, and $\mu_z=m$ on the H-type coordinates. Ψ_4 is expanded in terms of four-body basis functions:

$$\Psi_3 = \sum_{c=1}^{18} \Phi^{(c)}(\vec{x}_c,\vec{y}_c,\vec{z}_c).$$

Each of these component functions is expanded in terms of the Gaussian basis functions associated with the K-type and H-type Jacobi coordinates, in analogy with the three-body case. In the similar way, the five-body wave function can be calculated. The five-body problem has three additional degrees of freedom and employs 120 component functions, each of which is associated to one set of 4 Jacobi coordinates.

3. Results

In this work, we have carried out three-body calculations as well as code tuning of the four- and five-body computer codes. We have treated three-body systems such as the helium trimer and its isotope as well as the ones that consist of two helium atoms and one alkali-metal atom. Such three-body atomic systems are known to be weakly-bound molecules, and therefore their calculations become difficult due to the diffuse nature of their wave function. We have calculated the bound state energy levels of the $^4He_3$, and $^4He_2{}^3He$, and $^4He_2{}^7Li$ molecules. Our finding is that $^4He_3$, and $^4He_2{}^3He$, and $^4He_2{}^7Li$ have respectively two, one and two $J^\Pi=0^+$ bound states. The $^4He_3$ ground and excited state energy levels are found to be respectively -127.45 mK and -2.4505 mK, while we have found the $^4He_2{}^3He$ energy level to be -14.224 mK. The $^4He_2{}^7Li$ ground and excited state energy levels are -76.32 mK and -5.51 mK.

On the other hand, we have also carried out tuning of the four- and five-body computer codes on the Earth Simulator 2 (ES2). Typically, each execution of the five-body code took more than 200 hours. We have eliminated several wasteful calculation and vectorized the most expensive part of the calculation. The vectorization percentage has been raised to more than 99%, and the average vector length to more than 255. Then, the five-body code necessitates only 2 hours and 50 minutes per each run.

References

[1] M. Kamimura, Phys. Rev. A 38, 621 (1988); M. Kamimura, Muon Catalyzed Fusion 3, 335 (1988).

[2] E. Hiyama, Y. Kino, and M. Kamimura, Prog. Part. Nucl. Phys. 51, 223 (2003); E. Hiyama and M. Kamimura, Phys. Rev. A 85, 022502 (2012).

[3] H. Suno, E. Hiyama, and M. Kamimura, Few-body Syst. DOI 10.1007/s00601-013-0708-z (2013).

ガウス関数展開法による少数粒子系の精密計算と冷却原子系への応用

プロジェクト責任者
肥山詠美子　　理化学研究所　仁科加速器研究センター
著者
肥山詠美子 *1，数納　広哉 *2, 1，上村　正康 *1
*1　理化学研究所　仁科加速器研究センター
*2　理化学研究所　計算科学研究機構

ガウス関数展開法（Gaussian Expansion Method; GEM）は少数多体系の束縛状態や散乱状態を計算する強力な手法であり、主にハイパー核、クォークなどの原子核・素粒子分野およびエキゾチック原子分子の分野で用いられてきた。本プロジェクトの目的はこのガウス関数展開法を用いて冷却原子系を研究することである。これまでは、原子核分野に応用するための 3 体、4 体、5 体の数値計算プログラムが開発されているが、地球シミュレータ上で冷却原子系に応用するためにはさらなる高度化・最適化が必要であった。我々は $^{4}He_{3}$、$^{4}He_{2}{}^{3}He$ や $^{4}He_{2}{}^{7}Li$ などの 3 体系の束縛状態計算を行うと同時に 4 体系、5 体系の高度化、最適化を行った。

キーワード:冷却原子, 弱結合分子, 変分計算