APPLICATION OF ATMS TO THE $^4$He TRIMER AND TETRAMER

S. Nakaichi, Y. Akaishi and H. Tanaka

Department of Physics, Hokkaido University, Sapporo 060, Japan

and

T. K. Lim

Department of Physics and Atmospheric Science, Drexel University
Philadelphia, Pa. 19104, USA

Using the recently proposed realistic diatomic potentials the binding energies of $^4$He trimer and tetramer were calculated. The results are $0.08 \sim 0.2$ $^0$K for the trimer, and $0.4 \sim 0.7$ $^0$K for the tetramer, and their existence is established.

In this letter we report on the result of a variational calculation of the ground state energy of the three $^4$He atom system and that of the four $^4$He atom system. The emphasis of the work is to determine how well the four body system is bound.

Any cluster of helium atoms is largely a quantum mechanical system, and recent experiments do not resolve whether the two helium atom system has a bound state [1]. On the other hand, possible clustering has been discussed in relation to the behaviour of the thermodynamical quantities of $^4$He gas at extremely low temperatures. In particular, Larsen [2] has pointed out that the change of sign of the third virial coefficient of $^4$He gas can be explained by assuming a bound three body state. Now the $^4$He-$^4$He interatomic interaction has been investigated in great detail from both the theoretical and phenomenological points of view using the concept of a shallow local potential. Thus it is interesting to see if we could establish the existence of the three body bound state, determine its energy, and further evaluate the binding of the four body system, on the basis of these potentials.

To perform these calculations, however, high accuracy of the method is required because cancellation between the kinetic and potential energies renders the binding energy very small. We used the method of ATMS [3]. In a previous report [4] we treated the three alpha particle system by this method. And by applying an integrodifferential Euler equation we showed that the method solves this dynamical system very accurately. However, in order to treat the four body system, we had to return to the original scattering equation [3]. Solving the two body correlation functions of the ATMS wave function using this equation rather than the Euler equation, for the same $^{12}$C system, we found an upper bound of $-5.16$ MeV and a lower bound of $-5.6$ MeV for the ground
state energy which are to be compared with $-5.18$ MeV and $-5.3$ MeV, respectively, previously obtained. Thus, we believe that by this scheme we can solve the dynamical systems of three and four atoms with essentially the same accuracy as by the Euler equation scheme.

An important characteristic of the helium molecules is their large size which is due to the extremely small binding they possess. A great deal of consideration must be paid to this feature to assure the convergence of the numerical calculations, particularly in the Quasi Random Number integration [5] routines for the four body calculation. To achieve sufficient numerical accuracy, we took a transformation of variables which carefully takes in the appreciable amplitude of the wave function at large interparticle distances. This is quite a different circumstance from the cases of systems of nucleons and alpha particles. In fig. 1 we show the convergence behaviour of the expectation values versus the number of integration mesh points in the four body calculation. It should be noted that the convergence of the total energy is very good compared to that of the kinetic and potential energies. This is because the variation of the integrand of the total energy is small [5]. Thus we find the numerical accuracy in our calculation is sufficiently reliable especially for the total energy.

We show our results for the three body system in table 1, and those for the four body system in table 2, where the diatomic potentials are the Smith-Thakkar [6], MDD-2 [7], Beck [8], Lennard-Jones [9] and ESMMSV [10] potentials. The three body binding energy ($-0.105 \text{ O}\text{K}$) in the case of the MDD-2 potential is slightly superior to that of the variational calculations of Lim et al. ($-0.091 \text{ O}\text{K}$) [11], and Bruch and McGee ($-0.078 \text{ O}\text{K}$) [12], and the Faddeev-UPE calculation ($-0.087 \text{ O}\text{K}$) [11]. For the Lennard-Jones potential, Schmid et al.[13] performed a variational calculation for three through ten $^4\text{He}$ atom systems. Their values for the three and four body systems are $-0.067 \text{ O}\text{K}$ and $-0.376 \text{ O}\text{K}$, respectively. Since the dynamical parameters they took in their calculation are slightly different from ours, we recalculated with their parameter values and obtained $-0.067 \text{ O}\text{K}$ and $-0.384 \text{ O}\text{K}$, respectively. With this agreement, we contend that the present results represent fairly reliable values for the energies of the $^4\text{He}$ molecules.

We note here that the general trend of binding energy values among the realistic potentials chosen for this study is the same in the two systems. In particular, the Smith-Thakkar potential is clearly distinguished from the other potentials in both systems. It is perhaps pertinent to point out that a plot of our four body versus three body