ULTRACOLD ATOMIC CLUSTERS VIA FADDEEV DIFFERENTIAL EQUATIONS

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ABSTRACT

This work is aimed at the theoretical investigation of two- and three-atomic clusters of neon. Bound state energies and wave functions have been calculated. The modern realistic potential models are used for description the interatomic interaction.

Differential Faddeev equations in the total angular momentum representation are used for the binding energies calculations of neon trimer system. The results obtained are compared with previous published results.

INTRODUCTION

Small clusters of rare gas atoms are of a great interest in the recent years. They belong to a large class of molecules interacting via potentials of van-der-Waals type and have unique quantum properties.

One of these properties is the Efimov effect [1]. This unexpected and unnatural effect was predicted by the Russian theoretical physicist Vitaly Efimov in 1970. This effect reflects the difference in the properties of the two-body and the three - body systems. When there are at least two subsystems of zero binding energy, the three - body system has an infinite number of weakly bound states - this is the essence of the Efimov effect.

This effect was experimentally confirmed only in 2006 [2] in ultracold gas of ^{133}Cs atoms. One of the best theoretically predicted example for this phenomenon is the ^{4}He$_3$ helium trimer where an excited state is of Efimov nature [3]. The first experimental measurements of the exited state in helium trimer were done recently in [4]. Calculations of ultracold three-body clusters require methods suitable for solving three-body bound state and scattering problems in configuration space. The aim of this paper is to develop the numerical algorithm for solving differential Faddeev equations in the total angular momentum representation [5, 6] and to apply it to ^{20}Ne$_3$ neon triatomic system.

FORMALISM

Interatomic potentials

Realistic effective interatomic potentials allow us to reduce the study of rare gas atoms to a system consisting only of point structureless particles. Such a description is satisfactory at relatively low energies of atomic motion. Various potential models existed long before the first experiments: all of them differ in their form, but demonstrate strong repulsion near zero and long van der Waals tail at long distances. We use two potential models the Tang - Toennies [7] and Aziz [8] potential model.

The Tang - Toennies potential [7] is given by:

$$V(r) = V_{rep} + V_{att} = Ae^{-br} - \sum_{n=3}^{N} f_{2n}(br)\frac{C_{2n}}{r^{2n}}, \qquad (1)$$

where A and b parameters,the C_{2n} are the dispersion coefficient, $f_{2n}(br)$ – the damping function, which is given by the following expression:

$$f_{2n}(br) = 1 - e^{-br}\sum_{k=0}^{2n}\frac{b^k}{k!}.$$

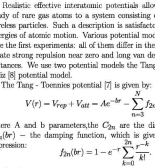

FIG. 1. The dependence of the interatomic potential Tang - Toennies [7], Aziz [8] and Lennard - Jones [9] (the value is in K) on the distance r (in Å) between the atoms.

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Method

The position of the three particles in configuration space after separating the center of mass is described by pairs of Jacobi coordinates $\vec{x}_\alpha, \vec{y}_\alpha$ ($\alpha = 1, 2, 3$):

$$\vec{x}_\alpha = \left[\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma}\right]^{1/2}(\vec{r}_\beta - \vec{r}_\gamma),$$

$$\vec{y}_\alpha = \left[\frac{2m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma}\right]^{1/2}\left(\vec{r}_\alpha - \frac{m_\beta\vec{r}_\beta + m_\gamma\vec{r}_\gamma}{m_\beta + m_\gamma}\right) \qquad (2)$$

where $\vec{r}_\alpha$ is radius vector of the particles with mass m_α and (α, β, γ) form a cyclic permutation of the atom numbers (1, 2, 3). A set of coordinates α describes a partition of three particles on a pair of particles $(\beta\gamma)$ and single particle α.

One of the effective methods for studying three - particle systems is based on using the differential Faddeev equations in the total angular momentum representation [5, 6, 10]. Three - particles system is described by the Hamiltonian:

$$H = H_0 + \sum_\alpha V_\alpha(x_\alpha)$$

where H_0 stands for the kinetic energy of the three particles, $V_\alpha(x_\alpha)$ is the interaction potential acting in the pair α. We consider the states with zero total angular momentum. The angular degrees of freedom corresponding to collective rotation of the three-body system can be separated and the kinetic energy operator reduces to:

$$H_0 = -\rho^{-5}\partial_\rho\rho^5\partial_\rho - \frac{4}{\rho^2}\sin^{-2}\chi_\alpha \times \left(\partial_{\chi_\alpha}\sin^2\chi_\alpha + \sin^{-1}\theta_\alpha\partial_{\theta_\alpha}\sin\theta_\alpha\partial_{\theta_\alpha}\right) \qquad (3)$$

where ρ, χ_α and θ_α are the hyperspherical coordinates expressed through standard Jacobi variables $\vec{x}_\alpha, \vec{y}_\alpha$, $\alpha = 1, 2, 3$:

$$\rho = \sqrt{x_\alpha^2 + y_\alpha^2}, \quad \tan\theta_\alpha/2 = x_\alpha/y_\alpha, \quad \cos\theta_\alpha = \frac{(\vec{x}_\alpha, \vec{y}_\alpha)}{x_\alpha y_\alpha}$$

$$x_\alpha = |\vec{x}_\alpha|, y_\alpha = |\vec{y}_\alpha|, \rho \in [0, \infty), \quad \{\chi_\alpha, \theta_\alpha\} \in [0, \pi] \otimes [0, \pi]. \quad (4)$$

The total wave function Ψ a three - body system can be written as the sum of Faddeev components Ψ_α:

$$\Psi(\rho, \chi_\alpha, \theta_\alpha) = \sum_\alpha \Psi_\alpha(\rho, \chi_\alpha, \theta_\alpha), \qquad (5)$$

satisfying Faddeev equations

$$(H_0 + V_\alpha - E)\,\Psi_\alpha(\rho, \chi_\alpha, \theta_\alpha) = -V_\alpha\sum_{\beta\neq\alpha}\Psi_\beta(\rho, \chi_\beta, \theta_\beta) \qquad (6)$$

where V_α is the potential of interaction in the pair α and E is the total energy of the system. For numerical solution it is suitable to substitute

$$\Psi_\alpha = \rho^{5/2}\sin\chi_\alpha\sin\theta_\alpha\psi_\alpha. \qquad (7)$$

The scaled components ψ_α satisfy the boundary condition:

$$\psi_\alpha(\rho = 0) = \psi_\alpha(\chi_\alpha = 0, \pi) = \psi_\alpha(\theta_\alpha = 0, \pi) = 0. \qquad (8)$$

Then Eqs.(6) are rewritten in terms of as follows:

$$\left(\hat{H}_0 + V_\alpha(x) - E\right)\Psi_\alpha(\rho, \chi, \theta) = -V_\alpha(x)\sum_{\beta\neq\alpha}\Psi_\beta(\rho, \chi_\beta, \theta_\beta), \quad (9)$$

where $\chi = \chi_\alpha$, $\theta = \theta_\alpha$, $x = \rho\cos(\chi_\alpha/2)$. The differential operator $\hat{H}_0$ is given by

$$\hat{H}_0 = -\partial_\rho^2 - \frac{4}{\rho^2}\left[\partial_\chi^2 + \sin^{-2}\chi\left(\partial_\theta^2 - \cot\theta\partial_\theta + \sin^{-2}\theta\right) + \frac{1}{16}\right]$$

RESULTS

Two - atomic clusters

First experimental measurements of the spectrum of neon dimer ^{20}Ne$_2$ were given in [11]. Discrete spectrum of neon dimer in the s-state contains three levels, two of which are experimentally measured in [12] and have the energy value 24.22 ± 0.02 K and 4.405 ± 0.02 K, respectively. For the energy of the second excited state only an upper bound, namely 0.14 K, was determined. In this paper [13] the binding energy, the average radius and the root mean square radius of Ne dimers calculated with the potentials TT [7] and HFD-B [8] are shown in Table 1.

Level	0			1			2		
Potent.	E_0	$\langle r\rangle$	$\sqrt{\langle r^2\rangle}$	E_1	$\langle r\rangle$	$\sqrt{\langle r^2\rangle}$	E_2	$\langle r\rangle$	$\sqrt{\langle r^2\rangle}$
TT	24.0598	3.3329	3.3471	4.2040	4.2849	4.3438	0.0181	12.4793	13.8709
HFD-B	24.3715	3.3309	3.3452	4.4527	4.2527	4.3100	0.0276	11.2127	12.2721

Table 1. Energy levels of the bound states E_n (K), the average radius $\langle r\rangle$ (Å) and the root mean square radius $\sqrt{\langle r^2\rangle}$ (Å) of Ne dimers, calculated with potentials TT [7] and HFD-B [8]. The energies are given in units of K and are relative to the three-body dissociation threshold.

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Neon dimer has three bound states for zero orbital angular momentum. Calculated binding energies and average distances are in a good agreement with the reported in [3, 14, 15]. Radial wave functions φ of all state of neon dimers are shown in Fig.1.

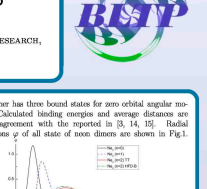

Fig.1. The radial wave functions φ of the ground and excited states of neon dimer, calculated with the TT [7] and HFD-B [8] potentials.

Three - atomic clusters

For the calculations of the spectrum of neon trimer we use finite-difference approximation for solving the differential equations (9) with the Dirichlet boundary conditions. To increase the speed of calculation we used the library Eigen [16] for linear algebra, OpenMP and CUDA technology. We have applied developed numerical algorithm for solving the above mentioned equations for the ^{20}Ne three - atomic system. Atomic masses for neon isotope were taken from [17]. To describe the interatomic interaction, the realistic potential model TT [7] and HFD-B [8] were used. Table 2 contain spectrum for neon trimer [13], which are in a good agreement with the results obtained using different methods by other authors.

E (K)	HFD-B	TT	[14]*	[15]*
E_0	74.13	74.07	74.10	74.11
E_1	52.44	52.37	52.41	52.43
E_2	49.25	49.19	49.23	49.24
E_3	45.53	45.49	45.51	45.52
E_4	40.37	40.31	40.34	40.35
E_5	34.67	34.62	34.65	34.66
E_6	32.33	32.27	32.30	32.31
E_7	31.54	31.48	31.51	31.52
E_8	27.66	27.61	27.64	27.65
E_9	26.20	26.16	26.17	26.18
E_{10}	24.95	24.92	24.93	25.03

* - HFD-B [8] potential model used.

Table 2. The bound states energy (in K) for ^{20}Ne$_3$ calculated with TT [7] and HFD-B [8] potentials.

Investigation of the ground state energy convergence with respect to the number of grid points demonstrates that $N_\rho = 250$ is sufficient to get up to four accurate figures for the energy of the ground state (see Fig. 2).

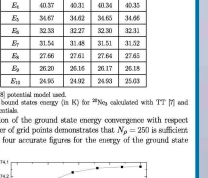

Fig. 2. Convergence of the neon trimer ground state energy on the grid points N_ρ for fixed value of $N_\theta = 100$ and $N_\chi = 10$.

CONCLUSION

In the course of this work we investigated the properties of neon clusters. Namely, we have calculated binding energy, the average radius and the root mean square radius for neon dimers and spectrum for neon trimer, using realistic potentials TT [7] and HFD-B [8]. In order to perform the calculations we developed numerical algorithm for solving the differential Faddeev equations in the total angular momentum representation. This algorithm has been realized in the programming language C++. Our results are in a good agreement with the results obtained by other methods. The developed numerically effective computational scheme, especially in combination with an option of using multiple processors, makes it possible to calculate wide range of three - body problems.

References

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