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Calculation of the van der Waals potential of argon dimer using a modified Tang-Toennies model

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Abstract. The Tang-Toennies (TT) potential model was modified based on the physical nature of the interatomic interaction to describe the Ar–Ar potential very accurately in the short range of the repulsive region. Using the modified TT potential model, the ground state van der Waals potential energy curve of Ar_2 was calculated. Compare to the experimental result, the current potential shows that the modified potential model not only gives the precise result in the long-range part, but also gives quite accurate result in the short-range repulsive part.

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Key words: modified TT potential model, argon dimer, van der Waals potential

1 Introduction

In recent years, with magneto-optical traps [1,2], a number of fields in ultracold atom physics, such as photoassociation [1, 3], optical frequency standards [4, 5], as well as possible Bose-Einstein condensates [6, 7], have been initiated. The accuracy of interaction potentials is necessary for these investigations.

The interatomic potentials are also necessary in the studies of new materials, atomic and molecular collisions. Usually, *ab initio* method is used to calculate the van der Waals potential of dimers, but it is very complicated, time consuming and difficult to apply to complex systems, so a relatively simple and reliable method of calculation is necessary.

Tang-Toennies (TT) potential model [8] is a relatively simple analytic function. It has been used to calculate a lot of two-atom interaction potentials successfully, such as recently to the van der Waals potentials of mercury [9, 10] and group IIA systems [11–13].

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In this paper, the repulsive part of the TT model is modified based on the physical nature of the interatomic interaction. This modified TT potential model (MTT) can describe entire part, especially the short-range repulsive part of Ar–Ar potential correctly.

2 Tang-Toennies potential model

In 1984, Tang and Toennies [8] proposed a potential model which consists of the sum of the short range repulsive Bon-Mayer potential Ae^{-bR} and the long range attractive potential of the damped asymptotic dispersion series

$$V(R)=Ae^{-bR}-\sum_{n=3}^{N_{\max}} f_{2n}(bR)\frac{C_{2n}}{R^{2n}}, \tag{1}$$

where R is the internuclear distance, A and b are the parameters of the Born-Mayer repulsive potential, C_{2n} are the dispersion coefficients, and $f_{2n}(bR)$ is the damping function

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

For many systems, the first three coefficients C_6, C_8 and C_{10} are available, higher accuracy additional terms can be generated by the recurrence relation

$$C_{2n}=\left(\frac{C_{2n-2}}{C_{2n-4}}\right)^3 C_{2n-6}. \tag{3}$$

3 The modified Tang-Toennies potential model

In 1995, K. T. Tang [14] obtained an exchange energy for two-atom systems based on a surface integral method [15]. This method calculates the exchange energy by a surface integral which accounts for the flux of electrons flowing from one atom to another. The analytical expression of this exchange energy is $TR^{7/2\beta-1}e^{-2\beta R}$, where T is the amplitude of the atom wave function, it may be calculated by a highly accurate CI calculation, $\beta=\sqrt{2\epsilon}$, with ϵ is the ionization energy of the atom. Since the exchange energy is the mainly contribution to the repulsive potential, we found that using $TR^{7/2\beta-1}e^{-2\beta-1}e^{-2\beta R}$ to replace $A\exp(-br)$ in the TT model and adjusting T and β by the experimental well depth and equilibrium distance R_e, the entire ground state potential curve of the argon dimer can be accurately described. We call this modified TT potential model as MTT model, that is

$$V(R)=TR^{7/2\beta-1}\exp(-2\beta R)-\sum_{n\geq 3}^{N_{\max}}\Big(f_{2n}(bR)\Big)\frac{C_{2n}}{R^{2n}}, \tag{4}$$