Few Helium Atoms in Quasi Two-Dimensional Space

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Abstract

Two, three and four ^3He and ^4He atoms in quasi two-dimensional space above graphite and cesium surfaces and in "harmonic" potential perpendicular to the surface have been studied. Using some previously examined variational wave functions and the Diffusion Monte Carlo (DMC) procedure, it has been shown that all molecules: dimers, trimers and tetramers, are bound more strongly than in pure two- and three-dimensional space. The enhancement of binding with respect to unrestricted space is more pronounced on cesium than on graphite. Furthermore, for $^3He_3$ ($^3He_4$) on all studied surfaces, there is an indication that the configuration of a dimer and a "free" particle (two dimers) may be equivalently established.

Key words: helium molecules; binding in quasi 2D space; dimerization

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1. Introduction

Few interacting helium atoms may be thought of as models for real many-body systems in a specific physical environment. Besides this, they form exotic molecules: dimers, trimers and tetramers, which are interesting physical systems in themselves as well. Helium molecules in infinite space have been the subject of research since the sixties. After experimental detection of helium 4 dimers and trimers [1], further consideration of these systems was initiated. It is shown that ^4He_N is bound for any N in three-dimensions (3D) [2]. Due to a smaller mass and the Pauli principle, it takes at least 35 atoms of ^3He to form a bound state in 3D [3].

In 2D space, which serves as a model for helium atoms on smooth strongly binding substrates, some molecules are bound more strongly than in 3D [4]. Furthermore, variational calculations have showed that both ^3He dimer and trimer are bound in 2D [5]. Quite recently, using the Monte Carlo (MC) procedure, the binding of helium trimers and tetramers in infinite 2D, in confined 2D, and quasi-2D space has been demonstrated [6]. In this paper, we enlarge our previous research of two, three and four helium atoms and study their behaviour in quasi two-dimensional space above graphite and cesium and in "harmonic" substrates. In particular, we obtain binding energies and structures of these exotic systems.

2. Basic expressions, results and discussion

The hamiltonian of our systems reads

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{n}\Delta_i + \sum_{i<j=1}^{n} V(r_{ij}) + \sum_{i=1}^{n} V_{ext}(r_i) \qquad (1)$$

where, with the corresponding mass and $n = 2, 3, 4$, hamiltonian is adapted to the molecules of two, three and four helium atoms. For interaction potential $V(r_{ij})$ we take the one by Korona et al. [8]. $V_{ext}(r_i)$ is an external holding potential and three types of it are considered independently: 1. graphite [9] , 2. cesium [10] and 3. "harmonic" $V_{ext}(z) = m\omega^2 z^2/2$ with variable width $a = (\hbar/m\omega_0)^{\frac{1}{2}}$. We use the trials which combine the products of the two-body Jastrow-

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Table 1
The helium molecules binding energies (in mK) in quasi-2D infinite space. Results ^{a} are taken over from [7]

molecule	harmonic (a=3Å)	graphite	cesium
$^3He_2$	-8.25^a	-0.053(7)	-6.2(3)
$^4He_2$	-101.84^a	-43(2)	-101(4)
$^3He_3$	-9.1(5)	-0.022(7)	-6.2(3)
$^4He_3$	-489(3)	-188(3)	-452(5)
$^3He_4$	-18(1)	-0.05(2)	-12.9(4)
$^4He_4$	-1200(20)	-477(5)	-1040(10)

Feenberg-Bruch (JFB) correlation functions and one-particle wave functions on the appropriate substrate [6]:

$$\Psi_0 = \prod_{i<j}^{n} F(r_{ij}) \prod_{i=1}^{n} \phi(z_i), \qquad for\ \ bosons \qquad (2)$$

$$\Psi \ = \ X(spin, space)\ \Psi_0\ , \qquad for\ \ fermions; \quad (3)$$

the explicit forms of the functions $F(r)$, $X(spin, space)$ and $\phi(z_i)$ in cases of graphite and harmonic potential are cited in paper [6]. For cesium, the single-particle functions are obtained by solving the differential equation of a single particle in that potential and by fitting the obtained data set with the function

$$\phi(z) = exp\left[-\left(\frac{a_2}{z}\right)^{a_3} - a_4 z^{a_5}\right].$$

In extensive MC calculations which have been performed in two successive stages, simple variational MC and DMC, we have obtained ground state energies and distribution functions. For fermions we have used fixed-node DMC. Some of the results are presented in Table 1 and in Figures 1 and 2. Errorbars on these Figures range from 2-8%.

Our results show that helium molecules in quasi-2D real space above graphite are more bound than in pure infinite 2D space. In the study of the binding of helium dimers in a model harmonic potential, the strongest binding was obtained for $a \approx 3$Å[7]. Similar enhancement of binding is observed here for trimers and tetramers. The binding energies above cesium are comparable with those for the harmonic potential ($a = 3$Å). All molecules are floppy but not as large as in pure 2D space. Above all considered substrates, the energy of ^{3}He trimers is close to the dimer energy, and the energy of ^{3}He tetramers is close to twice the dimer energy; this is the indication of a kind of dimerised structure. The same behaviour is confirmed by the formation of two maximums in the pair distribution function (Fig. 2).

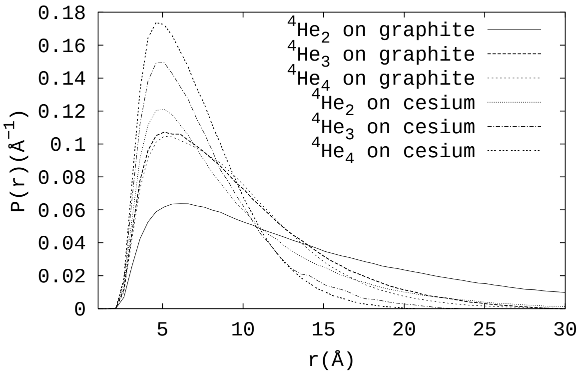

Fig. 1. The pair distribution function for ^{4}He dimers, trimers and tetramers on graphite and cesium. $\int P(r)dr = 1$

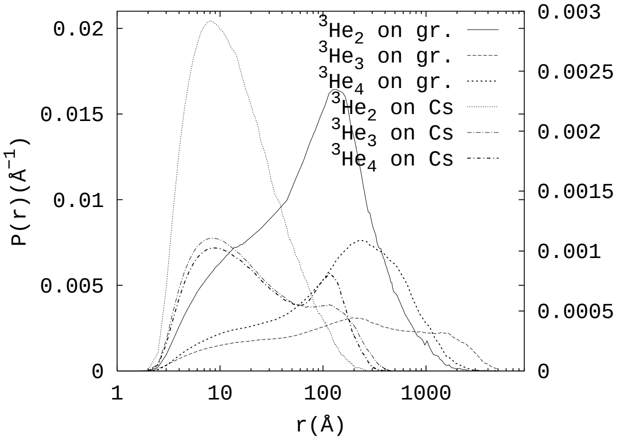

Fig. 2. The same as Fig.1 for ^{3}He dimers, trimers and tetramers on graphite (right scale) and cesium (left scale) .

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