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ATOMS, MOLECULES, OPTICS

MOLECULES OF REPELLING ATOMS ADSORBED ON SURFACES AND THREADS

© 2024 A. V. Maksimychev[a*], L. I. Menshikov[a, b**], P. L. Menshikov[a, b***]

[a]National Research University MPTI 141701, Dolgoprudny, Moscow region, Russia
[b] National Research Centre Kurchatov institute 123182, Moscow, Russia
*e-mail: maksimychev.av@mipt.ru
** e-mail: mleonid1954@mail.ru
*** e-mail: menshikov2005@mail.ru

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Abstract. The interaction of two slow atoms adsorbed on a surface or thread is considered. It is shown that, for any sign of the scattering length, this system has a bound state. In particular, such a state exists for two atoms with interaction in the form of a spherical potential with an infinitely high wall.

Keywords: *zero radius potential, bound states of atoms, quasimolecule, adsorption, scattering length, Efimov effect*

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1. INTRODUCTION

One of the unexpected results of quantum mechanics is the Efimov effect — the presence of bound states in a system of three repulsive particles [1] (see also works [2–5]). In this article, which is a further development of work [6], a similar phenomenon is indicated: the possibility of the existence of a bound state (van der Waals molecule) of repulsive atoms adsorbed on a surface or filament, acting as a third body.

In work [6], a pair of such atoms with mass m, interacting with the surface through an oscillator potential

$$u(z) = m\omega^2 z^2 / 2$$

was considered (z-axis is directed perpendicular to the surface).

It is known [7] that the scattering length a is the only parameter that determines the interaction of two atoms at low energy. Based on this, to describe the motion of atoms, the authors applied in [6] the method of zero radius potentials [8], i.e., imposed a boundary condition on the wave function (WF) of the atom pair

$$\lim_{r\to 0}\left(\frac{1}{\varphi}\frac{\partial\varphi}{\partial r}\right) = \gamma. \tag{1}$$

Here

$$\varphi = r\psi, \quad \gamma = -1/a,$$

$$r = |\mathbf{r}|, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 = (z, \rho),$$

$z = z_1 - z_2, \rho = (x_1 - x_2, y_1 - y_2)$ is a two-dimensional vector characterizing the relative motion of atoms along the surface. According to [6], the dissociation energy of the adsorbed molecule equals

$$D = \kappa^2,$$

where κ is determined from the equation

$$f(\kappa) = \gamma. \tag{2}$$

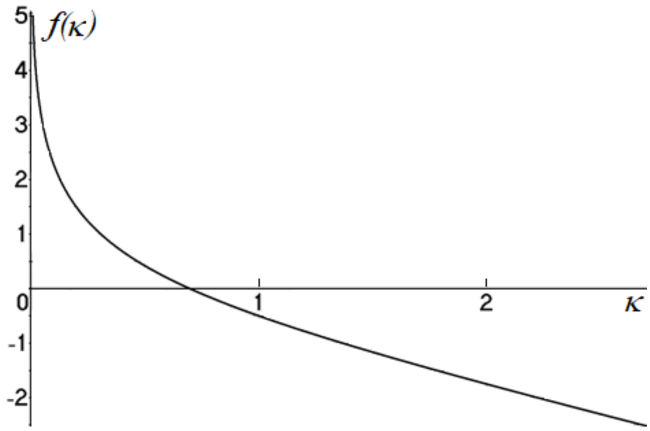

Fig. 1. Graph of function $f(\kappa)$ from (2)

The graph of function $f(\kappa)$ is shown in Fig. 1 (here and further we use units $\hbar = m = \omega = 1$).

From formula (2) and Fig. 1, it is evident that the bound state exists for any sign of γ, despite the fact that for $\gamma > 0$ (in paper [6] this case is called repulsion) such states do not exist for a pair of atoms in free space. Paper [9] considers attractive interaction between atoms in the form of a spherical well

$$V(r) = -u_0\theta(r_0 - r),$$

where $u_0 > 0$, θ – is the Heaviside function. It is indicated that depending on the parameter values u_0 and r_0, both cases $\gamma > 0$, and $\gamma < 0$. are possible. Hence, it is clear that the case $\gamma > 0$ does not always correspond to repulsion. It is clear, however, that $\gamma > 0$ can also correspond to explicit repulsion of atoms. Let's demonstrate this using an example of a definitely repulsive interaction

$$V(r) = +u_0\theta(r_0 - r). \qquad (3)$$

2. HARD SPHERE APPROXIMATION FOR ADSORPTION ON A PLANE

For a pair of free slow atoms, it is sufficient to consider s-wave. In their center of mass system

$$\varphi(r) = A\mathrm{sh}(qr), \quad r < r_0,$$

$$\varphi(r) = \sin[k(r - r_0) + \eta], \quad r > r_0.$$

Here k^2 is the kinetic energy of relative motion of atoms, $q = \sqrt{u_0 - k^2}$. Wave function matching at the boundary gives

$$\eta = \frac{q}{k}\mathrm{cth}(qr_0). \qquad (4)$$

At $r > r_0$ we get

$$\frac{\varphi'}{\varphi} = k[k(r - r_0) + \eta].$$

Condition $r \to 0$ in (1) should now be understood as $r \ll 1/k$. From (1) and (4) we obtain

$$\lim_{r\to 0}\frac{\varphi'}{\varphi} = k\cdot(-kr_0 + \eta). \qquad (5)$$

Statements [6] are valid if

$$\gamma(\kappa) = \mathrm{const}. \qquad (6)$$

This is satisfied at

$$kr_0 \ll 1,\ k \ll q_0, \qquad (7)$$

where $q_0 = \sqrt{u_0}$. In this case

$$\gamma = q_0\mathrm{cth}(q_0 r_0). \qquad (8)$$

Thus, if (6) is satisfied, which is true under conditions (7), then according to the conclusions of paper [6], even in case (3) there exists a bound state of the adsorbed quasi-molecule.

The value k corresponds to distances between atoms $r \sim 1/k$. For motion along the axis x $r \sim 1$, therefore from (7) we obtain the conditions for validity of this work's conclusions:

$$r_0 \ll 1,\ q_0 \gg 1, \qquad (9)$$

or, in conventional units,

$$r_0 \ll \sqrt{\frac{\hbar}{m\omega}},\ u_0 \gg \hbar\omega \qquad (10)$$

From (8) and (9) we conclude

$$\gamma > q_0 \gg 1. \qquad (11)$$

According to [6], in this limiting case

$$\mathrm{k} \sim \exp\left(-\gamma\sqrt{\frac{\pi}{2}}\right), \qquad (12)$$

therefore, considering (11), we come to the conclusion that the quasi-molecule size, determining the characteristic distance for longitudinal motion, is large and equals

$$r \sim \frac{1}{k} \sim \exp\left(\gamma\sqrt{\frac{\pi}{2}}\right) \gg 1.$$

Thus, for longitudinal motion, the conditions for satisfying (7) are less stringent compared to (10):

$$r_0 \ll \sqrt{\frac{\hbar}{m\omega}} \cdot \exp\left(\gamma\sqrt{\frac{\pi\hbar}{2m\omega}}\right),$$

$$u_0 \gg \hbar\omega \exp\left(\gamma\sqrt{\frac{\pi\hbar}{2m\omega}}\right),$$

The second condition (10) is typically satisfied under typical conditions, and the first one is the most stringent. Based on the known stability of bound states in two-dimensional and one-dimensional systems, it can be stated that such states can exist in case (3).

3. ADSORPTION ON A FILAMENT

Now let's direct the axis z along the filament, and for the adsorption potential, we'll again adopt the oscillator approximation

$$u(\rho) = \rho^2 / 2, \quad \rho^2 = x^2 + y^2.$$

According to formula (8) from work [6], the WF of relative motion of atoms is given by the expression

$$\psi(\mathbf{r}) \propto G(\mathbf{r}),$$

where $G(\mathbf{r})$ is found from the equation

$$\left(-\Delta_r + \frac{1}{4}\rho^2 - 1 + \kappa^2\right)G(r) = \delta(x)\delta(y).$$

Now we need to perform a Fourier transform over z, after which, similar to [6], we obtain, omitting constant factors

$$\psi = \int_0^\infty \frac{d\tau}{\sqrt{\tau}(1 - e^{-2\tau})} \exp\left(-\kappa^2\tau - \frac{1}{4}\rho^2 cth\tau - \frac{z^2}{4\tau}\right).$$

When substituting into (1) here we can set $\rho = 0$, so that $r = |z|$, and also apply the identity

$$\frac{1}{1 - e^{-2\tau}} = \frac{1}{2\tau} + \left(\frac{1}{1 - e^{-2\tau}} - \frac{1}{2\tau}\right).$$

The integral of the first term is solved analytically and equals

$$\frac{\sqrt{\pi}}{r} e^{-kr} \approx \sqrt{\pi}\left(\frac{1}{r} - \kappa\right).$$

The second term is non-singular, and we can set $z = 0$. in it. This gives for the filament equation (2), in which

$$f(\kappa) = -\kappa + \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{d\tau}{\sqrt{\tau}} e^{-k^2\tau} \left(\frac{1}{1 - e^{-2\tau}} - \frac{1}{2\tau}\right).$$

The graph of this function is similar to that shown in Fig. 1, i.e., again the solution (2) exists for any sign of γ. For large γ instead of exponential smallness (12), characteristic for the two-dimensional case, we obtain power-law smallness of binding energy $\kappa \approx 1 / \gamma$.

4. CONCLUSIONS

From the above, we conclude that restricting the motion of atoms in one or two directions can lead to the appearance of a bound state absent in a pair of free atoms or to an increase in the binding energy of the quasi-molecule they already form.

Let's apply our model to describe experiments [10–12] with a two-dimensional gas of spin-polarized hydrogen atoms adsorbed on the surface of liquid helium.

For the applicability of the zero-radius potential approximation (1), it is required that the characteristic size of r_0 pair interaction $u(r)$ between hydrogen atoms in the triplet state should be small compared to both the amplitude of z_{ads} atomic oscillations in the adsorption potential (r_0 / z_{ads} = 1), and the characteristic de Broglie wave length of hydrogen atoms under experimental conditions [10–12], that is $kr_0 \ll 1$, where $k \sim \sqrt{2mT} / \hbar$ is the characteristic wave vector of hydrogen atoms with mass m. The experiments were conducted at temperature $T \sim 0.15$ K, therefore $k \sim 6 \cdot 10^6$ cm^{-1}. According to [13], at

$$r_0 = 7.85a_0, \tag{13}$$

where a_0 is the Bohr radius, the potential energy $u(r)$ has a minimum $u(r_0) = -u_0$, where $u_0 = 6.2$ K. In this adsorption potential, hydrogen atoms have only one bound state with binding energy $E_q = 1.14$K [14]. From this, we conclude that

$$z_{ads} \sim z_{in} + z_{out} \sim 20a_0,$$

where $z_{\text{in}} \sim 10a_0$ is the characteristic oscillation amplitude in the classically accessible region of hydrogen atoms motion in the adsorption state and $z_{out} \sim \hbar / \sqrt{2mE_a} \sim 10a_0$ is the characteristic depth of their penetration under the potential barrier in the classically inaccessible region of motion. Thus,

$$r_0 / z_{ads} \sim 0.3 \tag{14}$$

Taking (13) as the characteristic size of pair interaction between hydrogen atoms in the triplet state, we obtain

$$kr_0 \sim 0.2 \tag{15}$$

We should add that condition (15) also allows us to neglect the correction terms $\sim kr_0$ to formula (1) (see [15], as well as formulas 133.9, 133.10, and 133.14 from work [16]).

Within our adopted oscillator approximation for the adsorption potential, the distance from the adsorption level to the bottom of the well should be equal to $\hbar\omega/2$. According to the data provided above, it amounts to $u_0 - E_a \approx 5$ K, which corresponds to $\omega \approx 1.3 \cdot 10^{12}$ s^{-1}. From this, we find the unit of length used in calculations:

$$L = \sqrt{\frac{\text{h}}{m\omega}} \approx 4a_0.$$

The scattering length of hydrogen atoms in the state with total spin $S = 1$ equals $a \approx 1.2a_0$ [17]. In our units, this equals $a \approx 0.3$, which corresponds to

$$\gamma = -\frac{1}{a} \approx -3.3.$$

From Fig. 1, we conclude that $k \approx 2.5$, therefore the binding energy of the adsorbed quasi- molecule equals

$$D = \hbar\omega \cdot \text{k}^2 \approx 60\text{K}$$

As noted in work [6], this conclusion may indicate the instability of Bogoliubov two-dimensional Bose-condensates obtained in experiments [10–12], formed by hydrogen atoms adsorbed on the surface of liquid helium

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