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THE MOLECULE OF TWO ^{4}He ATOMS

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ABSTRACT

The possibility of existence of a bound state of two ^{4}He atoms is considered by making use of variational method based on asymptotic wave functions at small and large interatomic distances. The result is negative.

1. INTRODUCTION

The system of ^{4}He atoms is extensively investigated during a long period of time. The reasons for this are exceptional properties of the system. Due to weak attractive interaction and relatively small mass the system does not have a solid state. The investigations are mostly concentrated on large homogeneous system. The existence of a bound state of a small number of ^{4}He atoms is not investigated. One of the first questions in this sense is the existence of a molecule of two ^{4}He atoms. E. Feenberg has mentioned in [1] that such a molecule exists. In this article we consider this problem on the basis of asymptotical properties of weve functions at small and large interatomic distances. Having known these asymptotic functions we formulate a variational ansatz and evaluate the expectation value of energy.

In Section 2 we consider the linear system and show that a bound state very likely doesn't exist. Section 3 contains three dimensional motion and solutions of two-particle wave equation for small and large interatomic distances. In Section 4 we formulate the variational ansatz for the ground state wave function and evaluate the expectation value of the energy. In last Section we give comments.

2. THE LINEAR MOTION OF TWO ^4He ATOMS

In order to get insight in the problem we consider at the beginning linear motion of this system.

The interaction between two ^4He atoms we take to be given by Yntema-Schneider [2]. A particular choice of existing potentials is of no importance for our analysis. The Yntema--Schneider potential is

$$V(r) = A e^{-\alpha r} - \frac{a}{r^6} - \frac{b}{r^8} , \tag{2.1}$$

where $A=1200\cdot10^{-12}$ ergs, $\alpha = 4,717(\text{Å})^{-1}$, $a= 1,24\cdot10^{-12}$ ergs, $b = 1,89\cdot10^{-12}$ ergs and r is given in Å.

For linear analysis this potential can be substituted by the Morse potential

$$V(x) = D\left(e^{-2\beta x} - 2e^{-\beta x}\right)$$

or in our case

$$V(x) = D\left[e^{-2\beta(x-a)} - 2e^{-\beta(x-a)}\right], \tag{2.2}$$

where D, β, a are constants which have to be determined from the Yntema-Schneider potential. We take $2\beta = \alpha$, $D = -V_{min}^{Y-S}$, $a = r_{min}$ of the Yntema-Schneider potential. These values are $\beta = 2,358\cdot10^{8}\,cm^{-1}$, $D= 11,31\cdot10^{-16}$ ergs and $a = 3,00\cdot10^{-8}$ cm.

The Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + V(x)\right]\varphi(x) = E\varphi(x), \tag{2.3}$$

where $\mu = 1/2\, M_{^4He}$ is reduced mass, can be exactly solved.

The substitution

$$\xi = \frac{2\sqrt{2\mu D}}{\beta\hbar}\, e^{-\beta(x-a)}$$

gives

$$\varphi'' + \frac{1}{\xi}\varphi' + \left(-\frac{1}{4} + \frac{n+s+\frac{1}{2}}{\xi} - \frac{s^2}{\xi^2}\right)\varphi = 0 \qquad (2.4)$$

where

$$s = \frac{\sqrt{-2\mu E}}{\beta\hbar}\ , \quad n = \frac{\sqrt{2\mu D}}{\beta\hbar} - \left(s+\frac{1}{2}\right).$$

The solution of (2.4) is given in [3]. The energy spectrum is

$$E_n = -D\left[1 - \frac{\beta\hbar}{\sqrt{2\mu D}}\left(n+\frac{1}{2}\right)\right]^2 . \qquad (2.5)$$

If

$$\frac{\sqrt{2\mu D}}{\beta\hbar} < \frac{1}{2} \qquad (2.6)$$

there is no bound state. The left side of (2.6) for the potential (2.2) is 0,35 . From this we conclude that there is no bound state for linear motion of two ^{4}He atoms.

The substitution of the Yntema-Schneider potential by the Morse potential is not quite correct. However, the value of $\frac{\sqrt{2\mu D}}{\beta\hbar}$ is so small that one can not expect something else from a better calculation.

3. ASYMPTOTIC WAVE FUNCTIONS

The stationary states of three dimensional motion of two ^{4}He atoms are determined by

$$\left[-\frac{\hbar^2}{2\mu}\Delta + V(r)\right]\psi = E\,\psi(r)\ , \qquad (3.1)$$

where r is the relative coordinate and μ is reduced mass.

In the limit $r \to 0$ we have

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + A e^{-\alpha r}\right]\psi_{r\to 0} = 0\ . \qquad (3.2)$$

The solution of this equation is [4]

$$\Psi_{r\to 0}(r) = \text{const}\cdot e^{-Be^{-\frac{\alpha}{2}r}} , \tag{3.3}$$

where

$$B = \frac{2\sqrt{MA}}{\hbar\alpha} \tag{3.4}$$

Therefore, (3.3) gives the short-range asymptotic wave function.

In the limit $r \to \infty$ Eq (3.1) becomes

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\Psi_{r\to\infty} = E\,\Psi_{r\to\infty} . \tag{3.5}$$

The solution of this equation is

$$\Psi_{r\to\infty} = \text{const}\cdot e^{-\gamma r} , \tag{3.6}$$

where $\gamma = \frac{\sqrt{-2\mu E}}{\hbar}$, ($E<0$). Therefore, $\Psi_{r\to\infty}$ given by (3.6) is long range wave function. Inthe next we take these two asymptotic wave functions for the construction of a variational ansatz.

4. THE VARIATIONAL CALCULATION OF THE GROUND STATE ENERGY

Having known the asymptotic wave functions at small and large interatomic distances we write the variational ground state wave function in the form

$$\Psi_0(r) = N\, e^{-Be^{-\frac{\alpha}{2}r}}\, e^{-sr} , \tag{4.1}$$

where N is the constant of normalization and s is the variational parameter.

The expectation value of the Hamiltonian of the problem

$$H = -\frac{\hbar^2}{2\mu}\Delta + V(r)$$

for $\psi_0(r)$ is

$$\bar{E}_0(s) = \frac{\int \psi_0^*(r)\, H\, \psi_0(r)\, d\vec{r}}{\int \psi_0^*(r)\, \psi_0(r)\, d\vec{r}} \qquad (4.2)$$

or

$$\bar{E}_0(s) = \frac{J_1(s)}{J_2(s)}$$

where

$$J_1 = \int_{r_0}^{\infty} r^2 e^{-2Be^{-\frac{\alpha}{2}r} - 2sr} \cdot \left\{ -\frac{\hbar^2}{M} \cdot 10^{16} \left[s^2 - \right.\right.$$

$$\left. - B\alpha s e^{-\frac{\alpha}{2}r} - \frac{B\alpha^2}{4} e^{-\frac{\alpha}{2}r} + \frac{2}{r}\left(\frac{B\alpha}{2} e^{-\frac{\alpha}{2}r} - s\right)\right] -$$

$$\left. - \frac{a}{r^6} - \frac{b}{r^8} \right\} dr \,,$$

$$\mathcal{J}_2 = \int_{r_0}^{\infty} r^2 e^{-2Be^{-\frac{\alpha}{2}r} - 2sr} dr ,$$

and r_0 is radius of the ^{4}He atom.

The integrals $\mathcal{J}_1$ and $\mathcal{J}_2$ are evaluated nummericaly for various s .

The results are presented in the Fig. 1.

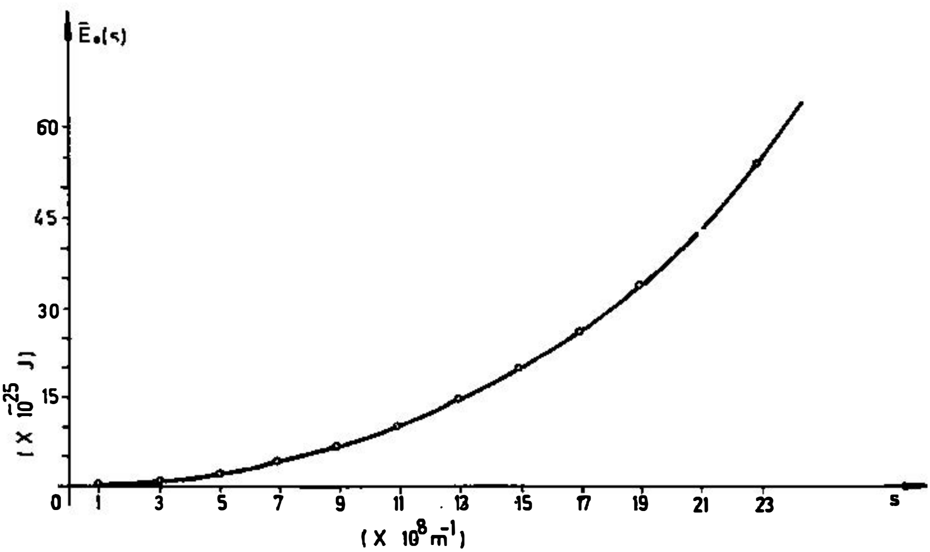

Fig. 1.

5. CONCLUSIONS

We conclude that there is no bound state of two ^{4}He atoms.

The given analysis is approximative. However, it contains correct properties of the wave functions at small and large interatomic distances. Due to this fact we dor't expect changes in the final result in any better calculation. Therefore, we tend to conclude that there is no bound state of two ^{4}He atoms.

There is also no experimental evidence of $(^4\mathrm{He})_2$ molecule.

References

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MOLEKULA OD DVA ATOMA ^4He

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Sadržaj

Razmatran je problem postojanja vezanog stanja od dva ^4He atoma. Najprije je analizirana jednodimenzionalno kretanje posredstvom Morseovog potencijala i nadjeno je da tada nema vezanog stanja.Zatim je razmotreno trodimenzionalno kretanje upotrebom varijacione metode u kojoj je varijaciona funkcija osnovnog stanja konstruisana posredstvom asimptotske valne funkcije na malim i velikim medjuatomskim udaljenostima.

Za tako odredjenu valnu funkciju izračunata je očekivana vrijednost hamiltonijana i ona je minimizirana s obzirom na varijacioni parametar.

U ovom postupku nadjeno je da ne postoji molekula od dva ^4He atoma. Budući da postupak sadrži ispravna asimptotska svojstva valne funkcije na velikim i malim udaljenostima, mi smo skloni da zaključimo da ni bilo koji bolji račun neće izmjeniti konačni rezultat.