

THE MOLECULE OF TWO He³ ATOMS

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ABSTRACT.

The bound state of two He³ atoms is considered by making use of variational method. It is found that such a molecule exists. The cohesion energy is of order $-0,4689 \cdot 10^{-19}$ ergs.

Liquid He³ is extensively investigated. However, the knowledge of systems with small number of He³ atoms is poor. One of the first question is the existence (He³)₂ molecule. The subject of this paper is the analysis of this problem.

The stationary states of two He³ atoms are given by

$$\left[-\frac{\hbar^2}{2\mu} \Delta + V(r) \right] \psi(r) = E \psi(r) \quad (1)$$

where μ is reduce mass ($\mu = 1/2 M_{\text{He}^3}$) and

$$V(r) = A e^{-\alpha r} = \frac{a}{r^6} - \frac{b}{r^8} \quad (2)$$

with $A = 1,2 \cdot 10^{-9}$ ergs, $\alpha = 4,717 \cdot 10^8 \text{ cm}^{-1}$, $a = 1,24 \cdot 10^{-12}$ ergs, $b = 1,89 \cdot 10^{-12}$ ergs and r is given in Å [1].

We investigate the ground state by making use the variational method. The variational ansatz we construct by means of asymptotic wave functions at small and large interatomic distances [2]:

$$\psi_0(r) = N e^{-\beta e^{-\frac{1}{2}r} - \gamma r} \cdot \varphi(r_1, r_2) \quad (3)$$

where γ is the variational parameter and $\varphi(r_1, r_2)$ is antisymmetric spin wave function.

The expectation value of the Hamiltonian

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

for the wave function (3) is

$$\bar{E}_0(r) = \frac{J_B(r)}{J_N(r)}, \quad (4)$$

where are

$$J_B(r) = -\frac{\hbar^2}{M} \cdot 10^{16} \int_{r_0}^{\infty} r^2 e^{-2Be^{-\frac{d}{2}r} - 2\gamma r} \cdot$$

$$\cdot \left[(\gamma^2 - B d \gamma e^{-\frac{d}{2}r} - \frac{B d^2}{4} e^{-\frac{d}{2}r}) + \frac{2}{r} \left(\frac{B d}{2} e^{-\frac{d}{2}r} - \gamma \right) - \frac{a}{r^6} - \frac{b}{r^8} \right] dr$$

$$J_N(r) = \int_{r_0}^{\infty} r^2 e^{-2Be^{-\frac{d}{2}r} - 2\gamma r} dr. \quad (5)$$

The integrals (5) were evaluated numerically. The minimum of $\bar{E}_0(r)$ is at $\gamma = 8 \cdot 10^4 \text{ cm}^{-1}$ and with the value $-0,4689 \cdot 10^{-19}$ ergs.

From this result we conclude that there is the $(\text{He}^3)_2$ molecule. Due to very small cohesive energy of two He^3 atoms these atoms tend to form large bound systems (liquid He^3).

References

- [1] J.L.Yntema, W.G.Schneider, J. Chem. Phys. 18 (1950) 641.
- [2] S.M.Sunarić, FIZIKA (1976), submitted for press.