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Features of the structure of the self-consistent field of molecules in a liquid

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Abstract

The model of condensed matter is considered. In this model, the particles oscillate with a limited amplitude in a self-consistent field. Each particle moves in a certain local volume of the electromagnetic field, which is formed by the particles surrounding it. All particles are identical, the particle size is independent of temperature and external pressure. Collisions of molecules occur absolutely elastically, the RMS velocity in collisions is proportional to the temperature of the substance.

A numerical calculation of the interaction energy between molecules is performed on the basis of the spherically symmetric pair potential of Mi-Lennard-Jones. The total potential energy of a molecule in a local field is calculated in accordance with the principle of superposition.

The amplitudes of the motion of particles in the condensed state are much smaller than the average distances between their centers. The changing electromagnetic field is replaced by a stationary field averaged over time. The molecules that create this field are fixed in their oscillation centers (in equilibrium positions). The field parameters are determined by the interaction and arrangement of the particles, this field is self-consistent.

Calculations for one-, two- and three-dimensional models were performed. It is revealed that at small oscillation amplitudes, the center of each particle moves in the potential well. The average width of potential wells is equal to two amplitudes of limited oscillations. In this state, the particle system simulates a solid.

As the amplitude of the oscillations increases, the equilibrium position of each molecule becomes unstable. The resultant force of attraction from the surrounding particles tends to remove the central particle from the equilibrium position. This state of the system simulates fluid. In a fluid, the particles move relative to the positions of unstable equilibrium on potential "hills". The detected transformation makes it possible to explain the properties of the substance in the liquid state: the disordered arrangement of molecules, fluidity, the impossibility of the existence of a liquid at low temperatures and in the absence of external pressure.

In a liquid and in an amorphous substance, the arrangement of particles is disordered, but in a fluid the molecules move relative to the positions of unstable equilibrium, and in an amorphous substance the particles move in potential wells.

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