The structure and spectral properties of two-dimensional dipole systems

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Abstract. A molecular dynamics simulation of two-dimensional dipole systems was performed. The influence of particles dipole moment (PDM) on structures and spectral properties of the systems was analyzed. It was found that increase of PDM leads to qualitative changes in systems structure and spectrum. There is a critical ratio between temperature and PDM at which the system is polymerized. It was also shown that the spectral properties of the system are extremely sensitive to PDM.

1. Introduction

Processes occurring in condensed matter, especially in liquids, play an important role in modern engineering and technical issues [1]-[4]. However, despite the efforts made in this area complete theory about disordered states fluid and phase transition still does not exist. This is due to the fact that such theory must be able to describe the great variety of dynamic structures that can occur in condensed matter. Study of the liquid phase's properties, especially liquid water has received considerable attention. Water has several of anomalous properties. This is probably due to the fact that water molecules are connected by a network of hydrogen bonds can be formed in a very complex cluster groups, and various other structures. A large number of articles devoted to the study of structures that occur in liquid water (for example [5]-[7]).

Many studies in the field of condensed matter physics are performed by computer simulation in particular by molecular dynamics methods (MD). There are many models of water used in similar problems. For example review article [13] contains 46 different models of water. Most models of water are multisite. This allows more accurately reflect some of the properties of real water. However it also leads to a large amount of computer time necessary for calculation of interaction forces which imposes certain restrictions on the size of simulated system and simulation time.

There are a number of problems the study of which requires the simulation of large systems for long intervals of time. For example the existence of long-lived nanosized cavities in real water [11].

One of the simplest models of liquid is a system of particles interacting through Lennard-Jones potential (LJ) [8]. However, long-lived cavity in such systems is not observed. One of the features of water is the large dipole moment of the water molecule. Therefore there is a problem of investigating possibility that the existence of cavities is mainly due to the fact that the water molecules have a large dipole moment.

Therefore, it becomes necessary to perform a series of simulations of LJ systems the particles of

which have a dipole moment. This model is probably closest to the SSD model [12] excluding torsion forces. In this study the influence of PDM values on structure and spectral properties of the system was analyzed.

2. Description of the modelling process

The system consists of uniform spherical particles, the centers of which interact through LJ potential:

$$U(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

All particles have a fixed value of the dipole moment which contributes to the interaction energy of each i-th and k-th particle is given by expression:

$$_{pp} = \frac{1}{r^3}\left(\vec{p}_k * \vec{p}_j\right) - \frac{3}{r^5}\left(\vec{p}_k * \vec{r}\right)\left(\vec{p}_j * \vec{r}\right)$$

Where $\vec{p}_k$ and $\vec{p}_j$ - dipole moments of the i-th and k-th particle respectively, $\vec{r} = \vec{r}_k - \vec{r}_j$, $r = |\vec{r}|$. Modeling was performed in LJ units: $\sigma = 1$, $\varepsilon = 1$. The simulations were performed for two-dimensional systems with particle concentration $n = 0.8$. The initial velocity distribution was specified in accordance with the Maxwell distribution. The dipole moments of the system in the initial state are oriented randomly. Temperature of the system was maintained at T = 1, for this Brendstone thermostat was used. After setting the initial state of the system modeling was performed during $t = 100$ in LD units in order to obtain the equilibrium state. Then simulation of system was performed during $t = 500$ in LD units in order to obtain experimental data.

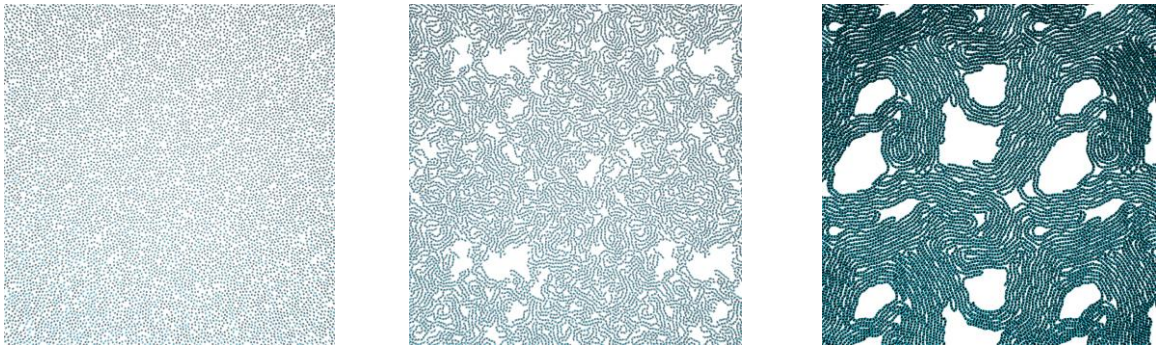
In the second phase of modeling at each simulation step calculation of average value of dipole moment $\langle\vec{p}_k(t)\rangle$, average speed of rotary motion of the particles $\Omega(t) = \langle\omega(t)\rangle$ and the quantities $P(t) = (\langle\vec{p}_k(t)\vec{p}_k(0)\rangle$ was performed (the brackets $\langle\ \ \rangle$ denote averaging over all systems particles).

The simulations were performed for different PDM values varying in the range from 0.1 to 2.5 in increments of 0.1 in LD units. The MD simulations are performed using the LAMMPS simulation package [9]. Visualization of the resulting structures was performed in the package VMD [10].

3. Results

Figure 1 shows snapshots of the systems structures obtained for different values of the PDM. System has a rather homogeneous structure at low values of PDM (Fig. 1a). Movement of particles leads to the appearance of cavities in systems structure. However they have relatively small size and very short lifetime. Increasing the value of PDM leads to changes in systems structure: lifetime of cavities increases significantly and their sizes increased up to a few interatomic distances (figure 1b). It is also possible to observe the formation of dipole chains, but they have very small length and lifetime. At some critical value of PDM occurs systems polymerization: stable long dipole chains are formed in system (figure3b). Also, there are large long-lived cavities in system.

Figure 2 shows the autocorrelation function (ACF) P (t) for systems with different values of PDM. It should be noted that form of ACF P (t) varies continuously when PDM changed in $p \lesssim 2.1$ region. However form of ACF P(t) varies discontinuously and oscillations P (t) become highly correlated when p ~ 2.1 which corresponds to system polymerization.



(a) **(b)** **(c)**

Figure 1. Snapshots of the system structure for different values of PDM: а – $p = 0.5$; б – $p = 1.5$; г – $p = 2.5$.

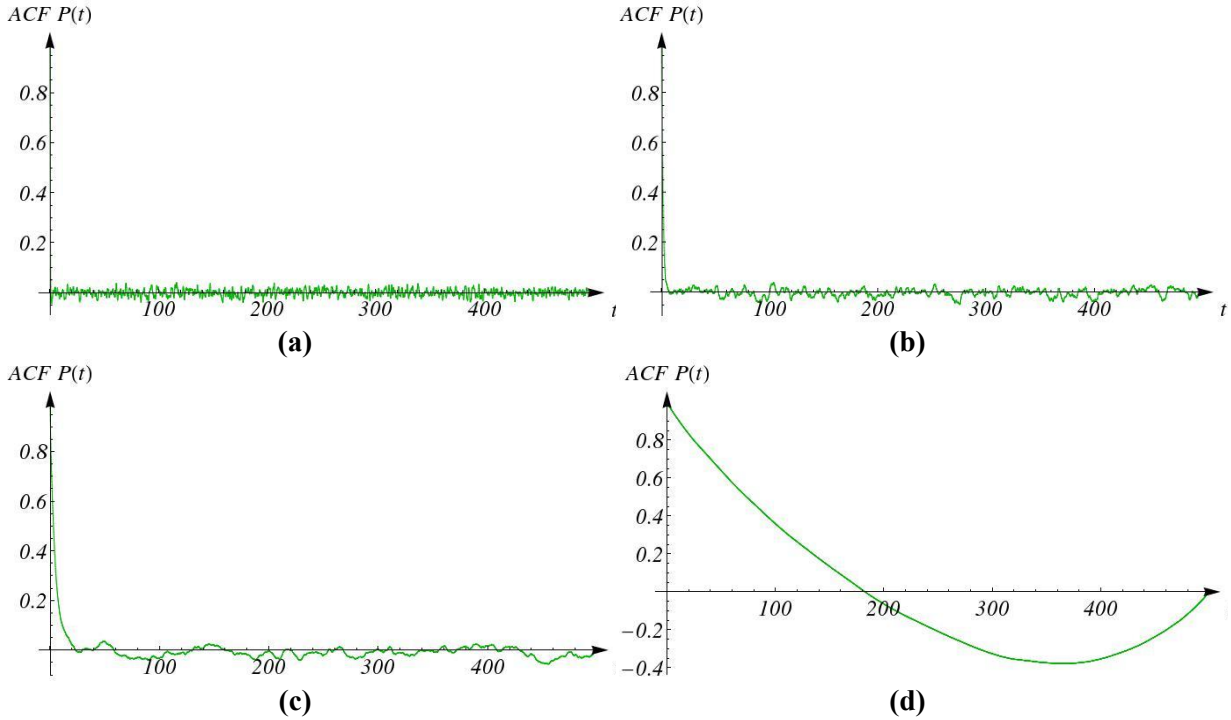


Figure 2. Autocorrelation functions of the P(t) for systems with different values of PDM: a – $p = 0.5$; b – $p = 1.5$; c – $p = 2.0$; d – $p = 2.5$

In figures 3-4 shows power spectrum of Ω (t) and P (t), respectively, for systems with different values of PDM. It can be seen that increasing of PDM values leads to a shift of the Ω(t) power spectrum into high-frequency region, while the P(t) power spectrum is shifted to lower frequencies.

Conclusions

Thus it was shown that the increase of PDM values leads to formation of long-lived cavities whose sizes are comparable with several interatomic distances. Also increasing of PDM values leads to a shift of the Ω(t) power spectrum into high-frequency region, while the P(t) power spectrum is shifted to lower frequencies. It has been shown that there is a critical ratio between the temperature and PDM values at which system is polymerized and ACF P(t) undergoes discontinuous change due to the fact that oscillations of the dipole moments become strongly correlated.

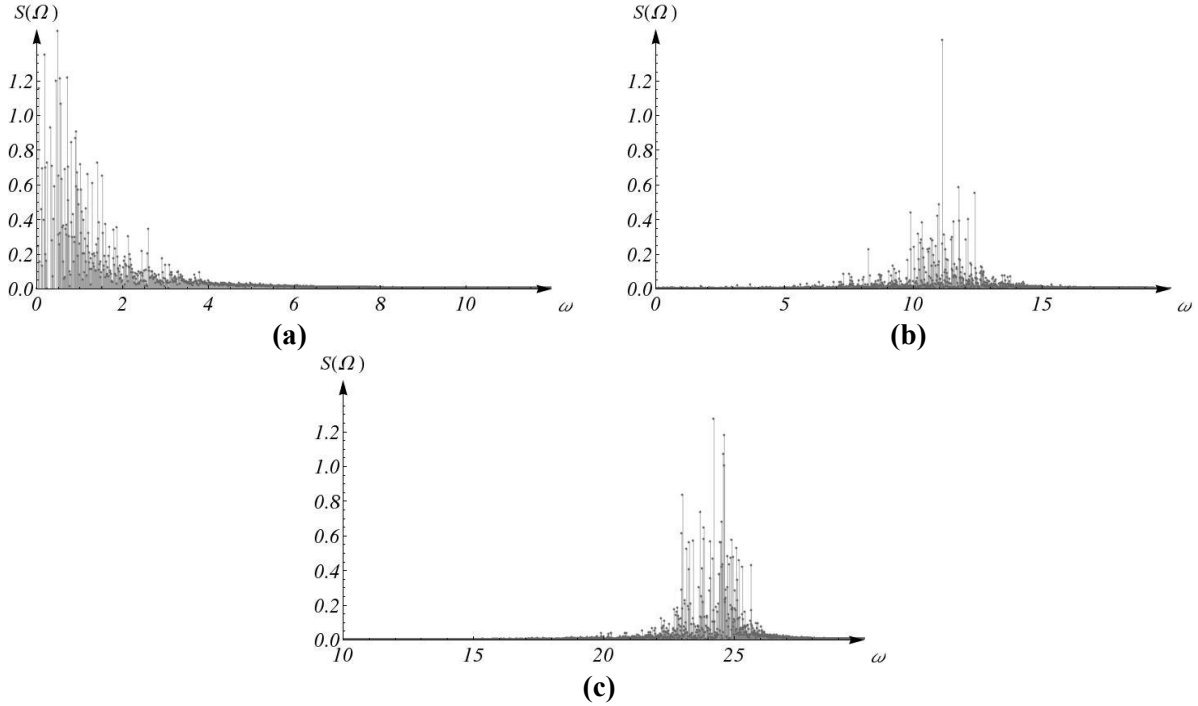


Figure 3. Power spectrum of Ω(t) for systems with different values of PDM: a - 0.5; b - 1.5; c - 2.5

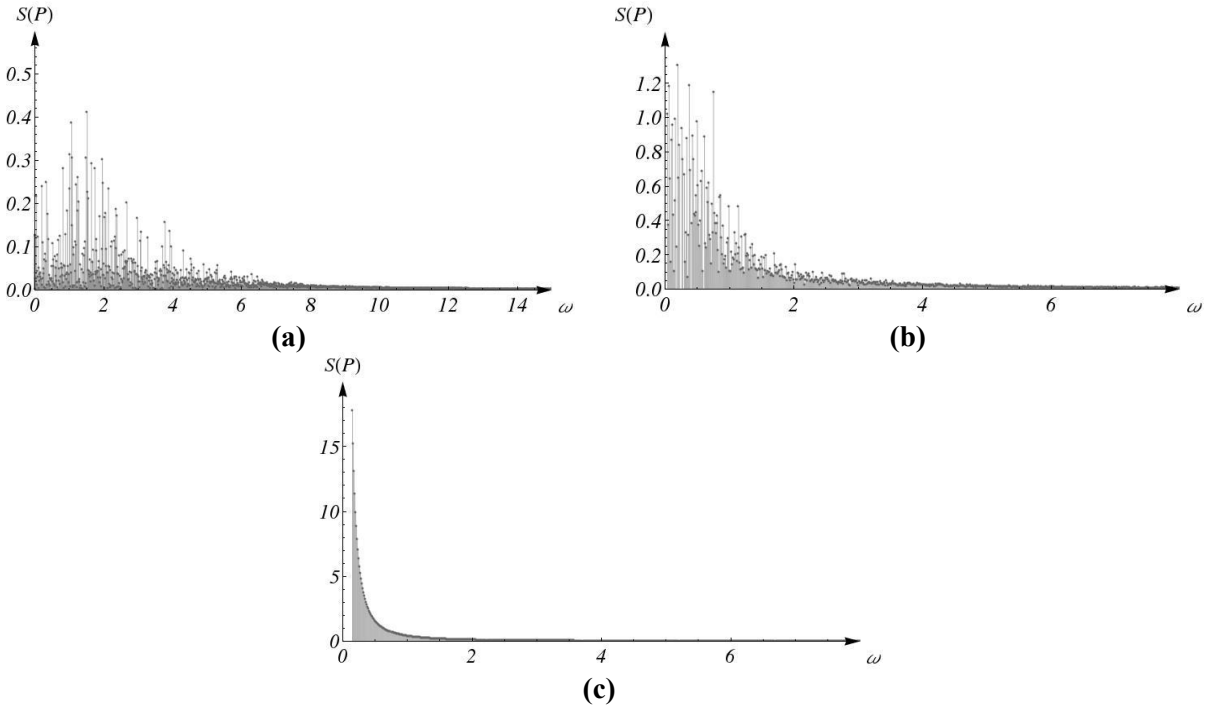


Figure 4. Power spectrum of P(t) for systems with different values of PDM: a - 0.5; b - 1.5; c - 2.5

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