was computed for the densities from $\rho = 0.1$ to $\rho = 1.0$ with the step of 0.1 for the isotherms $T = 0.04; 0.05; 0.06; 0.07; 0.1; 0.2; 0.3; 0.4; 0.5; 1.0; 2.0$. The calculation of the diffusion coefficient and excess entropy was carried in the same way as for Herzian spheres.

The last system considered in the present work is the continuous repulsive shoulder system introduced in the article [41]. The potential of this system has the form

$$U(r) = (\frac{\sigma}{r})^{14} + \frac{1}{2}\varepsilon \cdot [1 - tanh(k_0\{r - \sigma_1\})], \quad (8)$$

where $k_0 = 10.0$. As it was reported in the paper [45] this system demonstrates anomalous behavior due to its quasibinary nature. Here we extend the investigation of the diffusion anomaly in the repulsive shoulder system with $\sigma_1 = 1.35$ and check the Rosenfeld relations for this system in the anomalous region.

For the simulation of the repulsive shoulder system we used parallel tempering technic [68]. The details of the simulation were described in [45]. We computed the diffusion coefficients along different isochors starting from the density $\rho = 0.3$ to $\rho = 0.8$ with the step 0.05. A set of 24 temperatures between $T = 0.2$ and $T = 0.5$ was simulated. Taking into account the exchange of the temperatures at the same density more then a hundred runs at the same isochor was done. This allowed us to collect a good statistics on the temperature dependence of the diffusion coefficient. The diffusion coefficient along an isochor was approximated by a $9-$th order polynome of the temperature. The excess entropy was calculated in the way described above.

Usually excess entropy can be well approximated by the pair contribution only: $S_{ex} = S_{pair} + S_3 + ... \approx S_{pair}$, where

$$S_{pair} = -\frac{1}{2}\rho \int d\mathbf{r}[g(\mathbf{r})\ln(g(\mathbf{r})) - (g(\mathbf{r}) - 1)], \quad (9)$$

where ρ is the density of the system and $g(\mathbf{r})$ is the radial distribution function. We did not use the pair contribution to the excess entropy for the GCM and Herzian spheres because of the considerable overlap of the particles for the bounded potentials.

Since the potentials studied in the present work have negative curvature regions or are bounded they can not be approximated by an one component hard spheres system. It allows us to pose a question about the applicability of the entropy scaling to these systems both in Rosenfeld and Dzugutov forms. Note that Dzugutov relation (Eq. (5)) involves the size of the particles σ which is ill defined for the negative curvature and bounded potentials systems. This makes problematic to apply the Dzugutov scaling rule to them. Because of this only Rosenfeld relations were used in this work.

In this paper we use the dimensionless quantities: $\tilde{\mathbf{r}} = \mathbf{r}/\sigma$, $\tilde{P} = P\sigma^3/\varepsilon$, $\tilde{V} = V/N\sigma^3 = 1/\tilde{\rho}$, $\tilde{T} = k_BT/\varepsilon$. Since we use only these reduced units we omit the tilde marks.

III. RESULTS AND DISCUSSION

This section reports the simulation results for the diffusion coefficient and excess entropy of the three models described above and checks the validity of the Rosenfeld relation for these systems.

Herzian spheres

Low temperature behavior of the diffusion coefficient of Herzian spheres system was already reported in the work [67]. As it is seen from this publication the diffusivity shows even two anomalous regions at the temperature $T = 0.01$ where diffusion coefficient grows with growing density. In the present work the dependence of the diffusion coefficient on density along several isotherms was monitored. The simulation data are presented on the Fig. 1 (a) - (b).

One can see from these figures that at low temperatures (Fig. 1(a)) the diffusion is non monotonic, while at high temperatures it monotonically decays with increasing density (Fig. 1(b)) and comes to a constant value (see inset of the Fig. 1(b)).

It is worth to note that the melting temperatures of Herzian spheres reported in the work [67] are of the order of 10^{-3}, so the temperatures about 0.1 are extremely high for this model. This is easily seen from the Fig. 2 (a) - (b) where the radial distribution functions for the density $\rho = 6.0$ are shown for the same set of temperatures. One can see that at $T = 0.01$ the liquid has short range structure which rapidly decays with increasing temperature. At the temperature $T = 0.1$ the liquid looks almost like an ideal gas since $g(r)$ comes to unity very quickly.

Excess entropy also shows non monotonic dependence on density along an isotherm (Fig. 3(a) -(b)). One can see from these figures that at low temperatures excess entropy has two minima and a maxima in the investigated density range while at high temperature the first minima is depressed and the curves just change the slope smoothly.

Now we turn to the Rosenfeld relation for the Herzian spheres system. The dependence of the reduced diffusion (see formula (1)) on the excess entropy along some isotherms is shown in the Fig. 4 (a) - (b). Looking at the curve for $T = 0.01$ (Fig. 4 (a)) one can divide it into three distinct regions with different slopes which we denote as '1', '2' and '3'. The density increase corresponds to moving along the curves from right to left, i.e. region 2 corresponds to the higher densities then 1, and 3 - higher densities then 2. As is seen from the plots the region 3