Non-Gaussianity of translational and rotational degrees of freedom in supercooled liquid

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The non-Gaussian behaviors of diatomic Lennard-Jones system have been studied by molecular dynamical simulation. Non-Gaussian parameters(NGP) were defined separately for translation(T) and rotation(R). The two different critical temperatures, $T_C^{(T)}$ and $T_C^{(R)}$, were obtained by scaling the maximum time $t_{max}^{(T)}$ and $t_{max}^{(R)}$ of translational and rotational non-Gaussian parameters, respectively. Figure shows the NGP for the rotational degree of freedom at several temperatures, T=36, 42 48, 54, 60, 66 from bottom to top. Both the peak values and $t_{max}^{(R)}$ are increased with decreasing the temperature. The obtained relaxation time $\tau^{(T)}$ obeys the Vogel-Tammann-Fulcher law, while the τ^{R} obeys the Arrhenius law. This result suggests that the translational and the rotational dynamics play dominant roles in the α and the slow β-processes, respectively.

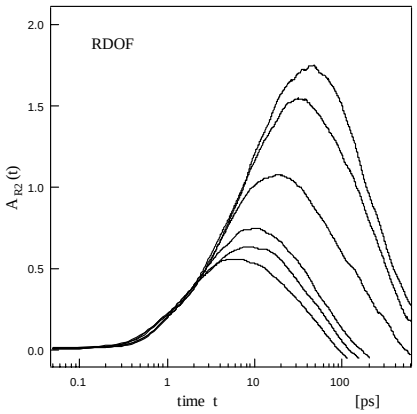

Figure Non-Gaussian parameter for rotational degree of freedom at several temperatures.