

explicitly considered in the path integral and in the transition region, in the coarse grained region they are neglected by the fact that the forces acting on them are not calculated and only the dynamical evolution of the coarse-grained sphere is considered.

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- [28] In fact for  $T_1$  the radial distribution function of the molecular center of mass of the path integral simulation (not shown here) is very close to that of the classical simulation. This means that the coarse-grained potential is very similar to that of the classical case and that the rings are rather stiff and thus the molecular representation in terms of path integral is very close to the atomistic one. We have looked also at the comparison between a full atomistic simulation and a full path integral simulation, at the two temperatures, for the intramolecular bond distribution. For  $T_1$  we have a broader distribution of the path integral simulation compared to the classical one, however the peak is located more or less at the same point, thus the path integral approach and the classical one will still be relatively close. For  $T_2$  the distribution is much broader and the peak is shifted and thus represents a test for the validity of the AdResS procedure in this context.
- [29] This in general is acceptable but not highly accurate for realistic applications; anyway we have done extended tests using liquid systems of simple spheres employing  $n = 20$  and  $n = 30$  and we obtain basically the same results as  $n = 10$ . Note that the arbitrary choice of  $T_1$ ,  $T_2$  and  $n$  is possible because we study a toy model without a specific physical meaning; in real systems  $k$  is defined by the physics of the system.
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