

thermodynamic equilibrium. The coarse-grained potential is obtained from a reference all atom simulation at the given thermodynamic condition via an iterative inverse Boltzmann procedure employing the molecular center of mass radial distribution [27]. For the case of the path integral description we have exactly the same procedure as for the classical case but with the difference that instead of a classical atomistic representation of the molecule we have a molecular representation where the atoms are described as polymer rings in a path integral approach (see Fig.1). It follows that the coarse-grained model is derived from a full path integral reference simulation at the given thermodynamic condition. Given the framework reported above the coupling between the path integral representation and the coarse-grained model occurs via the interpolation according to w between \mathbf{F}^{pi} acting on the beads of the rings (which now plays the equivalent role of \mathbf{F}^{atom} in Eq.1) and the \mathbf{F}^{cg} derived from the coarse grained potential acting among the centers of mass of the molecules. We tested this idea studying a liquid of tetrahedral molecules whose atomistic model was used in the original development of AdResS (see Fig.1(b)).

Results of the Path integral-coarse-grained Adaptive Resolution Simulation: We studied a system of thousand molecules at two different temperatures, indicated as T_1 and T_2 . T_1 is the same temperature employed in the previously studied classical model and $T_2 = \frac{T_1}{\sqrt{10}}$. In the Lennard-Jones units of this paper (see the Appendix or Ref.[21]) $T_1 = 1$ and consequently $T_2 = \frac{1}{\sqrt{10}}$. The different temperatures are directly related to the elastic constant of the polymers and thus, for the same number of beads per ring ($n = 10$), a lower temperature means more flexibility of the polymer rings, thus we have $k_2 = \frac{k_1}{10}$. For the testing purpose we have deliberately chosen T_2 because it mimics the thermodynamic conditions of a "more quantum" system than T_1 (see also [28]). Given the computational cost of path integral simulations and the very extended range of tests we have used, for both systems, the number of beads per polymer, n , equal to 10 [29]. Fig.2 reports the radial distribution functions (RDF) and the density distribution of the AdResS simulation of thousand molecules compared to a full path integral simulation for the temperature T_1 . They show that indeed this coupling procedure displays the desired behaviour. In particular, in Fig.2(b), the comparison between the bead-bead radial distribution function obtained with AdResS in the quantum region and that obtained from a full path integral simulation shows that indeed the very quantum nature of the particles in the quantum region of AdResS is very well described and thus the "classical bath" of the coarse-grained molecules is indeed