MAR14-2013-002860

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Path-Integration Computation of the Transport Properties of Polymers Nanoparticles and Complex Biological Structures

JACK DOUGLAS, Material Science and Engineering Division, NIST

One of the things that puzzled me when I was a PhD student working under Karl Freed was the curious unity between the theoretical descriptions of excluded volume interactions in polymers, the hydrodynamic properties of polymers in solution, and the critical properties of fluid mixtures, gases and diverse other materials (magnets, superfluids,etc.) when these problems were formally expressed in terms of Wiener path integration and the interactions treated through a combination of epsilon expansion and renormalization group (RG) theory. It seemed that only the interaction labels changed from one problem to the other. What do these problems have in common? Essential clues to these interrelations became apparent when Karl Freed, myself and Shi-Qing Wang together began to study polymers interacting with hyper-surfaces of continuously variable dimension where the Feynman perturbation expansions could be performed through infinite order so that we could really understand what the RG theory was doing. It is evidently simply a particular method for resuming perturbation theory, and former ambiguities no longer existed. An integral equation extension of this type of exact calculation to "surfaces" of arbitrary fixed shape finally revealed the central mathematical object that links these diverse physical models- the capacity of polymer chains, whose value vanishes at the critical dimension of 4 and whose magnitude is linked to the friction coefficient of polymer chains, the virial coefficient of polymers and the 4-point function of the phi-4 field theory,. . . Once this central object was recognized, it then became possible solve diverse problems in material science through the calculation of capacity, and related "virials" properties, through Monte Carlo sampling of random walk paths. The essential ideas of this computational method are discussed and some applications given to non-trivial problems: nanotubes treated as either rigid rods or ensembles worm-like chains having finite cross-section, DNA, nanoparticles with grafted chain layers and knotted polymers. The path-integration method, which grew up from research in Karl Freed's group, is evidently a powerful tool for computing basic transport properties of complex-shaped objects and should find increasing application in polymer science, nanotechnological applications and biology.