LIMIT OF MANY MOLECULES DYNAMICS WITH RIGOROUS MACROSCOPIC RESULTS

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ABSTRACT

The thesis builds on recent ideas that combine work by C.B. Morrey (1955) and D.W. Jepsen & D. ter Haar (1962) with more recent analytic techniques: measure disintegration, PDEs for measures, etc. (M.I. Vishik & A.V. Fursikov 1988, L. Ambrosio et. al. 2005).

In particular, it is shown that sufficient assumptions for rigorous, non phenomenological, macroscopic equations for mass and momentum as the limit of Hamiltonian dynamics are indeed satisfied by a class of initial conditions and rescalings of interaction potentials, including all $1/r^p$, $p > 3$ potentials. The total energy equation is also obtained. The averages naturally defined by this method are shown to be abstract Reynolds averages in the sense of Kampe’ de Feriet, Rota, and Moy, both in terms of abstract Reynolds properties and as conditional expectations with respect to the correct $\sigma$-algebra. Further, a close examination of the disintegration theorem provides justification for Reynolds’s insistence on space averages.

Finally, a certain approximation of the non-linear velocity term, close to equilibrium and in terms of Hermite polynomials, satisfies Landau-Lifschitz type formulas, ostensibly leaving room for non-thermal fluctuations. With an eye to applications and insisting on space averages, the thesis avoids Gibbs ensembles and the Liouville equation, as well as the Boltzmann equation. The approach is entirely not quantum and non-relativistic.