Interactions from structural data: historical overview of simulation assisted methods

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Large part of statistical mechanics is concerned with determination of condensed matter structure on the basis of known microscopic interactions. In the last decades an increasing emphasis was put on the opposite situation, too. Structural data, e.g. pair-distance statistics determined by diffraction methods are known, and one looks for the corresponding interaction functions in case of the so-called inverse problem. Theoreticians, experimental scientist, and researchers on the field of computer simulations are affected. The solution was searched for within the integral equation theories of condensed matter in the early investigations[1], but before long a computer simulation assisted method was suggested by Schommers [2]. After the attempts appeared in the late eighties[3] the interest to this field shows an increasing trend. Several methods was published in the nineties[4], and yearly one-two methods appeared nowadays[5].

We would like to give a comprehensive and historical overview on the solution of the inverse problem by simulation assisted methods in our presentation. Emphasis will be put on the theoretical grounds of the methods, e.g. the links to integral equation theories, to polydisperse grand canonical theories, and to numerical mathematical methods. Different features of the methods will be mentioned, as the choice of possible input structural functions, as the numerically local or global schemes of the potential modifications, and as the advantages and limits of the different methods. We would like to discuss the connection of these methods to the reverse Monte Carlo simulation[6], too. Reverse Monte Carlo simulation is way to obtain three-dimensional particle configurations on the basis of known pair-distance statistics, that opens some other ways to the solution of the inverse problem [7]. Finally, we would like to present statistical data on the use of the different methods.

[1] J.P. Hansen and I.R. McDonald, Theory of simple liquids, Academic (Oxford), 1986.

[2] W. Schommers, Phys. Lett. 43A, 157 (1973).

[3] W. Schommers, Phys. Rev. A, 28, 3599 (1983), D. Levesque et al., Phys. Rev. Lett., 54, 451 (1985).

[4] A. P. Lyubartsev and A. Laaksonen, Phys. Rev. E, 52, 3730 (1995), A.K. Soper, Chem. Phys., 202, 295 (1996), T. Yamaguchi et al., Mol. Phys. 96, 1159 (1999).

[5] G. C. Rutledge, Phys. Rev. E, 63, 021111 (2001), G. Tóth, J. Chem. Phys., 115, 4770 (2001), N.G. Almarza and E. Lomba, Phys. Rev. E, 68, 011202 (2003), E. Bourasseau, J. Chem. Phys., 118, 3020 (2003), G. Tóth, J. Chem. Phys. 118, 3949 (2003), N.B.Wilding, J. Chem. Phys., 119, 12163 (2003), N.G. Almarza et al., Phys. Rev. E 70, 021203 (2004), C. Russ et al., Europhys. Lett., 69, 468 (2005).

[6] R.L. McGreevy and L. Pusztai, Mol. Simul. 1, 369 (1988).

[7] G. Tóth and A. Baranyai, Mol. Phys., 97, 339 (1999), G. Tóth, poster planned at this conference