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This Week's Citation Classic®

Barker J A & Henderson D. What is "liquid"? Understanding the states of matter. *Rev. Mod. Phys.* 48:587-671, 1976.
[IBM Research Laboratory, San Jose, CA]

A century of effort has led to a fairly complete basic understanding of the static and dynamic physicochemical properties of liquids. The study of intermolecular forces as well as advances in statistical mechanics and in experimental techniques have contributed to this knowledge. This paper is a survey, with particular emphasis on equilibrium properties, of the theory that underlies this basic understanding of liquids. [The *SCI*® indicates that this paper has been cited in over 645 publications.]

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When we were invited to write this review paper we had accumulated between us about 35 man-years of work on various aspects of the theory of liquids, covering many different approaches: cell, hole, and "tunnel" models; the virial series; integral equations; thermodynamic perturbation theories; and Monte Carlo and molecular dynamics simulation methods. Thus, almost everything that we wrote had benefited from "hands-on" experience, and we knew what did not work in the theory of liquids about as well as what did work.

The paper was written at a propitious time, following two decades of increasing activity in computer simulation of liquids that resulted in new insights and, incidentally, coming almost 10 years after our previous *Citation Classic*[1] on the perturbation theory of liquids using a hard-sphere reference fluid, which led to a great deal of activity and a major growth in the understanding of the liquid state. As a result of these factors, one could feel by 1976 that the problem of the theory of simple liquids, at least as far as equilibrium properties were concerned, was essentially a solved problem, whereas even 15 years earlier the very existence of liquids had seemed a little mysterious. Our title echoes the puzzlement of an alien character in "Star Trek" faced with human emotions and asking "What is 'love'?"

We aimed to give a unified account of the statistical mechanics of condensed phases and to show how the solid-liquid-gas phase diagram could be predicted in a favorable case.[2] It was our intention to discuss both the use of simple model potential functions and more realistic detailed potentials, including many-body potentials. We did our best to give a comprehensive survey of the many approaches to the theory of liquids, and we examined many possible extensions of existing theories. We gave a bibliography and listed something over 600 references, thus providing an entry to the very extensive literature on the subject. As a result, our paper has become recognized alongside the book of J.P. Hansen and I.R. McDonald[3] as the "standard reference" for the theory of liquids.[4]

1. **Barker J A & Henderson D.** Perturbation theory and equation of state for fluids. II. A successful theory of liquids. *J. Chem. Phys.* 47:4714-21, 1967. (Cited 460 times.) [See also: **Barker J A & Henderson D.** Citation Classic. (Thackray A, comp.) *Contemporary classics in engineering and applied science.* Philadelphia: ISI Press, 1986. p. 310.]
2. **Hansen J-P & Verlet L.** Phase transitions of the Lennard-Jones system. *Phys. Rev.* 184:151-61, 1969. (Cited 245 times.)
3. **Hansen J P & McDonald I R.** *Theory of simple liquids.* London: Academic Press, 1986. 395 p.
4. **Tildesley D & Adams D J.** *Computer simulation of liquids.* Oxford, England: Clarendon Press, 1987. 385 p.

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