Fig. 1 Radial distribution function for liquid with 6:12 interactions (depth ε, diameter σ) for $T^* = kT/\varepsilon = 0.72$, $\rho^* = N\sigma^3/V = 0.85$. Dotted curve, zero order hard sphere distribution function; solid curve, first order distribution function. The circles are molecular dynamics results of Verlet[20].

before modern computers permitted the explicit demonstration of the full richness of content of statistical mechanics.

The same article suggests that the "random geometric" approach to liquids, ably propounded by Bernal and his co-workers[7-9], is unexplored because it is unorthodox. In fact the importance of random packing of hard cores in determining the properties of liquids has been recognized since the time of van der Waals[10], who incorporated this concept in his well known equation of state. More recently the ideas of van der Waals have been developed by Longuet-Higgins and Widom[11] and by Guggenheim[12], and have been given a rigorous basis in statistical mechanics by the development of perturbation theories[13-19] using the hard sphere fluid as the unperturbed system. The latter approach has led to a quantitatively satisfactory and qualitatively appealing theory of liquids; the properties of a fluid are determined by expansion in powers of parameters representing the strength of the attractive forces and the softness of the repulsive potential. In zero order the structure of the fluid is determined by the random packing of hard spheres (given a precise definition by the statistical mechanics of Gibbs); in first order the structure is somewhat modified by the attractive forces and the softness of the repulsive potential, and it turns out that higher order terms are negligible. Both the zero order and the first order radial distribution functions are shown in Fig. 1. The first order curve is in excellent agreement with the "quasi experimental" results calculated by the method of molecular dynamics by Verlet[20]. (Actually the method of molecular dynamics rests ultimately on the ideas of Boltzmann, but comparison with a real experiment would lead to identical conclusions.) The calculation of these curves[21] relied on detailed knowledge of the relevant aspects of the "statistical geometry" of hard spheres derived from Monte Carlo computer calculations[19-21] using the statistical mechanics of Gibbs. There is also an integral equation theory[22] which gives an excellent approximation to the properties of the hard sphere fluid.

There are two obstacles to the fruitful implementation of Bernal's polyhedron statistics approach to statistical geometry in the theory of liquids. The first is that "random packing" is not a precisely defined concept until one specifies some ensemble (Gibbs ?) or population from which one is choosing randomly—this point was made clearly by Bernal[8] in connexion with the reproducibility of measures. The second is that no one has yet found a fully satisfactory way of using the polyhedron statistics description to make progress. It may be that the route lies in homology theory[19], but homology theory may well be as discouraging to a molecular physics correspondent as configuration integrals. It is perhaps these difficulties that have prevented progress rather than an unyielding orthodoxy; if there is an orthodoxy in the theory

of liquids, one surely expects it to be fluid and eclectic rather than rigid.

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OUR molecular physics correspondent writes: On the whole, I am unrepentant. What worries me in the above is the pious implication that we should be content with one particular mathematical method said, with rather slim justification, to give birth to a "complete description" (no less) of the states of matter and their phase equilibria. Precisely what sense are the words "complete" and "description" supposed to carry in this context? Would Barker and Henderson accept, at least for the purposes of my article, that there is an element of difference between a "description" of the states of matter and an "understanding" of them, just as it is by "predictive" rather than "descriptive" power that any theory must ultimately stand or fall, even in a field as difficult as the theory of liquids?

The use of computers for molecular dynamic calculations has undoubtedly revitalized the classical theory, but the effect of this will be less telling if it leads to the neglect or undervaluation of alternative approaches, particularly those which, for want of a label, might be called information theoretic in standpoint. And, in speaking of undervaluation, I would specifically include the tendency to see a radical innovation such as Bernal's as just another formulation of received ideas. In the end this attitude, fluid and eclectic perhaps, could be as inhibiting to original work as the outright intolerance which so often went with orthodoxy in Gibbs's day.

My prediction, from a relatively detached position, is that information theoretical methods will prosper in the long run, that their advance will be only marginally dependent on computer technology and that the heterodox views of the Birkbeck school will be a historically significant, though probably not a central, feature of this trend. Whatever else, Bernal's theory of liquids is imaginative—in several flavours of the word—and, pending final justice, should be welcomed as such.