



Fig. 2. The P - V curve at high pressures. The solid line represents the results of the present theory. The dots represent the theoretical calculations of Pollock *et al.*¹⁴

calculated kinetic energy to the potential energy decreases monotonically as the pressure increases. The onset of classical behavior is easily recognized. The lack of theoretical agreement with experiment at higher pressures may well be due to the use of an inadequate interaction potential. This interpretation is particularly plausible since our calculation agrees so closely with other quite different theoretical approaches at high pressures. The success of the theory at low pressures is interesting.

Finally, an interpretation of the pressure dependence of the pair correlation function $f(r)$ in Eq. (1) is possible in terms of this theory. The boundary condition $\phi(x) = 0$ for $x > a/\sigma$ can be interpreted as equivalent to a step-function form for $f(r)$. The pressure dependence of $f(r)$ is then determined by the behavior of a . Our calculations show that a decreases by approximately a factor of two as the volume is reduced from 22 to 11 cm³/mole. The location of the step in f is shifted from $x = 0.895$ to $x = 0.83$ as the volume is decreased in this interval. In terms of Eq. (1) the particles become more localized as the pressure is increased, as evidenced by the narrowing of $\phi(x)$. In addition, as the pressure increases, the position of the step in $f(r)$ is shifted further into the region containing the strong repulsive potential core. These results tend to support the notion that the shape of $f(r)$ is fairly sensitive to changes in the volume.

REFERENCES

1. W. C. DeMarcus, *Astron. J.* **63**, 2 (1958).
2. See M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, Oxford, England, 1954).
3. F. W. deWette and B. R. A. Nijboer, *Phys. Letters* **18**, 19 (1965).
4. J. A. Krumhansl and S. Y. Wu, *Phys. Letters* **28A**, 263 (1968).
5. L. H. Nasanow, *Phys. Rev.* **146**, 120 (1966).
6. J. W. Stewart, *J. Phys. Chem. Solids* **1**, 146 (1956).
7. T. A. Bruce, Cornell University, Ithaca, New York, 1971, preprint.
8. J. P. Hansen and D. Levesque, *Phys. Rev.* **165**, 293 (1968).
9. C. Ebner and C. C. Sung, *Solid State Commun.* **8**, 1903 (1970).
10. R. A. Guyer and L. I. Zane, *Phys. Rev.* **188**, 445 (1969).
11. N. Bernardes, *Phys. Rev.* **120**, 1927 (1960).
12. N. Bernardes, *Phys. Rev.* **120**, 807 (1960).
13. J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, New York, 1954).
14. E. L. Pollock, T. A. Bruce, G. V. Chester, and J. A. Krumhansl, Cornell University, Ithaca, New York, preprint.