Radial Distribution Functions in Crystals and Fluids,* J. L. LEIBOWITZ, Yeshiva University, J. K. PERCUS, New York University Institute of Mathematical Sciences, I. J. ZUCKER†, Yeshiva University.

We are investigating the qualitative nature of the two particle distribution function $n_2(r_1,r_2)$ with particular reference to its long range behaviour in crystals and fluids. Starting with an $N$-particle system in a box with periodic boundary conditions the two particle distribution will always have translational invariance and in the limit of the system becoming infinite will only depend on the distance between the particles, i.e. $n_2(r_1,r_2) = n^2 g(r)$. The question we ask is what, if any, qualitative differences are there between the $g(r)$ in the fluid and crystalline states. One method of approach is through $\sigma(k)$ the Laplace transform of $g(r)$ which is related to the expectation value $\langle \rho_k \rho_{-k} \rangle$ where the $\rho_k$ are the Fourier transforms of the microscopic density. In the crystalline case these may be evaluated for low values of $k$ in terms of the usual crystalline normal coordinates. This yields the moments of $(g(r)-1)$ which may give information on the existence of long range order in crystals. For a one dimensional system with nearest neighbor forces $\sigma(k)$ is given directly in terms of the thermodynamic parameters of the system; $\sigma(k) = \frac{1}{n \exp(\mu(p+k) - \mu(p)) - n}$, where $\mu$ is the chemical potential and $p$ is the pressure measured in units of temperature, from which the moments of $(g-1)$ may be computed explicitly. These systems, as is well-known, always remain in the fluid state. The above expression for $\sigma(k)$ may be compared with that obtained when only harmonic forces are used.
