

Phase Transition in a Model Quantum System : Quantum Corrections to the Location of the Critical Point*

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It was proved by Lebowitz, Penrose, and Lieb that the pressure of a system with an interparticle potential $v(r)$ of the form $v(r) = q(r) + \gamma^v \varphi(\gamma r)$, where v is the dimensionality of the space considered and γ^{-1} is the range of φ , is given in the limit $\gamma^{-1} \rightarrow \infty$ by applying the Maxwell equal-area construction to the generalized van der Waals pressure $\tilde{p}(T, \rho) = p^0(T, \rho; h) + \frac{1}{2}\alpha\rho^2$. Here T is the temperature, ρ the particle density, h Planck's constant, $p^0(T, \rho; h)$ the pressure of a system with interparticle potential $q(r)$ and $\alpha = \int \gamma^v \varphi(\gamma r) d\mathbf{r} \equiv \int \varphi(y) dy$. This system will have a first-order phase transition for $\alpha < 0$. In this paper we apply the above results to obtain the properties of a one-dimensional quantum system for which $q(r)$ is a hard-core potential of "diameter" a . For this system $p^0(T, \rho; h)$ is known exactly and we can thus find how the properties of the phase transition depend on the quantum parameter $\lambda = (h^2/mkT^*)^{1/2}/d^*$, the ratio of the de Broglie wavelength to the interparticle separation evaluated at the classical critical point, i.e., at the critical point found in the limit $h \rightarrow 0$. We compute in particular the fractional changes in the critical temperature $T_c(\lambda)/T_c^*$, critical density $\rho_c(\lambda)/\rho_c^*$, and the critical ratio $(p_c/\rho_c kT_c)/(p_c^*/\rho_c^* kT_c^*)$. We find that $T_c(\lambda)/T_c^* \sim \rho_c(\lambda)/\rho_c^*$ decreases rapidly from unity as λ increases, approaching zero as $\lambda \rightarrow \infty$. The critical ratio on the other hand varies only slightly with λ , decreasing from one to about 0.98 as λ varies from 0 to ∞ . When we compare this behavior of this model system with that observed experimentally in fluids expected to obey the law of corresponding states, the resemblance is very striking. Taking xenon as our "classical system" to fix the values of T_c^*, ρ_c^*, p_c^* and comparing its critical parameters (in reduced units) with those of argon, neon, and the isotopes of hydrogen and helium we find again $T_c(\lambda)/T_c^* \sim \rho_c(\lambda)/\rho_c^*$ decreasing to less than half as we go from Xe to He³, the corresponding values of λ increasing from 0.04 to 1.90. On the other hand, the critical ratio varies by only about 5% (increasing from Xe to He³).

I. INTRODUCTION

IT was recently shown by Lebowitz and Penrose¹ that a generalized form of the van der Waals-Maxwell theory of the liquid-vapor transition can be made rigorous by considering a system of N particles confined to a box of volume Ω , $N = \rho\Omega$, and interacting with a pair potential $v(r, \gamma)$ of the form

$$v(r) = q(r) + \gamma^v \varphi(\gamma r). \quad (1.1)$$

Here $q(r)$ is a "short-range" potential which drops off sufficiently rapidly as $r \rightarrow \infty$, v is the dimensionality of the space considered, and γ is a parameter which measures the range of the long-range potential $\varphi(y)$. The integral of the long-range potential is independent of γ

$$\int \gamma^v \varphi(\gamma r) d\mathbf{r} \equiv \int \varphi(y) dy \equiv \alpha. \quad (1.2)$$

They found [for a wide class of potentials $q(r)$ and $\varphi(y)$], that in the van der Waals limit $\gamma \rightarrow 0$, taken after the thermodynamic limit $\Omega \rightarrow \infty$, the Helmholtz free energy per unit volume

$$a(\rho, 0+) \equiv \lim_{\gamma \rightarrow 0} a(\rho, \gamma) \equiv \lim_{\gamma \rightarrow 0} \lim_{\Omega \rightarrow \infty} \left[\frac{A(\rho\Omega, \Omega, \gamma)}{\Omega} \right] \quad (1.3)$$

has the form obtained by applying the double tangent construction or Gibbs construction to the generalized

van der Waals free energy

$$\tilde{a}(\rho) = a^0(\rho) + \frac{1}{2}\alpha\rho^2.$$

Here $A(N, \Omega, \gamma)$ is the Helmholtz free energy of the system with N particles at some temperature T (not indicated explicitly), $a^0(\rho)$ is the Helmholtz free energy per unit volume in the reference system, i.e., the system with interparticle potential $q(r)$, and α is defined in (1.2).

The corresponding pressure $p(\rho, 0+) = \lim_{\gamma \rightarrow 0} p(\rho, \gamma)$ is given by $p(\rho, 0+) = \rho^2(\partial/\partial\rho)[a(\rho, 0+)/\rho]$ which corresponds to applying the Maxwell equal-area construction to the generalized van der Waals pressure $\tilde{p}(\rho) = p^0(\rho) + \frac{1}{2}\alpha\rho^2$, i.e.,

$$p(\rho, 0+) = p^0(\rho) + \frac{1}{2}\alpha\rho^2 + [\text{Maxwell rule}]. \quad (1.4)$$

The results of Lebowitz and Penrose were shown by Lieb² to apply also to quantum systems. A knowledge of $a^0(\rho)$ as a function of Planck's constant, will thus yield information about quantum effects on the liquid-vapor transition, particularly on the critical constants which are almost always treated, as far as they can be treated theoretically at all, by classical mechanics. Of particular interest in this connection are deviations from the law of corresponding states for the noble gases and inert molecules. It is difficult to decide *a priori* how much of these deviations are due to quantum effects and how much to the failure of the interparticle potential to obey a law of corresponding states. Also, the discrepancy between theoretical computations (classical) and the behavior of substances like argon have cast doubt on

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¹ J. L. Lebowitz and O. Penrose, *J. Math. Phys.* **7**, 98 (1966).

² E. Lieb, *J. Math. Phys.* **7**, 1016 (1966).

whether the properties of these gases can be represented to all by a pair potential.³ Here too the deviations might be due, in part at least, to quantum effects. It should be pointed out, however, that the analytical behavior of the thermodynamic functions in the immediate vicinity of the critical point is, for the systems considered here (infinite-range potential), not affected by quantum mechanics but is always van der Waals-like, e.g., the critical-point exponents are independent of the quantum parameter. This follows from the fact that $a^0(\rho)$ is analytic in the vicinity of ρ_c , there being no special significance to the density ρ_c in the reference system. Our model van der Waals system thus differs qualitatively in this respect from the behavior of real fluids. The same is not true, however, of the grosser features of the phase transition,⁴ e.g., the variation of the critical constants and the over-all shape of the co-existence curve with the quantum parameters, which is what we shall now investigate.

To obtain explicit results for our model systems it is necessary to know explicitly the behavior of the reference system, e.g., $a^0(\beta, \rho)$; β is the reciprocal temperature. This requirement restricts us effectively to a reference system of one-dimensional hard rods,⁵ i.e.,

$$\begin{aligned} q(x) &= \infty, \quad |x| < a \\ &= 0, \quad |x| > a. \end{aligned} \quad (1.5)$$

For this system $a^0(\beta, \rho)$ is known both classically and quantum mechanically.⁶ We shall use this system, with an added long-range attractive potential, to find the fractional changes in the critical temperature T_c , density ρ_c , as well as the critical ratio $\tilde{p}_c/\rho_c kT_c$ as a function of the quantum parameter

$$\lambda = h/d^*(mkT_c^*)^{1/2}, \quad (1.6)$$

where T_c^* and d^* are the values of the temperature and interparticle spacing at the critical point, in the classical limit, i.e., when $h \rightarrow 0$.

The principal result of our computation is that ρ_c and T_c change drastically and in an almost identical manner with λ , both approaching zero as $\lambda \rightarrow \infty$, while the critical ratio ($\tilde{p}_c/\rho_c kT_c$) remains essentially unchanged (decreasing by about 2% as λ varies from zero to infinity).

³ J. A. Barker and P. J. Leonard, Phys. Letters **13**, 127 (1964); P. G. Mikolaj and C. J. Pings, Phys. Rev. Letters **16**, 4 (1966); L. Verlet (private communication).

⁴ For a discussion of the possible quantum effects on the critical indices see M. E. Fisher, Phys. Rev. Letters **16**, 11 (1966).

⁵ When $\varphi(\gamma, r)$ is non-negative definite it is possible to use the ideal gas, $q(r) = 0$, as a reference system (Ref. 1). In this case, however, $\alpha \geq 0$, and there is no vapor-liquid transition. When $\alpha < 0$ it is generally necessary that $q(r)$ contain a hard core. In the limit of the hard-core diameter $a \rightarrow 0$, our one-dimensional reference system becomes identical to an ideal Fermi gas whose critical parameters are given at the end of Sec. II. A three-dimensional Fermi ideal gas reference system would collapse to infinite density for arbitrary $\alpha < 0$ while a two-dimensional ideal gas reference system would collapse completely for $T < T_c$.

⁶ For a classical system there are good approximations to $a^0(\beta, \rho)$ available for hard spheres in two and three dimensions. This is not so for quantum systems, however.

This is qualitatively very similar to the behavior of real fluids as we go from Xe to He³ (λ changing from 0.04 to 1.90) cf. Fig. 2. (The "classical" T_c^* and d^* for a system with a Lenard-Jones potential with parameter ϵ and σ were taken to be those corresponding to Xe which presumably is quite classical). We also find that for our system the critical parameters are analytic functions of λ and we give the first few terms in their expansion.

II. ANALYSIS OF ONE-DIMENSIONAL SYSTEM

For a one-dimensional system of hard rods of length a the classical free-energy density, at temperature T and particle density ρ , is

$$a^0(\rho) = kT\rho \left\{ \ln \left(\frac{\rho}{1-\rho a} \right) - \frac{1}{2} \ln \left(\frac{mkT}{2\pi\hbar^2} \right) - 1 \right\}. \quad (2.1)$$

The pressure of this system with an added long-range potential is obtained from (1.4) by applying Maxwell's rule to the generalized van der Waals pressure

$$\tilde{p} = - \frac{\partial}{\partial \rho^{-1}} \left\{ \frac{1}{\rho} [a^0(\rho) + \frac{1}{2}\alpha\rho^2] \right\} = \frac{kT\rho}{1-\rho a} + \frac{1}{2}\alpha\rho^2. \quad (2.2)$$

The conditions for a critical point

$$\partial \tilde{p} / \partial \rho^{-1} = \partial^2 \tilde{p} / \partial (\rho^{-1})^2 = 0 \quad (2.3)$$

lead to the following values for the classical critical density, temperature, and pressure, for $\alpha < 0$:

$$\rho_c^* = \frac{1}{3a}, \quad T_c^* = \frac{4|\alpha|}{27ka}, \quad \tilde{p}_c^* = \frac{1|\alpha|}{54a^2}, \quad (2.4)$$

and the dimensionless quantity, the critical ratio

$$\tilde{p}_c^*/kT_c^*\rho_c^* = \beta_c^*\tilde{p}_c^*/\rho_c^* = \frac{3}{8}. \quad (2.5)$$

Lieb² has shown that the free-energy density of the corresponding quantum-mechanical system (apart from a trivial constant contribution to the entropy caused by any spins which may be present) is given by

$$\begin{aligned} a^0(\rho) &= kT\rho \left\{ \ln z - \left(\frac{1-\rho a}{\pi\rho} \right) \left(\frac{2mkT}{\hbar^2} \right)^{1/2} \right. \\ &\quad \left. \times \int_0^\infty dt \ln(1+ze^{-t^2}) \right\}, \end{aligned} \quad (2.6)$$

where $z(\rho, T)$ is the solution of

$$1 = \left(\frac{1-\rho a}{\pi\rho} \right) \left(\frac{2mkT}{\hbar^2} \right)^{1/2} \int_0^\infty \frac{ze^{-t^2}}{1+ze^{-t^2}} dt. \quad (2.7)$$

The critical point is no longer given by (2.4) but is a function of the dimensionless parameter

$$\Lambda = (\hbar^2/ma|\alpha|)^{1/2}$$

[which, for this system, is related to λ defined in (1.6) by $\lambda = \sqrt{3}\pi\Lambda$]. The case $\Lambda = 0$, i.e., $\hbar = 0$, reduces to the classical situation.

The analysis is simplified if we introduce the dimensionless quantities

$$x = \rho a, \quad \nu = (\hbar^2 \beta / 2ma^2)^{1/2}, \quad y = \nu x / (1-x) \quad (2.8)$$

and consider y and ν as independent variables. If we define

$$I(z) = \int_0^\infty dt \ln(1 + ze^{-t^2}), \quad (2.9)$$

then (2.6) and (2.7) may be rewritten as

$$\beta a^0 / \rho = \ln z - (1/\pi y) I(z(y)) \quad (2.10)$$

and

$$\pi y = z \partial I / \partial z. \quad (2.11)$$

The van der Waals pressure can be expressed in dimensionless form:

$$\beta a \tilde{p} = \frac{I(z)}{\pi \nu} - \frac{\nu^2}{\Lambda^2} \left(\frac{y}{y+\nu} \right)^2. \quad (2.12)$$

Application of the conditions (2.3) enables us to eliminate Λ and obtain the following equation for the critical values of y and ν :

$$(2y-\nu) \frac{dI}{dy} + y(y+\nu) \frac{d^2 I}{dy^2} = 0, \quad (2.13a)$$

wherein I is regarded as a function of y given implicitly by (2.11). The solution of Eq. (2.13) provides values of the critical density and temperature⁷ subject to the physical restriction that $0 \leq x \leq 1$. The first critical-point condition, namely $\partial \tilde{p} / \partial \rho^{-1} = 0$, gives the value of Λ associated with a particular T_c and ρ_c

$$\Lambda^2 = \frac{2\pi y \nu^4}{(y+\nu)^3 dI/dy}. \quad (2.13b)$$

The classical limit $\Lambda \rightarrow 0$ corresponds to $y \rightarrow 0$ since in this limit y is proportional to Λ . Using the expansion

$$I(z) = -\frac{\sqrt{\pi}}{2} \sum_{n=1}^{\infty} \frac{(-z)^n}{n^{3/2}}$$

valid for $|z| < 1$, and Eq. (2.11), we can expand I in powers of y and hence in powers of Λ . Therefore for small values of Λ it is possible to write the free energy and other physical quantities as a series in Λ . When $\Lambda = 0$ the classical results (2.1), (2.2), and (2.4) are re-

⁷ It is easy to show by a tedious and, therefore, unilluminating demonstration that a critical point exists for all values of T , m , α , and a . We have not succeeded in proving that there is only one critical point, although the numerical results indicate that this is surely the case.

gained and to first order in Λ

$$\begin{aligned} \frac{\beta a^0}{\rho} &= \frac{\beta a^{0*}}{\rho} + \frac{3}{8} (3\pi)^{1/2} \Lambda, \\ \frac{\rho_c}{\rho_c^*} &= \frac{T_c}{T_c^*} = \frac{\beta_c p_c}{\beta_c^* p_c^*} = 1 - \frac{3}{4} (3\pi)^{1/2} \Lambda, \\ \nu_c &= \left(\frac{3}{2}\right)^{1/2} \Lambda, \end{aligned} \quad (2.14)$$

whereas the critical ratio $\beta_c p_c / \rho_c$ has no linear term. As before, asterisks denote classical ($\hbar = 0$) values.

The numerical results discussed below show that in the quantum limit $\Lambda \rightarrow \infty$, ρ_c and T_c approach zero, but that the critical ratio goes to a constant approximately 0.978 of its classical value. In this case y approaches a limiting value of approximately 0.303 and by expanding I about this value one can show that in the quantum limit ρ_c , T_c , and $\beta_c p_c$ behave like Λ^{-2} so that the critical ratio will go to a constant.

For intermediate values of Λ a numerical solution of Eq. (2.13) was carried out and the results are shown in Fig. 1. Since it turns out that ρ_c / ρ_c^* and T_c / T_c^* , as functions of Λ , are almost equal, the latter lying below the former by at most 5%, we have shown the behavior of ρ_c / ρ_c^* only. Thus the critical temperature and density drop sharply from their classical value as Λ increases

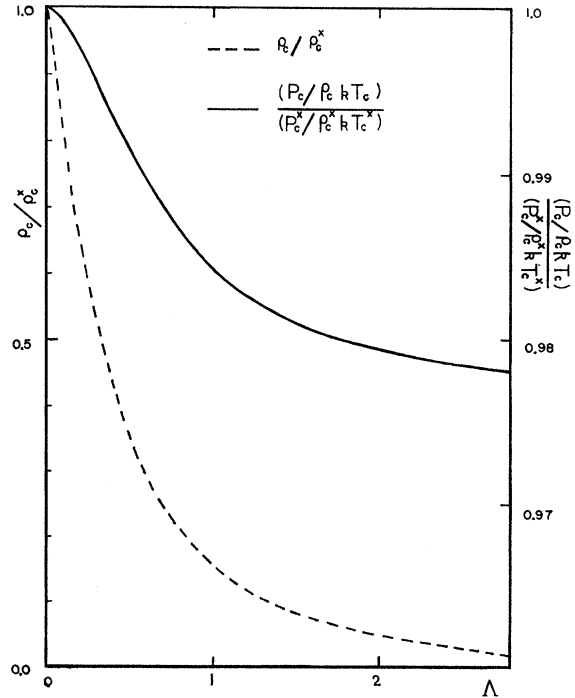
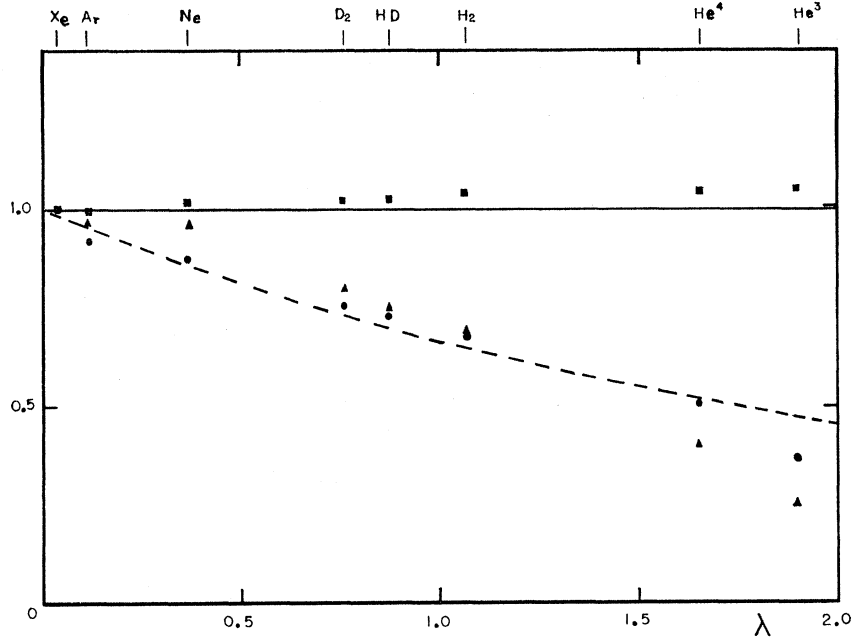


FIG. 1. The critical density and critical ratio, divided by the corresponding values for $\hbar = 0$, as a function of $\Lambda = (\hbar^2 / ma |\alpha|)^{1/2}$ for a one-dimensional system of hard rods with an infinite-range attractive potential. The value of T_c / T_c^* is almost equal to ρ_c / ρ_c^* for all values of Λ .

FIG. 2. The reduced critical parameters ρ_c/ρ_c^* , T_c/T_c^* , and $(\beta_c p_c/\rho_c)/(\beta_c^* p_c^*/\rho_c^*)$, denoted by circles, triangles, and squares, respectively, for the noble gases and hydrogen isotopes compared with results of the model system. [Data taken from Ref. 8 and from A. S. Friedman *et al.*, J. Chem. Phys. 19, 126 (1951). Krypton has been omitted because of difficulty in obtaining a consistent Lennard-Jones potential for this gas; cf. E. A. Mason, J. Chem. Phys. 32, 1832 (1960).]



and monotonically approach zero as $\Lambda \rightarrow \infty$. However, the critical ratio decreases very slowly and, as we mentioned above, even in the limit $\Lambda \rightarrow \infty$ it is only about 2.2% less than its classical value.

In the limit where the hard-core diameter $a \rightarrow 0$, our reference system reduces to an ideal Fermi gas in one dimension.⁵ The critical point will occur for the value of y , say $y = y_0$, where

$$\frac{d^2 I}{dy^2} - \frac{1}{y} \frac{dI}{dy} = 0$$

which corresponds to the quantum limit $\hbar \rightarrow \infty$ of the system with finite a ($y_0 \approx 0.303$). The critical parameters are given by

$$\rho_c = \frac{2\pi y_0^2 m |\alpha|}{I_0' \hbar^2} \approx 0.076 \frac{m |\alpha|}{\hbar^2},$$

$$T_c = 2 \left(\frac{\pi y_0}{I_0'} \right)^2 \frac{m |\alpha|^2}{\hbar^2 k} \approx 0.032 \frac{m |\alpha|^2}{\hbar^2 k},$$

$$\frac{\beta_c p_c}{\rho_c k T_c} = \frac{1}{2\pi y_0} [2I_0 - y_0 I_0'] \approx 0.365 \approx 0.978 \times \frac{2}{3},$$

where I_0 and I_0' denote the values of I and dI/dy at $y = y_0$.

III. RELATION TO THE CRITICAL PROPERTIES OF REAL FLUIDS

It is generally believed⁸ that the interparticle potentials $v(r)$ of the inert gases (as well as that of many

⁸ See, e.g., J. O. Hirschfelder, C. F. Curtis, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954).

molecular substances) may be represented to a good approximation in the form $\epsilon f(r/\sigma)$. Here f is a universal function (usually taken as a Lennard-Jones potential) and ϵ and σ are energy and length parameters which differ for each substance. Hence if the world were classical these substances would have the same critical temperature T_c^* and density ρ_c^* , in units of ϵ and σ^{-3} respectively, as well as the same numerical critical ratio. The deviations from these universal values may then be attributed to quantum effects. These effects will depend (disregarding statistics and spin forces) on the dimensionless parameter $\Lambda^* = h(\sigma^2 m \epsilon)^{-1/2}$.

We shall now try to relate the fractional changes of T_c/ϵ , $\rho_c \sigma^3$, and $\beta_c p_c/\rho_c k T_c$ for these substances from their classical universal values T_c^*/ϵ , $\rho_c^* \sigma^3$, and $\beta_c^* p_c^*/\rho_c^* k T_c^*$ (taken to be those for Xe), to our model. (Such fractional changes are clearly the most suitable to try to understand with our simple model.) In order to do this we need to know how to relate Λ^* , defined in terms of the parameters of the Lennard-Jones potential, to Λ defined in terms of our one-dimensional-model system. This is of necessity somewhat arbitrary and we chose to use the model-independent physical parameter λ , defined in (1.6), as a universal measure of the quantum nature of a system.

Taking xenon as our reference classical system, the following relations hold between the classical critical temperature and interparticle spacing and the parameters of the Lennard-Jones (6-12) potential⁸:

$$\epsilon = 0.77kT_c^*, \quad \sigma = 0.703d^*,$$

so that

$$\lambda = 0.618\Lambda^* = \pi\sqrt{3}\Lambda,$$

where the second equality follows from (2.4). In Fig. 2

we have plotted the reduced temperatures and densities and also the critical ratios of various substances against λ and compared these with the results of our model.⁹ In the case of the critical ratio there is experimentally an increase of about 5% as λ increases from Xe to He³,

⁹ After completion of this paper M. E. Fisher supplied us with more recent experimental data collected by him for Ref. 4. However, use of those results makes only about 1% change to Fig. 2.

whereas the model shows a decrease of 0.5% over the same range of λ . Thus our model agrees with the experiment by giving only a small variation of the critical ratio due to quantum effects. When the reduced critical temperatures and densities of the noble gases and hydrogen isotopes are plotted against λ , the agreement of the results with those of the model is remarkably good, especially for the dependence of critical density on λ .

Temperature Dependence of the Structure of Liquid Indium*

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The x-ray diffraction pattern of liquid indium were measured at 170, 280, 390, 500, and 650°C. For comparison, liquid mercury was measured at room temperature. All data were taken with a θ - θ diffractometer from the open surface of the melt between values of $K = 4\pi \sin\theta/\lambda = 1.5$ and 15 \AA^{-1} . Absolute intensity data $I_{\text{e.u.}}^{\text{coh}}$ were obtained by scaling the measured intensity of In to that of liquid mercury (coh = coherent, e.u. = electron units). The values of $I_{\text{e.u.}}^{\text{coh}}$ for $K > 12$ did not show extensive modulation and were in good agreement with the square of the dispersion-corrected scattering factor f of In. The interference function $I(K)$ was calculated by dividing the $I_{\text{e.u.}}^{\text{coh}}$ values by the theoretical f^2 values. Fourier transform of $I(K)$ yielded the radial distribution function $\text{RDF} = 4\pi r^2 \rho(r)$ and pair probability function $g(r) = \rho(r)/\rho_0$, where ρ_0 is the atomic density. The RDF curve of Hg is completely free of ripples below $r < D$, where D is the hard-sphere diameter, indicating that $I_{\text{e.u.}}^{\text{coh}}$ and f^2 were determined accurately. In the case of In, ripples were found below the first peak in the RDF. We conclude that these ripples are a consequence of the use of inappropriate f^2 values rather than errors in $I_{\text{e.u.}}^{\text{coh}}$, since Hg and In were measured under identical conditions. Fourier transform of the ripple-free RDF yielded an $I(K)$ curve which was about 10% higher in the region of the first peak. Dividing $I_{\text{e.u.}}^{\text{coh}}$ by the corrected $I(K)$ leads to values of the scattering factor which are 5% lower in the range of $K = 1.5$ to 8 \AA^{-1} than the Dirac-Slater scattering factors. The distribution of the atoms in liquid In can be approximately described by the hard-sphere model with a packing density of 0.45 compared to 0.74 in the solid. This density corresponds to a hard-sphere diameter $D = 2.86 \text{ \AA}$, which is the first value of r in the RDF where $\rho(r) = \rho_0$. The interatomic distances r_1 taken as the position of the first peak maximum in the RDF and the coordination number CN decrease with increasing temperature. Both variations are a consequence of the excess or free volume created in the liquid. The electrical resistivity ρ_R and thermoelectric power Q of liquid In were calculated from the measured $I(K)$ and the theoretical values of the Fourier transform $U(K)$ of the pseudopotential for different temperatures. The predicted values of ρ_R are about 50% lower than those observed experimentally. The theory also underestimates the temperature dependence of the resistivity by about a factor of 3.

I. INTRODUCTION

THE liquid state of matter is the least understood of the three common states solid, liquid, and gaseous. The atomic arrangement in the liquid state represents a compromise between the long-range order characteristic of crystalline solids and total disorder characteristic of gases. There must be correlations between atoms separated by short distances in the liquid, but complete randomness between atoms or molecules separated by large distances.

The distribution of atoms as a function of the radial distance r about a given reference atom, i.e., $4\pi r^2 \rho(r)$, can be obtained from the x-ray intensity $I_N(K)$ scattered by N atoms with scattering factors f as a function

of the magnitude of the diffraction vector $K = 4\pi(\sin\theta)/\lambda$, where 2θ is the angle between the incident and diffracted x rays and λ is the wavelength¹⁻³:

$$4\pi r^2 \rho(r) = 4\pi r^2 \rho_0 + \left(\frac{2r}{\pi}\right) \int_0^\infty K [I(K) - 1] (\sin Kr) dK, \quad (1)$$

where ρ_0 is the average atomic density and $I(K)$ is the interference function given by

$$I(K) = I_N(K)/(Nf^2) = I_{\text{e.u.}}^{\text{coh}}(K)/f^2. \quad (2)$$

$I_{\text{e.u.}}^{\text{coh}}(K)$ is the coherent scattering from one atom in electron units.

¹ A. Guinier, *X-Ray Diffraction in Crystals, Imperfect Crystals, and Amorphous Bodies* (W. H. Freeman and Company, Inc., San Francisco, 1963).

² N. S. Gingrich, *Rev. Mod. Phys.* **15**, 90 (1943).

³ K. Furukawa, *Rept. Progr. Phys.* **25**, 395 (1962).

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