

range of temperature." Our Fig. 3 shows that when the classical van der Waals gas equations are solved exactly, X^3 is nearly linear between $0.8T_c$ and $0.95T_c$.

Edwards also presents plots for helium of X^2 , X^3 , and $X^2/(1-\ln X)$ within 250 mdeg of T_c . In our Fig. 4, we present similar plots for a van der Waals gas above $0.95T_c$. Figure 4 shows that X^2 is accurately linear above $0.98T_c$.

Edwards concludes that the functional form $X^2/(1-\ln X)$ is the best asymptotic form for the coexistence curve of helium, with the critical point lowered 6 to 8 mdeg below the T_{58} value. Moldover and Little⁶ have obtained experimental evidence from their specific-heat work that the critical point on the T_{58} scale is 10 mdeg below the presently accepted value.

The details of derivations and numerical val-

ues of the various thermodynamic functions calculated for a van der Waals gas will be published as a Bureau of Mines publication.

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EFFECTS OF A LONG-RANGE OSCILLATORY POTENTIAL ON THE RADIAL DISTRIBUTION FUNCTION AND THE CONSTANT OF SELF-DIFFUSION IN LIQUID Na†

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Johnson, Hutchinson, and March¹ (JHM) have recently reported the striking observation that an analysis of the experimental radial distribution functions of liquid metals yields a long-range oscillatory (LRO) interatomic pair potential for a number of metals but gives the usual van der Waals potential for liquid argon. While LRO potentials have been derived theoretically² and observed experimentally³ for solids, it is not obvious that these results can be extrapolated to the liquid state. Further, the JHM analysis of the data is based on the Born-Green⁴ and Percus-Yevick⁵ equations which in themselves may not be capable of yielding accurate enough information⁶ to give the pair potentials quantitatively.

In addition to the time-independent study of JHM, there is some information about the time-dependent behavior of the motions of the atoms in liquid Na. Randolph⁷ has analyzed the slow-neutron inelastic spectrum of liquid Na and

obtained the time-dependent mean square displacement of the atoms, $\langle r^2 \rangle$. He concludes that at times less than 10^{-13} sec the displacements show a gaslike behavior, while at longer times the displacements increase slowly and show a high degree of solidlike behavior. It has been conjectured that such a solidlike behavior of $\langle r^2 \rangle$ might result from the existence of a LRO potential in a liquid metal.

It has been demonstrated by Rahman⁸ that the radial distribution function and $\langle r^2 \rangle$ can be calculated on a computer using the method of molecular dynamics. In particular, he solved the classical equations of motion with periodic boundary conditions for a system of 864 particles interacting with a Lennard-Jones potential. Applying this method to argon, he was able to reproduce the experimental radial distribution function and D , the constant of self-diffusion, which is simply related to the asymptotic form of $\langle r^2 \rangle$. Using the same computation-

al technique, we have investigated the dynamics and structure of liquid Na using various LRO potentials. These calculations therefore complement the JHM calculations. The JHM analysis consisted in going from the radial distribution function $\rho(r)$ to a pair potential (using various liquid-state statistical theories) while our procedure consists in going from a pair potential to $\rho(r)$ (using the method of molecular dynamics). The present calculations check the consistency of the JHM work and further examine the time-dependent behavior of $\langle r^2 \rangle$.

The calculations parallel Rahman's,⁸ with parameters chosen to fit Na characteristics at 373°K. The system consists of 686 particles in a box of dimensions 30.449 Å along an edge, corresponding to a density of 0.0243 atoms/Å³. Periodic boundary conditions are used to eliminate the effects arising from a surface. The potentials used in the calculation are compared with that of JHM in Fig. 1. The

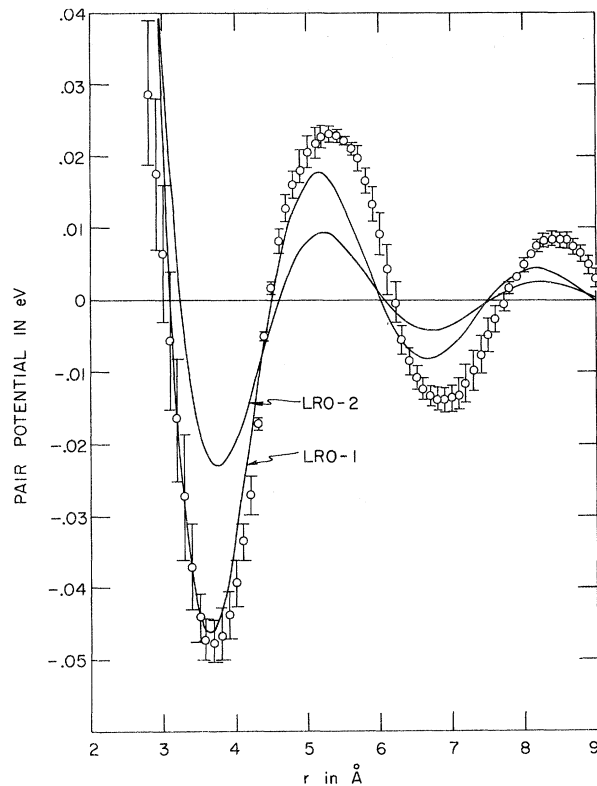


FIG. 1. The pair-potential curves for the JHM average potential (Φ) and the two LRO potentials used in the present calculations. LRO-1 was chosen to approximate the JHM potential while LRO-2 was chosen to yield a better fit to the experimental radial distribution function.

circles represent average values obtained by JHM using the Born-Green equation on data taken at 114 and 203°C (the horizontal bars associated with the circles give the range in potential values obtained at these temperatures). The LRO potentials used in our calculations were of the form $V = V_{\text{LRO}} + V_R$, where

$$V_{\text{LRO}} = -A(r_0/r)^3 \cos\{7.812[(r/r_0) + \beta]\}$$

and

$$V_R = 0.78 \exp(5.0724 - 10.7863r/r_0) \text{ eV.}$$

Here r is the interatomic distance, $r_0 = 3.72$ Å, and A and β are taken as adjustable parameters for varying the LRO part of the potential. The values of A and β used were $A = 0.048$ eV, $\beta = 0.5954$ for LRO-1 and $A = 0.027$ eV, $\beta = 0.5689$ for LRO-2. The Born-Mayer repulsive part of the potential,⁹ V_R , was included to take care of the hard core of the ions and insure the desired behavior at small distances. The parameters of V_R were those appropriate for Na⁹ and were the same for LRO-1 and LRO-2. The potentials thus constructed are compared with the JHM potential in Fig. 1. The LRO-1 potential was made to fit JHM in the region of the first minimum while LRO-2 was chosen to give a better fit to the observed radial density function.¹⁰ A comparison of theory (with potentials truncated at $r = 8.18$ Å) and experiment¹⁰ is shown in Fig. 2. It can be seen that the potential which more closely fits the JHM potential yields a ρ which is sharper and deviates from the average density ρ_0 by factor of about 1.6 more than the experimental value $\rho - \rho_0$ at the first maximum. The function ρ obtained from LRO-2 is a much better fit to the data. Several points are worth noting about these results: First, they demonstrate that, keeping a constant hard-core potential, the attractive part of the potential near the melting point can have an appreciable effect which suggests that the hard-sphere approximation¹¹ may be more unrealistic than is realized; second, the LRO-2 potential gives a better fit to the experimental $\rho(r)$ than the JHM potential; third, the LRO-2 potential has a quantitative resemblance in the region of the first minimum to the potential derived by Cochran⁹ from an analysis of the lattice dynamics of solid Na.

However, the agreement between LRO-2 and the observed structure is not⁹ a sufficient criterion for accepting the potential as a good ap-

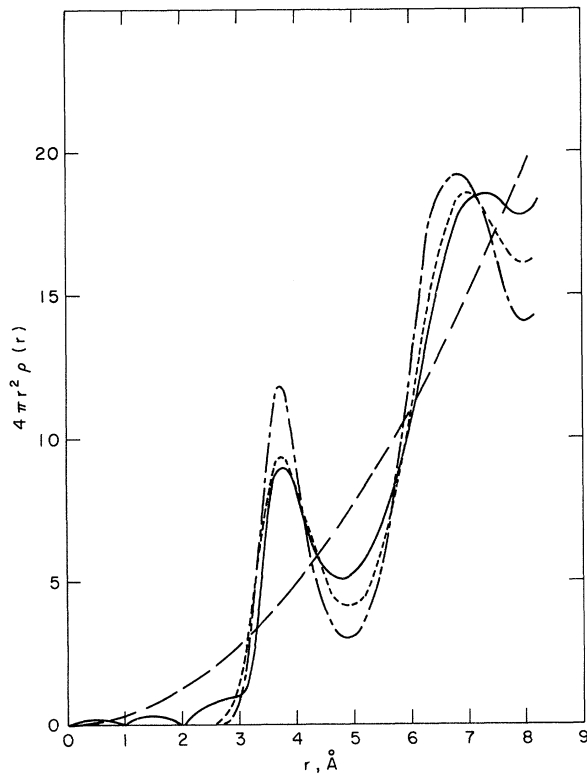


FIG. 2. The radial density function curves are shown for neutron diffraction experiment¹⁰ (solid curve), LRO-1 (dash-dot), LRO-2 (short-dashed), and the uniform density (long-dashed). The experimental results are given for 373°K and the calculated curves are for an average temperature of 371°K.

proximation. A further condition should be that the potential generate D , the constant of self-diffusion. In Fig. 3, we give the time-dependent behavior of $\langle r^2 \rangle$ for LRO-1 and LRO-2. The asymptotic behavior of $\langle r^2 \rangle$ yields D through the relationship $D = (\frac{1}{6})d\langle r^2 \rangle/dt$. We find the following values for D : $D(\text{LRO-1}) = 1.9 \times 10^{-5} \text{ cm}^2 \text{ sec}^{-1}$ and $D(\text{LRO-2}) = 5.8 \times 10^{-5} \text{ cm}^2 \text{ sec}^{-1}$, as compared with the experimental value¹² of $4.2 \times 10^{-5} \text{ cm}^2 \text{ sec}^{-1}$ at 100°C. Therefore, we see that the experimental value of D lies between the LRO-1 and LRO-2 values. For $t > 10^{-13}$ sec there is no evidence of the extreme solidlike behavior of $\langle r^2 \rangle$ reported by Randolph⁷ while for $t < 10^{-13}$ (i.e., in the region of gaslike behavior) there is over-all agreement between these results and Randolph's.⁷ While no evidence of extreme solidlike behavior is found, there are distinct oscillations in $\langle r^2 \rangle$ showing some evidence for residual solidlike behavior.

The curves in Fig. 3 are remarkably similar to the curve suggested by Vineyard¹³ from intuitive arguments. Such oscillations have not been observed in similar calculations on argon using the Lennard-Jones potential.⁸

On the basis of the present computations on Na, we have arrived at the following general conclusions: (1) At liquid densities, the Born-Green and Percus-Yevick equations do not allow the accurate determination of the pair potential; we have demonstrated that using the potential derived from these equations near the melting point of Na, we do not recover the radial distribution function. (2) If one uses D as a further check on the potential, comparing LRO results with Lennard-Jones results, we find that for Na a van der Waals type of potential is insufficient to match both the diffusion and the structure. Unlike argon, the diffusion and structure data seem to require a potential that has an attractive well followed by a repulsive region at larger distances (for examples of such potentials see Cochran⁹ and Ascarelli¹⁴). Such a potential might correspond to a highly damped oscillatory potential.

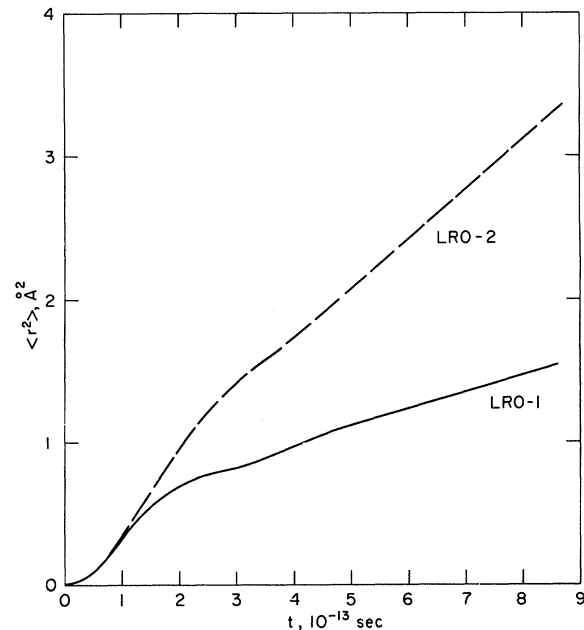


FIG. 3. The time dependence of the mean square displacements $\langle r^2 \rangle$ (averaged for 10 different origins in time) is given for LRO-1 (solid curve) and LRO-2 (dashed curve). The relatively sharp inflection in the LRO-1 curve at $t \sim 2 \times 10^{-13}$ sec is not a characteristic of $\langle r^2 \rangle$ obtained from the Lennard-Jones potential.

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OBSERVATION OF COOPERATIVE EFFECTS IN THE SCATTERING OF A LASER BEAM FROM A PLASMA

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Incoherent scattering of radiation from a plasma has been treated theoretically by a number of authors.¹ The spectral distribution of the scattered radiation is a function of the parameter

$$\alpha = \lambda_0 / 4\pi\lambda_D \sin^{1/2}\theta, \quad (1)$$

where λ_0 is the wavelength of the incident radiation, $\lambda_D = (kT_e/4\pi n_e e^2)^{1/2}$ is the Debye length in the plasma, θ the angle of observation of the scattering measured with respect to the forward direction, n_e the electron density, and T_e the electron temperature. For $\alpha \ll 1$, the spectrum reflects the electron velocity distribution and, for a thermal plasma, is a Gaussian centered on the wavelength λ_0 . This has been observed by a number of workers.²⁻⁵ For $\alpha \gg 1$, the spectrum is modified by cooperative interactions between the ions and electrons and consists of a central feature, whose width is of the order of the Doppler shift for ion thermal velocities, flanked by a pair of satellites, corresponding to scattering from longitudinal electrostatic oscillations in the plasma, which are displaced from the wave-

length of the incident beam by

$$\Delta\lambda = \frac{\omega_p}{2\pi c} \lambda_0^2 \left(1 + \frac{3}{\alpha^2}\right)^{1/2}, \quad (2)$$

where $\omega_p = (4\pi n_e e^2/m_e)^{1/2}$ is the plasma frequency. The central ion peak has been observed in radar backscatter from the ionosphere.⁶

For a thermal plasma only $1/\alpha^2$ of the scattered radiation lies in the satellites and, as a result, these have so far only been observed^{7,8} under conditions in which the level of electron density fluctuations is enhanced by nonthermal processes, although observation of the emergence of the satellites under conditions such that $\alpha \sim 1$ has been reported by Kunze, Fünfer, Kronast, and Kegel,³ by Kunze,⁴ and by Ramsden and Davies.⁹ Experiments designed to observe cooperative effects in the forward scattering of a ruby-laser beam from a plasma have been reported by DeSilva, Evans, and Forrest⁴ and by Bartoli, Katzenstein, and Lovisetto,¹⁰ and evidence has been obtained for a narrow central ion peak when $\alpha > 1$. We have been carrying out a similar experiment and wish to report measurements which show