

## SHORT-RANGE ORDER PARAMETER FOR LIQUID <sup>4</sup>He, Ne, AND Ar.

ПАРАМЕТР БЛИЗКОГО ПОРЯДКА ДЛЯ ЖИДКОФАЗНЫХ <sup>4</sup>He, Ne и Ar.

DUŠAN KORÝTÁR\*, PETER MRAFKO\*, Bratislava

In liquids only some short-range order of atoms is present, which fact is demonstrated by several diffuse maxima and minima in interference and pair correlation functions.

In [1] a short-range order parameter (SRO-parameter), the value of which increases with an increasing short-range order, has been introduced by means of pair correlation functions  $g(r)$ . The present work deals with the SRO-parameter for various states of liquid <sup>4</sup>He, Ne, and Ar.

The phase diagram of <sup>4</sup>He is shown in Fig. 1, where  $P$  is the pressure,  $T$  the temperature in the absolute scale, and the  $\lambda$ -line represents the transition between the normal and the superfluid <sup>4</sup>He ( $\lambda$ -transition). Neutron diffraction measurements in several thermodynamic states below and above helium  $\lambda$ -transition were performed by Mozer et al. [2]. By the Fourier transformation of the resulting interference functions, the corresponding pair correlation functions  $g(r)$  were computed by Mountain and Raveché [3]. Brostow and Sochanski [4] fitted them by an analytical expression with 10 parameters. By comparing their correlation functions with Table 2 in [3] one can find that pair correlation functions corresponding to states 13 and 14 must be in [4] interchanged [8].

Neutron diffraction measurements on liquid neon were performed by de Graaf and Mozer [5], the corresponding pair correlation functions were fitted by an analytical expression with 10 parameters [4], as well as results of X-ray diffraction measurements on liquid Ar, performed by Kirstein and Plügg [6].

The fitted analytical expressions of pair correlation functions were used in computing SRO-parameters by [1].

After re-scaling for the first peak, the pair correlation functions were substituted into the expression

$$D(s) = \int_0^s C(r)C(r+s) dr,$$

where  $R = 5$  (in the most probable atomic separation units) and

$$C(r) = g(r) - 1.$$

The SRO-parameter has the form

$$SRO = \int_0^R D^2(s) ds.$$

\* Fyzikálny ústav SAV, Dúbravská cesta, CS-899 30 Bratislava.

Computed values of the SRO-parameter as well as quantities characterizing the state of liquid <sup>4</sup>He, Ne, and Ar are tabulated in Tables 1, 2, and 3. There are presented also values of the integral

$$B = \int_0^R |C(r)| dr.$$

Table 1 shows the very interesting behaviour of the SRO-parameter for liquid <sup>4</sup>He:

1. The SRO-parameter above the  $\lambda$ -transition decreases with increasing temperature at a fixed density (states 16, 17, 18).
2. Above the  $\lambda$ -transition it decreases with an increasing density at a fixed temperature (18, 20, 22).
3. Below the  $\lambda$ -transition it increases with an increasing temperature at a fixed density (13, 14, 15).
4. It increases if the temperature is increased from below to above the  $\lambda$ -transition at a fixed density, provided we are close enough to the  $\lambda$ -line (13, 14, 15—16, 19—20, 21—22). If we are farther from the  $\lambda$ -line the statement does not hold (15—18). We can easily ascertain that the integral  $B$  does not behave in the same way.

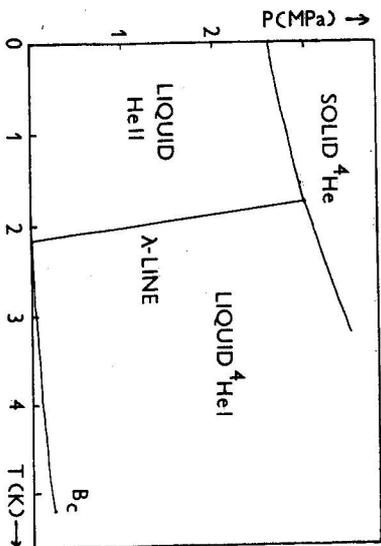


Fig. 1. Phase diagram of liquid <sup>4</sup>He.  $T$  — temperature,  $P$  — pressure. The  $\lambda$ -line represents the  $\lambda$ -transition between the normal and the superfluid state.

It is seen from Table 2 that in the case of liquid neon the SRO-parameter increases with an increasing density (at a fixed temperature).

Table 3 shows values of the SRO-parameter for the same state of liquid Ar, calculated from two independently measured  $g(r)$ . Considerable dispersion of the SRO-parameter in the case of independent measurements in the same state does not give us possibility of interpreting them, esp. if we do not know further details of measurement or calculation of the pair correlation functions.

The above mentioned results for liquid <sup>4</sup>He are consistent with the statement of Raveché and Mountain [7] who claim that because of the relatively light mass of helium and the symmetry of the Bose-Einstein statistics the deviation of  $g(r)$  from unity is a decreasing function of a decreasing temperature at a fixed density (whereas for classical fluids it increases with a decreasing temperature at a fixed density). Moreover, it decreases as the temperature of the liquid is lowered from above to below the superfluid transition.

The first part of their statement has been illustrated by the magnitude of the first maximum and minimum of  $g(r)$  [7] and corresponds to point 3 (see above). Point 4 corresponds to the second part of

Table 1

N	$\rho_0(\text{atm}^{-3})$	T(K)	$P(\times 10 \text{ MPa})$	B	SRO-par.
13	0.0230	1.86	4.31	0.8975	0.097 792
14	0.0230	2.05	3.96	0.8797	0.099 144
15	0.0230	2.13	3.60	0.9211	0.101 386
16	0.0230	2.14	3.60	0.9208	0.101 762
17	0.0230	2.30	3.79	0.9199	0.101 411
18	0.0230	2.84	5.25	0.9175	0.101 047
19	0.0236	2.02	6.50	0.8868	0.096 510
20	0.0236	2.86	7.81	0.8951	0.096 790
21	0.0245	1.94	11.60	0.8859	0.093 597
22	0.0245	2.86	12.51	0.8972	0.094 462

Values of the integral  $B$  and SRO-parameters for various states of liquid  $^4\text{He}$ .  $T$ —temperature,  $P$ —pressure,  $\rho_0$ —mean number density of atoms. Numerated as in [4].

Table 2

$N(\rho_0(\text{atm}^{-3})/T(\text{K})P(\times 10 \text{ MPa})\text{BSRO-par.})$	
230.0346935.05	21.41.21200.145 819
240.0333835.05	79.01.23530.145 884
250.0316935.05	140.01.25970.146 797

Values of the integral  $B$  and SRO-parameters for three states of liquid neon. Numerated as in [4].

Table 3

N	$\rho_0(\text{gcm}^{-3})$	T(K)	B	SRO-par.
8	1.054	133.0	1.1211	0.133 547
9	1.054	133.0	1.1039	0.128 724

Values of the integral  $B$  and SRO-parameters for one states of liquid Ar from two independent measurements. Numerated as in [4].

their statement. However, the increase of the SRO-parameter when passing from below to above the  $\lambda$ -line is limited. This limitation is a consequence of point 1.

## REFERENCES

- [1] Korytár, D., Mrafko, P.: submitted to Acta phys. slov.
- [2] Mozet, B., Graaf, L. A., Le Neindre, B.: Phys. Rev. A9 (1974), 448.
- [3] Mounlain, R. D., Raveché H.: J. Res. Natl. Bur. Stand. U. S. A77 (1974), 725.
- [4] Brostow, W., Sochanski, J. S.: Phys. Rev. A13 (1976), 882.
- [5] De Graaf, L. A., Mozet, B.: J. Chem. Phys. 55 (1971), 4967.
- [6] Kirstein, B., Pings, C. J.: unpublished.
- [7] Raveché, H. J., Mounlain, R. D.: Phys. Rev. A9 (1974), 435.
- [8] Brostow, W.: private communication.

Received August 15<sup>th</sup>, 1977