Collective Motions in Classical Liquids (*).

III: Liquid Sodium (**).

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Summary. — The atomic dynamics of liquid sodium at high frequencies and short wavelengths is investigated on the basis of the theory developed for liquid argon in paper II of this series and using the static structure factor and the velocity autocorrelation function determined by Rahman and by Schiff by computer simulation with two different interionic potentials. Specifically, numerical calculations are presented for the spectral function of the longitudinal-current correlations, the quasi-elastic scattering and the scattering law in the range of momentum transfer \((0.3 \div 6) \text{ Å}^{-1}\). The results of the calculation appear to be in fair agreement with the rather scarce neutron scattering data which are available at present.

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1. - Introduction.

In paper I of this series a simple theory of high-frequency and short-wavelength collective motions in classical liquids, based on a generalized random-phase approximation, was given by Singwi, Sköld and Tosi (1). In paper II an improved version of this theory was presented by Pathak and Singwi (2). The latter theory satisfies exactly the low-order moments of the dynamic form factor $S(q, \omega)$ up to the fourth, and was successfully applied to explain the observed behaviour of $S(q, \omega)$ in liquid argon, for which there are now available fairly exhaustive and reliable data from computer simulations (3) and laboratory experiments (4).

In contrast to this, experimental data on liquid metals are meager. From a theoretical standpoint, the main difficulty is the lack of a reliable interionic potential. This fact, together with the long-range nature of the potential, has to some extent hampered progress in computer-simulated experiments in liquid metals. The purpose of this work is twofold: i) to present a numerical calculation of $S(q, \omega)$ for the simplest metal, liquid sodium, based on a two-body potential which is derived from first principles (5) and in whose validity some confidence has been gained (6-7); and ii) to stimulate further experimental work on liquid metals. The presently available data on liquid sodium (8-9) are in general agreement with the predictions of our theory, but they are neither exhaustive nor very reliable.

The theory of the dynamic structure factor applied in this paper requires a knowledge of the static structure factor. The latter for liquid sodium with the potential of Shyu et al. (6) was kindly provided to us by Rahman (10). In order to test the sensitivity of the results to the choice of the interionic potential, we have also performed the calculation with the model potential used by Schiff (11) in computer-simulated experiments to calculate the static correlation function for liquid sodium.

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