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1989 J. Phys.: Condens. Matter 1 9665

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## On the quasiparticle spectrum and maxima of the dynamic ion structure factor in liquid metals

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Received 4 October 1988

**Abstract.** The ion density–density retarded Green function of an elementary liquid metal has been investigated in terms of the electron–ion interaction pseudopotential. This notion has been used for studying the spectrum of quasiparticles due to ion excitations,  $\omega_i(k)$ , and its relation to the position of the maximum,  $\omega_{\max}(k)$ , of the dynamic ion structure factor. Numerical calculations for liquid rubidium show that the quasiparticles are well defined within the region of  $k \leq 1 \text{ \AA}^{-1}$ , where deviations are found from the acoustic-dispersion curve.

Detailed experimental information is available at present on the behaviour of the dynamic ion structure factor,  $S_{ii}(k, \omega)$ , in liquid metals as measured in the experiments on inelastic neutron scattering (Cocking and Egelstaff 1965, Gläser *et al* 1972, Copley and Rowe 1974). Considerable progress has also been made in theoretical examination of the function  $S_{ii}(k, \omega)$  (Rahman 1974, Goda and Osabe 1978), the examination being reduced to the description of  $S_{ii}(k, \omega)$  followed by the construction of the dependence  $\omega_{\max}(k)$  for the position of the maximum in  $S_{ii}(k, \omega)$ . The curve  $\omega_{\max}(k)$  for a given system is usually interpreted as the spectrum of quasiparticles in the system. It is natural in this connection to pose the question about quasiparticles in the ion subsystem of a liquid metal. This requires an examination of the complex poles,  $\omega_i(k)$ , of the ion density–density retarded Green function,  $L_{ii}^R(k, \omega)$ , that completely determines the spacetime behaviour of the mean ion density in a weak applied field and is directly related to the dynamic structure factor  $S_{ii}(k, \omega)$  (for real  $\omega$ ):

$$S_{ii}(k, \omega) = -2\hbar[1 - \exp(-\hbar\omega/T)]^{-1} \text{Im} L_{ii}^R(k, \omega) \quad (1)$$

$$L_{ab}^R(k, \omega) = \frac{i}{\hbar V} \int_0^\infty dt \exp(i\omega t) \langle [\hat{\rho}_k^a(t), \hat{\rho}_{-k}^b(0)] \rangle. \quad (2)$$

Here  $\hat{\rho}_k^a(t)$  stands for the Fourier component of the density (number of particles per unit volume) operator for the particles of type  $a$ , characterised by charge  $z_a$ , mass  $m_a$  and density  $n_a$ , in the Heisenberg representation;  $\langle \dots \rangle$  designates averaging with the equilibrium Gibbs operator corresponding to the exact Hamiltonian for the considered two-component plasma of the liquid metal, for which  $\sum_{a=e,i} z_a n_a = 0$ ,  $e$  denoting electrons, and  $i$ , ions;  $V$  is the volume of the system. The definition (2) is to be understood

in the limit of thermodynamics:  $V \rightarrow \infty$ ,  $n_a = N_a/V = \text{constant}$ . Naturally, quasiparticles can only exist if

$$\gamma_i = \text{Im } \omega_i(k)/\text{Re } \omega_i(k) \ll 1. \quad (3)$$

Thus, on defining  $L_{ii}^R(k, \omega)$  as a function of the complex variable  $\omega$ , one can examine  $S_{ii}(k, \omega)$  and determine the quasiparticle spectrum  $\omega_i(k)$  and the way it is related to  $\omega_{\text{max}}(k)$ .

For complex  $\omega$ , the retarded Green function  $L_{ii}^R(k, \omega)$  is the analytic extension of the corresponding temperature Green function,  $L_{ii}^T(k, i\Omega)$ , from the discrete set of points  $\Omega_n = 2\pi n/T$ ,  $n = 0, 1, \dots$ , into the upper half-plane of the complex  $\omega$ . Temperature Green functions can be calculated by means of the well developed diagram technique (Abrikosov et al 1962). The technique makes it easy to ascertain that

$$L_{ab}^T(k, i\Omega) = \Pi_{ab}^T(k, i\Omega) + \sum_{cd} \Pi_{ac}^T(k, i\Omega) U_{cd}(k) L_{db}^T(k, i\Omega). \quad (4)$$

Here  $U_{aa}(k) = 4\pi z_a^2/k^2$ ;  $U_{ei}(k) = 4\pi z_e z_i/k^2 + \varphi(k)$  is the local model pseudopotential of electron-ion interaction, with  $|\varphi(k \rightarrow 0)| < \infty$ ;  $\Pi_{ab}^T$  stands for the polarisation operator, which is the part of the Green function  $L_{ab}^T(k, i\Omega)$  irreducible in the 'k-channel' along one line of interaction. In the case of weak electron-ion interaction (in terms of the pseudopotential), the contribution of the functions  $\Pi_{ie}^T(k, i\Omega)$  and  $\Pi_{ei}^T(k, i\Omega)$  can be neglected and advantage can be taken of the approximate equality  $\Pi_{ee}^T(k, i\Omega) \approx \Pi_{ee}^{(0)}(k, i\Omega)$ , with  $\Pi_{ee}^{(0)}(k, i\Omega)$  denoting the exact polarisation operator for the electron fluid in the positive correcting background (Trigger 1976). As a result of the procedure of analytic extension, we obtain

$$L_{ii}^R(k, \omega) = \Pi_{ii}^R(k, \omega)(1 - U_{ee}(k)\Pi_{ee}^{(0)}(k, \omega))/F(k, \omega) \quad (5)$$

with

$$F(k, \omega) = 1 - U_{ee}(k)\Pi_{ee}^{(0)}(k, \omega) - U_{ii}(k)\Pi_{ii}^R(k, \omega) - \Pi_{ii}^R(k, \omega)\Pi_{ee}^{(0)}(k, \omega)(U_{ei}^2(k) - U_{ee}(k)U_{ii}(k)). \quad (6)$$

Taking into account the fact that  $|\omega_i(k)| \ll kv_F$ , where  $v_F = (\hbar/m_e)(3\pi^2 n_e)^{1/3}$  is the Fermi velocity of the free electron, we derive from (5), (6) that

$$L_{ii}^R(k, \omega) = \Pi_{ii}^R(k, \omega)(1 - U_{ii}^{\text{eff}}(k)\Pi_{ii}^R(k, \omega))^{-1} \quad (7)$$

with the effective potential of ion-ion interaction,  $U_{ii}^{\text{eff}}(k)$ , given by

$$U_{ii}^{\text{eff}}(k) = U_{ii}(k) + U_{ei}^2(k)\Pi_{ee}^{(0)}(k, 0)(1 - U_{ee}(k)\Pi_{ee}^{(0)}(k, 0))^{-1}. \quad (8)$$

Within the approximation in question, the function  $\Pi_{ii}^T(k, i\Omega)$  is no other than that part of the function  $L_{ii}^T(k, i\Omega)$  for the one-component ion fluid with the short-range interaction potential  $U_{ii}^{\text{eff}}(k)$  which is irreducible in the 'k-channel' along one interaction line. This accounts for the qualitative similarity in the behaviour of the dynamic structure in inert liquids and liquid metals. The difference is associated with the particular shape of the potential.

It follows from (7) that the poles  $\omega_i(k)$  of the Green function  $L_{ii}^R(k, \omega)$  can be determined from the expression

$$\varepsilon(k, \omega) = 1 - U_{ii}^{\text{eff}}(k)\Pi_{ii}^R(k, \omega) = 0 \quad (9)$$

which is equivalent to the equation for the natural longitudinal oscillations of charge in

the electron fluid (Silin 1971) and solved for real  $k$ . As mentioned above, quasiparticles are out of the question unless the condition (3) is satisfied. Therefore the quantity  $\text{Re } \omega_i(k)$  should be determined from the equation

$$\text{Re } \varepsilon(k, \omega) = 0. \quad (10)$$

In this case

$$\text{Im } \omega_i(k) = - \left( \frac{\partial \text{Re}(k, \omega)}{\partial \omega} \right)^{-1} \text{Im } \varepsilon(k, \omega) \Big|_{\omega = \text{Re } \omega_i(k)}. \quad (11)$$

Solving (9), (10) requires that the function  $\Pi_{ii}^R(k, \omega)$  be calculated for the case of strong interaction. By analogy with the electron fluid theory (Geldart and Vosko 1966), we shall allow for correlation effects by means of the function  $G_{ii}(k, \omega)$ :

$$\Pi_{ii}^R(k, \omega) = \Pi_{ii}^{\text{RPA}}(k, \omega) (1 + U_{ii}^{\text{eff}}(k) G_{ii}(k, \omega) \Pi_{ii}^{\text{RPA}}(k, \omega))^{-1} \quad (12)$$

where  $\Pi_{ii}^{\text{RPA}}(k, \omega)$  is the polarisation operator for the zero estimate of the interaction (random-phase approximation). Since  $|\hbar\omega_i(k)| \ll T$  for elementary liquid metals, we can confine ourselves to the case of classical statistics. Then (Sitenko 1965)

$$\begin{aligned} \Pi_{ii}^{\text{RPA}}(k, \omega) &= - (n_i/T) \{1 - \alpha(z) + i \pi^{1/2} z \exp(-z^2)\}; \\ \alpha(z) &= 2z^2 \exp(-z^2) \int_0^z dx \exp(x^2), \quad z = (m_i \omega / 2Tk)^{1/2}. \end{aligned} \quad (13)$$

It is natural to suppose that all the effects of the  $\omega$ -dependence of  $\Pi_{ii}^R(k, \omega)$  are included in  $\Pi_{ii}^{\text{RPA}}(k, \omega)$ , i.e.,  $G_{ii}(k, \omega) \approx G_{ii}(k)$ . Taking into account that, within the framework of classical statistics

$$\begin{aligned} S_{ii}(k, \omega) &= - (2T/\omega) \text{Im } L_{ii}^R(k, \omega) \\ n_i S_{ii}(k) &= \int_{-\infty}^{\infty} d\omega (1/2\pi) S_{ii}(k, \omega) = - TL_{ii}^R(k, 0) \end{aligned}$$

we arrive, from (7), (12), (13), at

$$G_{ii}(k, \omega) \approx (T/n_i U_{ii}^{\text{eff}}(k)) C_{ii}(k) + 1. \quad (14)$$

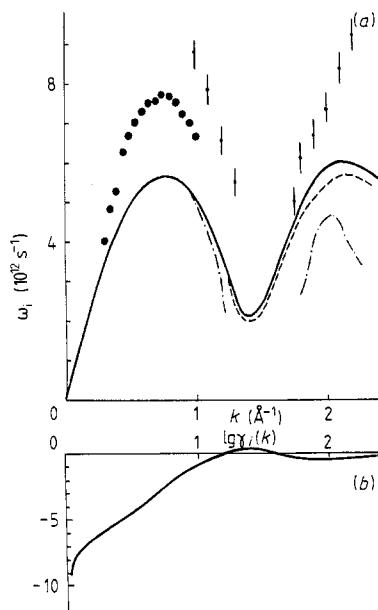
Here  $S_{ii}(k)$  is the static structure factor and  $C_{ii}(k)$  is the direct correlation function

$$C_{ii}(k) = (S_{ii}(k) - 1) S_{ii}^{-1}(k). \quad (15)$$

Note that the expression for  $S(k, \omega)$  obtained through the use of the approximation (14) coincides with that derived by Nelkin and Ranganathan (1967) with the aid of the kinetic equation. For small values of  $k$  there exists a solution of (10) that describes slow-damped acoustic vibrations in the liquid metal

$$\text{Re } \omega_i(k) \approx Sk. \quad (16)$$

For the calculations for liquid rubidium at  $T = 320$  K we make use of the pseudopotential due to Ashcroft (1968) with the parameter  $r_A = 2$  atomic units and the structure factor corresponding to the hard-sphere potential (Wertheim 1963). The packing parameter,  $\eta$ , was determined by the experimental value of the isothermal compressibility of liquid rubidium,  $\kappa_T$ , with the help of the relation  $\lim_{k \rightarrow 0} S_{ii}(k) = n_i T \kappa_T$  ( $\eta = 0.463$ ). The function  $\Pi_{ee}^{(0)}(k, 0)$  was calculated in the



**Figure 1.** The position of the maximum in the dynamic ion structure factor: full circles, the experimental data of Copley and Rowe (1974); vertical bars, the experimental data of Gläser *et al* (1972); chained curve, the present calculation; broken curve, the numerical solution of (10) with the RPA value of  $\Pi_{ee}^{(0)}(k, 0)$ ; solid line, the numerical solution of (10) with the value of  $\Pi_{ee}^{(0)}(k, 0)$  due to Geldart and Vosko (1966). The results of calculations for the damping factor  $\gamma_i$  are plotted on a logarithmic scale at the bottom.

random-phase approximation (RPA) using the expression derived by Geldart and Vosko (1966).

Figure 1 presents the results of calculations for liquid rubidium at a temperature of 320 K and the comparison with experimental data (Copley and Rowe 1974, Gläser *et al* 1972). First of all, it should be noted that the calculated  $k$ -dependence of the position of the peaks in the  $\omega$ -dependence of  $S_{ii}(k, \omega)$  is in satisfactory agreement with the experimental data. It is essential that the solution of (10) virtually coincides with the calculated  $k$ -dependence of the position of the peaks in  $S_{ii}(k, \omega)$ . But, as indicated above, the quasiparticles are well defined only if the damping factor  $\gamma_i$  is small. The calculation has shown that  $\gamma_i$  is quite a quickly increasing function of  $k$ . On the assumption that the condition of existence of the quasiparticles is given by  $\gamma_i \leq 1/10$ , the extreme magnitude of the wavevector for liquid rubidium under the specified conditions is  $k_{\max} = 1 \text{ \AA}^{-1}$ , the dispersion curve significantly differing at  $k \approx k_{\max}$  from the ordinary acoustic one, realised for small wavenumbers. Moreover, the one-to-one correspondence in the dispersion curve is not fulfilled in the region of well defined quasiparticles: two values of wavelength correspond to one value of  $\omega$ . Apparently, this effect can be directly investigated in the experiments on sound-wave propagation in liquid metals. It can be seen from the calculations that the break in the curve  $\omega_{\max}(k)$  is caused by the circumstance that  $\gamma_i \geq 1$  within a corresponding region of wavevectors. It is interesting that in this region the solution of (10) has the form similar to the minimum in the roton region in superfluid helium. However, in accordance with the above, rotons do not exist as quasiparticles in liquid metals. Note that the difference in the expressions used for  $\Pi_{ee}^{(0)}(k, 0)$  does not tell on the magnitude of the function  $\lg \lambda_i$ .

In conclusion, it should be noted that using the concept of quasiparticles in the excited ion subsystem of a liquid metal and the information concerning their spectra allows the thermodynamic characteristics of the ion subsystem to be considered in a similar manner to that for the case of solid metals, where phonons are introduced as quasiparticles.

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