Collective modes and gapped momentum states in liquid Ga: experiment, theory and simulation

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Collective excitations in liquids are important for understanding liquid dynamical and thermodynamic properties. Gapped momentum states (GMS) are a notable feature of liquid dynamics predicted to operate in the transverse sector of collective excitations. Here, we combine inelastic neutron scattering experiments, theory and molecular dynamics modelling to study collective excitations and GMS in liquid Ga in a wide range of temperature and k-points. We find that all three lines of enquiry agree for the longitudinal sector of liquid dynamics. In the transverse sector, the experiments agree with theory, modelling as well as earlier X-ray experiments at larger k, whereas theory and modelling agree in a wide range of temperature and k-points. We observe the emergence and development of the k-gap in the transverse sector which increases with temperature and inverse of relaxation time as predicted theoretically.

INTRODUCTION

Many important properties of solids are related to collective excitations, phonons 1. For example, solid energy and heat capacity are consistently understood on the basis of phonons. For a long time, it remained unclear whether this approach applies to liquids where dynamical disorder and the absence of a fixed lattice seemingly preclude the expansion of vibrational energy around a reference point required to derive phonons as in the solid theory. Calculating the liquid energy as an integral over correlation functions and the interaction potential is highly system-dependent due to strong interactions. For this reason, it is believed that liquid thermodynamic properties can not be calculated in general form, contrary to solids and gases 1. This singles out the liquid state as the state not amenable to general theoretical treatment. Known more generally as the absence of a small parameter in liquids, this was the long-standing problem in statistical physics research and teaching 2.

Phonons in the continuum or hydrodynamic limit of small frequency ω and wavevector k, are sound waves 3. As these phonons make negligible contribution to the density of states, they make only a small contribution to the liquid energy. An important question is whether liquids can support solid-like phonons with large k and ω approaching the zone boundary as in solids, therefore setting the system energy as in the solid theory. Experiments have ascertained that this is the case for longitudinal phonons 1,2, but solid-like transverse phonons have proved to be harder to detect experimentally and understand theoretically. Propagating transverse modes in liquids were first detected in viscous liquids. Later inelastic scattering experiments ascertained the same in low-viscosity liquids such as Na (see Ref. 4 for review). The transverse modes are important because (a) transverse modes have been traditionally viewed as a property of the solid state and are associated with the system having a well-defined shape set by the ability to support shear waves and (b) in solid theory, these modes contribute 2/3rds of the system energy and heat capacity.

As compared to solids, it took long time to understand the propagation of phonons and in particular solid-like transverse phonons in liquids. Generalised hydrodynamics 5 was a popular approach which aims to start with the hydrodynamic description where the low-frequency longitudinal sound is the only collective mode in the system and subsequently generalize it to include the non-hydrodynamic solid-like property of nonzero response to shear stress. This results in the prediction that liquids are able to support shear modes as solids do, but only above a finite critical value of the wavevector, k_g. This is in interesting contrast to the commonly held view that liquids are able to support transverse modes above a certain finite frequency ω = 1/τ rather than above a finite wavevector 3. In other words, liquids are predicted to have a gap in k-space, rather than ω-space.

The prediction of the k-gap was indirectly present in the Frenkel theory 6 which preceded generalized hydrodynamics by many decades. Using Maxwell interpolation to describe the viscoelastic liquid response, Frenkel represented viscosity as an operator in the Navier-Stokes
where \( c \) is the transverse speed of sound in the solid and \( \tau \) is liquid relaxation time.

In the Maxwell-Frenkel picture, \( \tau \) in Eq. (1) is \( \eta_s / G_\infty \), where \( G_\infty \) is the high-frequency shear modulus and \( \eta_s \) is shear viscosity. At the atomistic level, Frenkel theory identified \( \tau \) with liquid relaxation time, the average time between molecular jumps around quasi-equilibriums positions (1). This has become an accepted view (8).

Eq. (1) predicts that liquids are able to support propagating phonons but only with wavevectors above \( k_g \), where

\[
k_g = \frac{1}{2c\tau}
\]

which interestingly and importantly differs from solids where \( k_g \) is zero or, to be more precise, is a very small number set by the system size.

Gapped momentum states (GMS) are interesting on their own: for example, Eq. (1) implies an anomalous phase and group velocities as compared to the more common dispersion relation with the energy gap (11).

It has been realized that in addition to liquids, GMS emerge in a surprising variety of areas (11), including strongly-coupled plasma, electromagnetic waves, non-linear Sine-Gordon model, relativistic hydrodynamics and holographic models. In some of these areas, GMS are central to the system behavior and are actively studied. In other areas, GMS are not well understood and are often not discussed. A recent review (11) suggests that there is likely to be a common underlying mechanism for GMS in different areas.

As far as liquid theory is concerned, the dispersion relation (1) is important because it can be used to calculate the liquid energy as is done in solids (2, 12). This calculation predicts a decrease of constant-volume liquid heat capacity with temperature, as is seen experimentally. This decrease is caused by the reduction of the number of phonons propagating above \( k_g \) because, according to Eq. (2), the range of \( k \)-points where phonons propagate shrinks with temperature (\( \tau \) decreases with temperature) (12). In other words, the phase space of phonons in liquids decreases with temperature, in notable contrast to solids.

Although GMS have been seen in simulations of both liquids and supercritical fluids below the Frenkel line (12, 16), there is no experimental evidence for it in liquids. As recently reviewed (11), the only experimental evidence for GMS comes from imaging particles in strongly-coupled plasma (13). This has set one of the motivations behind this work.

Ga has a low melting point and is a convenient system in experimental scattering experiments. Ga is also a substance with a number of unusual properties. This trivalent element is one of the few metallic-like systems that does not crystallize into any simple structure. It shows an extremely rich polymorphism that includes a stable, low-pressure phase, \( \alpha \)-Ga (orthorhombic structure with eight atoms per unit cell), and two other phases which are stable at high pressure: \( \text{Ga-II} \) (a body centered cubic phase with twelve atoms per unit cell) and \( \text{Ga-III} \) (tetragonal phase). Furthermore, the phase diagram of gallium contains a number of metastable phases known as \( \beta, \gamma, \delta, \) and \( \epsilon \) with melting points of 256.8, 237.6, 253.8, and 244.6 K all well below that of 302.93 K for \( \alpha \)-Ga. The wide temperature range of the existence of the liquid phase (303 – 2500 K) and the low pressure of saturated vapors at \( T < 1400 \) K makes gallium a promising coolant with outstanding thermohydraulic properties. These properties, together with low melting point, make Ga an interesting and convenient system to study experimentally.

In this paper, we combine inelastic neutron scattering experiments, modelling, and theory to study phonons in liquid Ga in at a wide range of temperatures, frequencies, and wavenumbers. We find that all three methods agree for the longitudinal phonons. For transverse phonon branch, we find agreement between (a) our modelling and theoretical results with inelastic neutron and X-ray scattering at higher \( k \) and (b) theory and modelling data in the entire range of \( k \)-points showing the \( k \)-gap. We observe the increase of the \( k \)-gap with temperature and inverse of relaxation time, in agreement with Maxwell-Frenkel theory. This agreement, together with the agreement of all three lines of enquiry for the longitudinal mode, builds up the body of evidence for GMS. Our results serve as a stimulus for future inelastic neutron scattering experiments investigating transverse modes in liquids and its evolution in terms of gapped momentum states.

### INELASTIC NEUTRON SCATTERING EXPERIMENT

Seven molten gallium samples were prepared in vacuum-sealed quartz glass cylinders with 2.5 mm radius. The neutron scattering experiment (INS) was performed at the MARI chopper spectrometer at ISIS with incident
neutron energies of 7 meV and 40 meV$^1$. The energy resolution was $\Delta E = 0.3$ to 2 meV, for incident energies 7 to 40 meV at wavenumbers 0.4 to 1.5 Å$^{-1}$. We collected our data at 6 temperature points in a wide temperature range: 313, 400, 500, 600, 700 and 794 K.

The neutron scattering intensity $I(k, \omega)$ is related to the dynamic structure factor $S(k, \omega)$ through convolution with the experimental resolution function $R(k, \omega)$ $^{14}$:

$$I(k, \omega) \propto \int R(k, \omega - \omega') S_q(k, \omega') d\omega' + B(k, \omega), \quad (3)$$

$$S_q(k, \omega) = \frac{\hbar \beta \omega}{1 - e^{-\hbar \beta \omega}} \left[ \frac{\sigma_{coh}}{\sigma_{coh} + \sigma_{incoh}} S(k, \omega) + \frac{\sigma_{incoh}}{\sigma_{coh} + \sigma_{incoh}} S_s(k, \omega) \right] \quad (4)$$

$^{1}$ Professor Martin Dove et al; (2019): Phonon dynamics in liquid gallium, STFC ISIS Neutron and Muon Source, [https://doi.org/10.5286/ISIS.E.RB1820566]
Here, $S_q(k, \omega)$ and $S_s(k, \omega)$ are the quantum dynamic and self-dynamic structure factors, respectively; the term $B(k, \omega)$ corresponds to the background; $\beta = 1/(k_B T)$ is the reciprocal temperature; $\sigma_{\text{coh}}$ and $\sigma_{\text{incoh}}$ are the cross sections of coherent and incoherent scattering, respectively [for Ga $\sigma_{\text{incoh}}/\sigma_{\text{coh}} + \sigma_{\text{coh}} = 0.0658$].

The INS spectra of liquid gallium at the wave-numbers below the boundary of the first pseudo-Brillouin zone, $k_m/2$, are reported in Fig. [1]. Here, $k_m$ is the position of the principal maximum in static structure factor $S(k)$. The experimental scattering law was decomposed into partial components associated with various contributions of neutron scattering on matter: multiple, inelastic coherent and inelastic incoherent, quasi-elastic coherent and quasi-elastic incoherent scattering [16].

The intensity neutron scattering on matter: multiple, inelastic coherent and quasi-elastic incoherent scattering) were each fitted using a single Lorentzian function.

MOLECULAR DYNAMICS SIMULATIONS

Molecular dynamics (MD) simulations have been performed in the $NPT$-ensemble for the system consisting of 32000 particles interacting via the EAM potential [18] at the temperatures $T = [313, 400, 500, 600, 700, 794]$ K and pressure of about 1.0 bar.

The dynamic structure factor can be computed on the basis of MD results as

$$S(k, \omega) = \frac{S(k)}{2\pi} \text{Re} \int_{-\infty}^{\infty} \frac{\langle \delta \rho^*(k, 0) \delta \rho(k, t) \rangle}{\langle |\delta \rho(k, 0)|^2 \rangle} e^{i\omega t} dt.$$  \hspace{1cm} (6)

We also calculate the spectral densities

$$\widetilde{C}_\alpha(k, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} C_\alpha(k, t) e^{i\omega t} dt, \quad \alpha \in \{L, T\}$$  \hspace{1cm} (7)

of the time correlation functions (TCF) of the longitudinal current $C_L(k, t)$ and the transverse current $C_T(k, t)$,

$$C_L(k, t) = \frac{1}{N} \left\langle j_x(k, t) j_x(-k, 0) \right\rangle,$$  \hspace{1cm} (8)

$$C_T(k, t) = \frac{1}{2N} \left\langle j_x(k, t) j_x(-k, 0) + j_y(k, t) j_y(-k, 0) \right\rangle.$$  \hspace{1cm} (9)

Here, $\delta \rho(k, t)$ is the density fluctuations, $j(k, t)$ is the velocity current and the wave-vector $k$ is directed along the $z$-axis. Dispersion curves of longitudinal and transverse excitations are obtained from the location of maxima of the spectral densities $\widetilde{C}_L(k, \omega)$ and $\widetilde{C}_T(k, \omega)$ at various values of $k$. The longitudinal current spectra are related to the dynamic structure factor by the equation

$$\widetilde{C}_L(k, \omega) = \frac{\omega^2}{k^2} S(k, \omega).$$  \hspace{1cm} (10)

COLLECTIVE EXCITATIONS AND DISPERSION RELATION

According to the formalism of the time correlation functions [19], the spectral density of TCF of the longitudinal current spectra $\widetilde{C}_L(k, \omega)$ can be represented in the form of continuous fraction:

$$\widetilde{C}_L(k, \omega) = \frac{k_B T}{\pi m} \text{Re} \begin{pmatrix} \frac{1}{i\omega + \Delta_1(k)} \\ \frac{1}{i\omega + \Delta_2(k)} \end{pmatrix} \left( \frac{\Delta_1(k)}{i\omega + \Delta_2(k)} \right).$$  \hspace{1cm} (11)

Here, $\Delta_n(k), n = 1, 2, 3, \ldots$ are the relaxation parameters, which are related with the normalized frequency moments $\omega^{(2m)}_L(k)$ of $C_L(k, \omega)$:

$$\omega^{(2j)}_L(k) = \frac{\int \omega^2 \widetilde{C}_L(k, \omega) d\omega}{\int \widetilde{C}_L(k, \omega) d\omega}, \quad j = 1, 2, \ldots$$  \hspace{1cm} (12)

using the following expressions:

$$\Delta_1(k) = \omega^{(2)}_L(k),$$
$$\Delta_2(k) = \omega^{(4)}_L(k) - \omega^{(2)}_L(k),$$
$$\Delta_3(k) = \omega^{(6)}_L(k) - \omega^{(4)}_L(k)^2,$$
$$\ldots$$  \hspace{1cm} (13)

In the classical case, only the even frequency moments take non-zero values. The second moment of the spectral density $\widetilde{C}_L(k, \omega)$ in the case of a spherical pair potential of interatomic interaction $U(r)$ can be written as [20]

$$\omega^{(2)}_L(k) = \frac{3k_B T}{m} k^2 + \frac{\rho}{m} \int_{0}^{\infty} g(r) \left( 1 - \cos(kz) \right) \frac{\partial^2 U(r)}{\partial z^2} d^3r.$$  \hspace{1cm} (14)
FIG. 2: Intensity neutron scattering $I(k, \omega)$ in molten gallium. Solid purple line represents the dynamic structure factor calculated from molecular dynamics simulation data. The green line shows the resulting function containing partial components associated with various types of neutron scattering on matter: multiple, quasi-elastic coherent and quasi-elastic incoherent scattering. Dotted line depicts the spectrometer resolution function.

FIG. 3: Dynamic structure factor of liquid gallium calculated from molecular dynamics simulations.
Here, \( g(r) \) is the radial distribution function of two particles. The expressions for the moments of higher orders will contain integrals of many-particle distribution functions and higher order derivatives of the potential. The relaxation parameters can be determined numerically from molecular dynamics simulation data in accordance with the basic definitions [21]:

\[
\Delta_n(k) = \frac{\langle |A_n(k,0)|^2 \rangle}{\langle |A_{n-1}(k,0)|^2 \rangle}, \quad n = 1, 2, \ldots, (15)
\]

where

\[
A_0(k,t) = j_L(k,t), \\
A_1(k,t) = \frac{\partial A_0(k,t)}{\partial t}, \\
A_2(k,t) = \frac{\partial A_1(k,t)}{\partial t} + \Delta_1 A_0(k,t), \\
\ldots, \\
A_n(k,t) = \frac{\partial A_{n-1}(k,t)}{\partial t} + \Delta_{n-1} A_{n-2}(k,t). (16)
\]

The values of the relaxation parameters \( \Delta_1(k), \Delta_2(k), \Delta_3(k) \) and \( \Delta_2(k) \) were numerically computed from MD simulation data by means of relations (15) and (16).

According to self-consistent relaxation theory, the spectral density \( \tilde{C}_L(k,\omega) \) of longitudinal current is defined as

\[
\tilde{C}_L(k,\omega) = \frac{k_BT}{2\pi m} \frac{\Delta_1(k)\Delta_2(k)\Delta_3(k)\sqrt{4\Delta_3(k) - \omega^2}}{B_0(k) + B_2(k)\omega^2 + B_4(k)\omega^4}, (17)
\]

with

\[
B_0(k) = \Delta_1^2(k)\Delta_2^2(k), \\
B_2(k) = \Delta_3(k) \left[ \Delta_2(k) \left\{ \Delta_1(k) + \Delta_2(k) \right\} \right. \\
- 2\Delta_1(k)\Delta_3(k) \left. \right], \\
B_4(k) = \Delta_3(k) \left[ \Delta_3(k) - \Delta_2(k) \right].
\]

The maxima of longitudinal current spectra \( \tilde{C}_L(k, \omega) \) at different \( k \) give the dispersion law \( \omega_c^{(L)}(k) \). Solution of the following simple equation

\[
\frac{\partial}{\partial \omega} \left[ B_0(k) + B_2(k)\omega^2 + B_4(k)\omega^4 \right] \bigg|_{\omega = \omega_c} = 0, (18)
\]

gives the longitudinal dispersion relation as:

\[
\omega_{1,2}(k) = \pm i \sqrt{\frac{\Delta_2(k) \left[ \Delta_1(k) + \Delta_2(k) \right] - 2\Delta_1(k)\Delta_3(k)}{2 \left[ \Delta_3(k) - \Delta_2(k) \right]}} \\
= \pm i \omega_c^{(L)}(k). (19)
\]

Comparison of the theoretical results of the longitudinal current spectra \( \tilde{C}_L(k, \omega) \) of liquid gallium at \( T = 794 \) K according to equation (17) with INS and MD results is presented in Fig. 4, demonstrating good qualitative and quantitative agreement between all three methods.

The dispersion law \( \omega_c^{(L)}(k) \) for the liquid gallium at the temperature \( T = 794 \) K is given in Fig. 5. Here, results of molecular dynamics simulations, INS experiments, and inelastic x-ray scattering experiments (reproduced from [14]) are compared to theoretical results [19]. As seen, the calculated theoretical and MD dispersion curves are in a good agreement with the INS and IXS data.

**TRANSVERSE DISPERSION LAW AND GAPPED MOMENTUM STATES**

The transverse current TCFs (Eq. 9) were calculated from the MD simulations data at different temperatures. The dispersion law of the transverse collective mode calculated from the spectral densities of these TCFs at different temperatures is presented in Fig. 7 alongside experimental dispersion curves from inelastic X-ray experiments reported previously as well as earlier \textit{ab initio} modelling results [16].

At lowest temperature, we observe an agreement between the calculated dispersion curves and previous experimental results at large \( k \). We have attempted to extract the transverse dispersion curves from the current INS data by fitting to a two-oscillator model [29] and damped harmonic oscillator model [32], however the resolution and signal strength of the experimental data were lacking and the additional degrees of freedom available in the two-oscillator model resulted in overfitting.

We now focus on modelling and theoretical results for the transverse dispersion curve. First, we calculate the parameters in the predicted transverse dispersion curve [11]. We calculate \( \tau = E_s/G_\infty \), and \( \eta_s \) as

\[
\eta_s = \frac{V}{k_BT} \int_0^\infty \langle \sigma_{\alpha\beta}(t)\sigma_{\alpha\beta}(0) \rangle dt, (20)
\]

where angle brackets mean averaging over time and ensemble of particles, \( k_B \) is the Boltzmann constant, \( V \) is the volume, \( \sigma_{\alpha\beta} \) are the non-diagonal components of the stress tensor.

We subsequently calculate \( c \) as \( \sqrt{\frac{G_\infty}{\rho}} \), where the infinite-frequency shear modulus is evaluated as

\[
G_\infty = \frac{V}{k_BT} \langle |\sigma_{\alpha\beta}(0)|^2 \rangle. (21)
\]

Fig. 4 shows the calculated values of density, viscosity, \( G \), speed of sound and relaxation time as a function of temperature. As seen from the figure, the simulation results for the density and viscosity of liquid gallium are in
FIG. 4: Longitudinal current spectra \( \tilde{C}_L(k, \omega) \) calculated by equation (10) for liquid gallium at the temperature \( T = 794 \) K: circles – experimental results from inelastic neutron scattering; squares – the molecular dynamics simulation results; solid lines – theoretical results [Eq. 17].

qualitative agreement with the experimental data, correctly predicting the general trend with increasing temperature.

We now address the central point of this paper of how well the dispersion relation for GMS describes liquid dynamics. Our results enable us to study this point quantitatively and in detail.

We use three ways to study this. First, we plot Eq. (1) in Fig. 7 using the calculated \( \tau \) and \( c \). We observe a good agreement with (a) dispersion relation obtained from modelling in the wide rage of \( k \)-points including the \( k \)-gap at all temperatures and (b) experimental transverse points at the lowest temperature and higher \( k \).

Second, we plot the \( k \)-gap as a function of temperature in Fig. 8 and observe its increase. This is consistent with the prediction of Eq. (2) because \( \tau \) decreases with temperature.

Third and finally, Eq. (2) predicts the increase of \( k_g \) as \( 1/c\tau \). In Fig. 8 we plot \( k_g \) as a function of \( 1/c\tau \) and observe a linear dependence, consistent with the theoretical prediction.

DISCUSSION AND SUMMARY

This joint experimental, computational, and theoretical study represents further progress towards an understanding of collective modes in liquids and GMS in particular. With new INS data, the longitudinal and transverse collective modes predicted by the EAM potential for gallium enjoys agreement with both IXS and INS experiments. The longitudinal modes additionally sport very solid agreement from low-\( k \) up to and beyond the first BZ boundary. This increases our confidence that experiments, theory and modelling have now developed to the extent where they reliably describe the same physical mechanism. In the area of liquids, achieving this has remained a long-standing challenge from the point of view of experiment, theory and modelling [6].

Our current evidence for GMS comes from theory and modelling which agree well, as follows from our Figs. 7 and 8. Moreover, theory and modelling also agree with INS and IXS experiments at larger \( k \). Although we do not directly observe GMS in the current INS experiment (due persisting challenges of detecting a weaker trans-
verse mode in liquids at low $k$ \([7, 8]\), this agreement, together with the agreement of all three lines of enquiry for the longitudinal mode, builds up the body of evidence for GMS. Our results serve as a stimulus for future INS experiments investigating transverse modes in liquids at low $k$ and their evolution in terms of gapped momentum states.

We find that the theoretical prediction of GMS following from Maxwell-Frenkel theory describes liquid dynamics with a fairly high degree of accuracy. This is important for understanding most basic dynamical and thermodynamic properties of liquids as discussed in the Introduction. The overarching goal of this research programme is to reach the stage where, despite the complexity of their theoretical description \([1]\), liquids emerge as systems amenable to theoretical understanding at the level comparable to gases and solids.

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FIG. 6: Temperature dependencies of mass density $\rho(T)$ of the system (a), shear viscosity $\eta_s(T)$ (b), shear modulus $G$ (c) and relaxation time $\tau$ (c); solid triangles - molecular dynamics simulation results; solid squares and solid circles correspond to the experimental data [30] and [31], respectively. (e), Temperature dependencies of the sound velocity in liquid gallium: open squares – longitudinal waves open triangles – transverse waves.

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FIG. 7: The laws of dispersion of the transverse acoustic-like excitations of a gallium melt at various temperatures: open triangles show the results of molecular dynamics simulation; solid squares show the experimental data on inelastic neutron scattering [16]; solid circles show the experimental data on inelastic X-ray scattering [28]; solid diamonds are the results of the OF-AIMD simulation [28]; solid lines – theoretical results [Eq. 1].
FIG. 8: (a): Temperature dependence of the width of “gap” in the transverse dispersion law. The dashed line represents the linear fit $k_{\text{gap}} = \alpha \cdot T + k_0$ with the coefficients $\alpha = 9.12 \cdot 10^{-4} \text{ K}^{-1} \text{Å}^{-1}$, $k_0 = -0.12 \text{ Å}^{-1}$. (b): Relationship between the gap width and the characteristic quantity $1/c\tau$. The dashed line represents the linear fit $k_{\text{gap}} = 0.5/c\tau$. 