Comment on "Neutron Brillouin Scattering Study of Collective Dynamics in a Dense He-Ne Gaseous Mixture"

Bafile *et al.* [1] have recently reported the results of a neutron scattering study of a dense He-Ne mixture ($x_{\rm He} = 0.77$) at $T = 39.3$ K and wave vectors ranging between $k = 0.7$ nm^{-1} and $k = 1.8$ nm^{-1}. One of the conclusions in this paper is that the hydrodynamic behavior of the mixture persists up to k values which are much larger than those predicted by earlier theories and computer simulations. Bafile *et al.* [1] based their conclusion on the analysis of the $S^{\exp}(k,\omega)$ function obtained from experiments, which can be expressed as

$$S^{\exp}(k,\omega) = a_{\rm HeHe}S^{\rm HeHe}(k,\omega) + a_{\rm HeNe}S^{\rm HeNe}(k,\omega) + a_{\rm NeNe}S^{\rm NeNe}(k,\omega), \quad (1)$$

where $a_{\rm HeHe} = 0.63$, $a_{\rm HeNe} = 0.97$, and $a_{\rm NeNe} = 0.37$. Bafile *et al.* [1] did not observe any feature that could be attributed to the existence of fast propagating modes in the $S^{\exp}(k,\omega)$ functions up to $k = 1.8$ nm^{-1}.

We carried out a molecular dynamics (MD) study of the $\rm He_{0.8}Ne_{0.2}$ mixture at $T = 39.3$ K using a Lennard-Jones potential with the usual parameters and the Lorentz-Berthelot rule for the cross interactions. Our results are in good agreement with the MD findings for the same interaction potential by Enciso *et al.* [2]. The longitudinal dispersion curves for both the He and Ne particles were obtained from the position of the maxima of the partial longitudinal currents $C_L^{\rm HeHe}(k,\omega)$ and $C_L^{\rm NeNe}(k,\omega)$, respectively. As in Fig. 4 of Ref. [2] the frequencies for the fast propagating modes $\omega^{\rm HeHe}(k)$ are only slightly larger than those corresponding to the hydrodynamic sound, whereas $\omega^{\rm NeNe}(k)$ for the slow sound modes are markedly lower. The large differences between $\omega^{\rm HeHe}(k)$ and $\omega^{\rm NeNe}(k)$ at wave vectors larger than $k \approx 0.7$ nm^{-1} show that the hydrodynamic regime does not persist at these wave vectors.

We have calculated the longitudinal current $C_L^{\exp}(k,\omega) = \omega^2 S^{\exp}(k,\omega)$ defined according to Eq. (1). The position of the $C_L^{\exp}(k,\omega)$ peaks obtained by MD are consistent with the neutron scattering data [1]. The resulting function for a representative wave vector within the k interval explored by Bafile *et al.* [1] is shown in Fig. 1. The three contributions to $C_L^{\exp}(k,\omega)$ are also plotted in Fig. 1. As may be observed, the peak of $C_L^{\exp}(k,\omega)$ is located at slightly lower frequency than that of $C_L^{\rm HeHe}(k,\omega)$ and the contribution of the cross-correlation function $C_L^{\rm HeNe}(k,\omega)$ to $C_L^{\exp}(k,\omega)$ cannot be neglected. It should be noticed that the difference between $\omega^{\rm HeHe}(k)$ and the hydrodynamic dispersion is smaller than 0.1 ps^{-1} at $k = 1.4$ nm^{-1} (see Fig. 4 of Ref. [2]) and, then, hardly visible in $S^{\exp}(k,\omega)$. Hence, the absence in $S^{\exp}(k,\omega)$ of visible features that could be attributed to fast propagating modes should not be associated with a persistence of the hydrodynamic regime up to wave vectors higher than

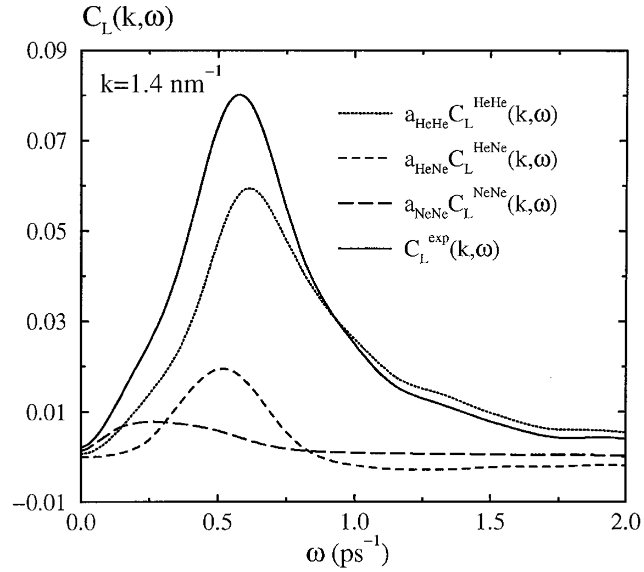

FIG. 1. Contributions of the partial longitudinal currents to the $C_L^{\exp}(k,\omega)$ function at $k = 1.4$ nm^{-1} obtained by MD simulation.

1.8 nm^{-1}, as concluded in Ref. [1]. It should be noted that experiments do not allow one to obtain the dispersion relations for He and Ne separately, being the existence of noticeable differences between these two curves the most suitable test to determine the limit of the hydrodynamic regime. Moreover, according to Fig. 1 the contribution of the slow sound mode, $\omega^{\rm NeNe}(k)$, to the experimental $S^{\exp}(k,\omega)$ function would be very small and, therefore, hardly detectable from neutron scattering measurements. It may then be concluded that the results in Ref. [1] are consistent with the MD findings but do not provide any definitive evidence on the upper limit of the hydrodynamic regime in dense He-Ne mixtures.

J. A. Padró and N. Anento
Departament de Física Fonamental
Universitat de Barcelona
Diagonal, 647, 08028 Barcelona, Spain

M. Canales
Departament de Física i Enginyeria Nuclear
Universitat Politècnica de Catalunya
Campus Nord. Sor Eulàlia d'Anzizu, B4-B5
08034 Barcelona, Spain

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