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# A molecular dynamics study of the collective correlation functions of a hard-core fluid with a Yukawa tail

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We present a molecular dynamics study of the collective correlation functions of a hard-core system with an attractive Yukawa tail, for various thermodynamic states in the fluid and liquid regions of the phase diagram. The results are compared with available information for hard spheres. The small-$q$ behavior of the intermediate scattering functions indicates the propagation of sound waves, i.e., phononlike collective excitations, in the hard-core Yukawa system. The upper limit of $q$ for these collective modes is practically independent of the thermodynamic state. The computed transverse current correlation functions show that at liquid densities the hard-core Yukawa system is able to sustain shear wave propagation above a critical $q$; the upper limit of $q$ for sound waves and the lower limit for shear waves nearly coincide. All of these features are qualitatively similar to those found for hard spheres. However, there are significant quantitative differences, which reflect the influence of the attractive Yukawa tail on the dynamical behavior of the system. © *1996 American Institute of Physics.* [S0021-9606(96)51542-4]

## I. INTRODUCTION

Information about the dynamic properties of fluids can be derived from neutron or light scattering experiments (see, e.g., Refs. 1, 2, and those cited therein). However, in some cases this experimental information is difficult or impossible to obtain, and the quasiexperimental molecular dynamics (MD) method provides an alternative approach, affording insight into the dynamical behavior of these systems. MD results based on a model intermolecular potential that accurately describes the physical system of interest allow assessment of the reliability of any available theoretical approximations.

Most computer simulation studies of the dynamic properties of fluids have been performed using continuous interatomic potentials. In particular, Lennard–Jones systems have been extensively investigated,[3–10] and a number of liquid alkali metals have recently been analyzed using effective interatomic pair potentials.[11–18] An MD study of the dynamical behavior of a hard sphere (HS) fluid has been carried out by Alley *et al.*[19]

In recent work,[20–22] we used MD simulations and the mean spherical approximation to investigate the static properties of one- and two-component fluids composed of hard spheres interacting through an attractive Yukawa tail; values of the self-diffusion constant of this kind of system were also computed.[20] The hard-core Yukawa (HCY) potential plays a prominent role in the physics of fluids due to its great versatility: By changing the inverse screening length, it can be varied from a Coulomb potential to a pure hard sphere interaction. Accordingly, the HCY potential has been used to describe a wide variety of physical systems, including liquid noble gases,[23] liquid metals,[24,25] astrophysical plasmas,[26] and colloidal dispersions.[27] However, systematic studies of the dynamic properties of HCY fluids have not yet been performed to our knowledge, perhaps partly because MD simu-

lations of this kind of system require different algorithms from the standard ones used for hard spheres or for systems interacting via continuous interatomic potentials.[20–22]

In this paper we report on an MD simulation study of the intermediate scattering function and the longitudinal and transverse current correlation functions of an HCY system for several thermodynamic states in the fluid and liquid regions of the phase diagram. These quantities are briefly introduced in Sec. II, where we also sketch the computational method used in this work (for a more detailed description of the collective correlation functions used in this paper we refer the reader to standard textbooks[1,2]). In Sec. III we present and discuss our MD results and compare them with available information for HS fluids. Finally, a summary of conclusions is given in Sec. IV.

It is perhaps worth pointing out that MD simulations with the HCY potential are much more time consuming that those using continuous interatomic potentials. An extensive study of the dynamical behavior of the HCY system, and of how this behavior depends on the value of the screening length, would be a major undertaking (particularly for the liquid region). The results reported in this paper nevertheless provide insight into the collective correlation functions of this kind of system and into the effect of the attractive Yukawa tail of the potential. Thus, the quasiexperimental results reported in this paper may orient theoretical studies of the dynamical properties of fluids described by the HCY potential.

## II. COMPUTATIONAL PROCEDURE AND THEORETICAL BACKGROUND

We considered a system of $N$ particles in a cubic box with periodic boundary conditions interacting through a pairwise HCY potential of the form

$$\phi = \infty \quad \text{for} \quad r < \sigma$$

$$= -(\epsilon\sigma/r)\exp[-\lambda(r-\sigma)] \quad \text{for} \quad r \geq \sigma, \qquad (1)$$

where $\sigma$ is the hard-core diameter of the particles, $\epsilon$ is the magnitude of the interaction at the hard core distance, and the Yukawa exponent $\lambda$ is the inverse range parameter. We adopted the same value of $\lambda$ as in our earlier study of the properties of an HCY fluid, $1.8/\sigma$.[20] This value makes the system qualitatively similar to argon as regards the densities and temperatures of the liquid in equilibrium with its vapor. The parameters $\sigma$, $\epsilon$, and $\tau(\equiv(m\sigma^2/\epsilon)^{1/2}$, where $m$ is the mass of the particles) were taken as units of length, energy, and time, respectively. For most runs $N$ was 108, but some calculations were also performed with $N=256$. The cutoff radius used in our calculations was, in each case, the maximum value allowed by the periodic boundary conditions, one-half the boxlength.

Computations were carried out for several values of the reduced density $\rho^*(\equiv N\sigma^3/V)$ and reduced temperature $T^*(\equiv kT/\epsilon$, where $k$ is the Boltzmann constant). More specifically, the states studied were $(\rho^*=0.3, T^*=1.5-7.0)$, $(\rho^*=0.5, T^*=1.5-4.0)$, and $(\rho^*=0.8, T^*=1.0)$. Since simulation studies performed by Smit and Frenkel[28] using the Gibbs ensemble technique show that the critical density and temperature of the HCY fluid with $\lambda=1.8/\sigma$ are $\rho_c^* = 0.294$ and $T_c^* = 1.192$, the low- and intermediate-density states studied in this paper lie in the fluid region of the phase diagram, and the highest-density state $(\rho^*=0.8, T^*=1.0)$ in the liquid region. Because the attractive part of the HCY potential is negligible at high temperature, the high temperature results for the HCY fluid should be compared with those of an HS system.

The computational procedure was as follows. For each fixed density and temperature, a canonical MD simulation was first carried out using the Nosé constant temperature technique.[29] Simulations started with the particles in an fcc configuration. The equations of motion were solved using a fourth-order Gear predictor-corrector algorithm[30] with a time step $t_s \leq 10^{-4}\tau$ depending on the next collision time (see below); for the state with $\rho^*=0.8$, $t_s \leq 0.5 \times 10^{-4}\tau$. A configuration was recorded every $\Delta t = 5 \times 10^{-3}$ time units. The energy of the system was then calculated by averaging over $5 \times 10^3$ configurations after an initial equilibration period of $5 \times 10^3$ configurations.

Calculation of collision times is one of the main problems in MD simulations.[30] The condition for collision between particles $i$ and $j$,

$$[\mathbf{r}_i(t) - \mathbf{r}_j(t)]^2 - \sigma^2 = 0, \qquad (2)$$

is quadratic for pure hard spheres, for which the particle position functions $\mathbf{r}_i(t)$ are simple linear functions of $t$. However, the trajectories of particles interacting via an attractive Yukawa potential are approximated by an equation of fourth degree with respect to time, making Eq. (2) an eighth degree polynomial. To compute the smallest positive root of Eq. (2) we used the Laguerre method,[31] which was applied to all particles pairs to obtain the collision time as the minimum of all these roots. If this value was $<10^{-4}\tau$

$(<0.5 \times 10^{-4}\tau$, for the state with density $\rho^*=0.8)$, then all the particles were moved forward for this time and the collision between the colliding pair was implemented; otherwise, the particles were all moved forward for a time of $10^{-4}\tau$ $(0.5 \times 10^{-4}\tau$, for the state with $\rho^*=0.8)$, and the next collision time was recalculated.

Starting now from a configuration with an energy equal to the average energy calculated as above, microcanonical MD simulation was carried out using a form of the velocity Verlet algorithm[30] adapted to the HCY potential in a way analogous to the above described modification of the Gear predictor-corrector algorithm. In this case, $35 \times 10^3$ configurations were generally recorded, one every $5 \times 10^{-3}$ time units, the first $5 \times 10^3$ of which were discarded for equilibration. Microcanonical simulations are better than canonical simulations for studying dynamical properties because of the difficulty of controlling the heat exchange rate variable in the Nosé method.[29] In order to be able to estimate the statistical uncertainty of the results of these microcanonical MD simulations, the dynamic properties of interest were averaged within each of the six groups of $5 \times 10^3$ configurations making up the total $3 \times 10^4$ postequilibration configurations (for some states, 12 of such groups of $5 \times 10^3$ configurations were acquired, without any significant improvement of the results).

The time-dependent correlation functions studied in this paper can be derived from the positions $\mathbf{r}_i(t)$ and the velocities $\mathbf{v}_i(t)$ of the particles during the microcanonical MD simulations. In particular, the intermediate scattering function $F(q,t)$ is defined as[1,2]

$$F(q,t) = \frac{1}{N}\left\langle \sum_{m,n} \exp\{i\mathbf{q}\cdot[\mathbf{r}_m(0) - \mathbf{r}_n(t)]\}\right\rangle, \qquad (3)$$

$\mathbf{q}$ being a wave vector compatible with the periodic boundary conditions, i.e., $\mathbf{q}=(2\pi/L)(n_x,n_y,n_z)$, where $L$ is the length of the simulation box, and $n_\alpha$ are integers. The angle brackets in Eq. (3) denote averaging both along the trajectories of the particles and over all the $N_q$ vectors $\mathbf{q}$ with the same modulus $q$; in the calculations carried out in this paper we ignored $q$ values with $N_q$ larger than 36.

The frequency spectrum $S(q,\omega)$ of the intermediate scattering function is its Fourier transform (FT):

$$S(q,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(q,t)e^{i\omega t}\,dt. \qquad (4)$$

$S(q,\omega)$ is the dynamic structure factor, the quantity directly determined by neutron or light scattering experiments.[1,2] We calculated $S(q,\omega)$ using the FFT (fast FT)[30] with a window function that removed cutoff noise. The static structure factor $S(q)$ may be defined by $S(q)=F(q,0)$.[1,2]

The longitudinal and transverse current correlation functions, $C_l(q,t)$ and $C_t(q,t)$, are defined by[1,2]

$$C_l(q,t) = \frac{q^2}{N}\left\langle \sum_{m,n} v_m^z(0)v_n^z(t)\exp\{i\mathbf{q}\cdot[\mathbf{r}_m(0) - \mathbf{r}_n(t)]\}\right\rangle \qquad (5)$$
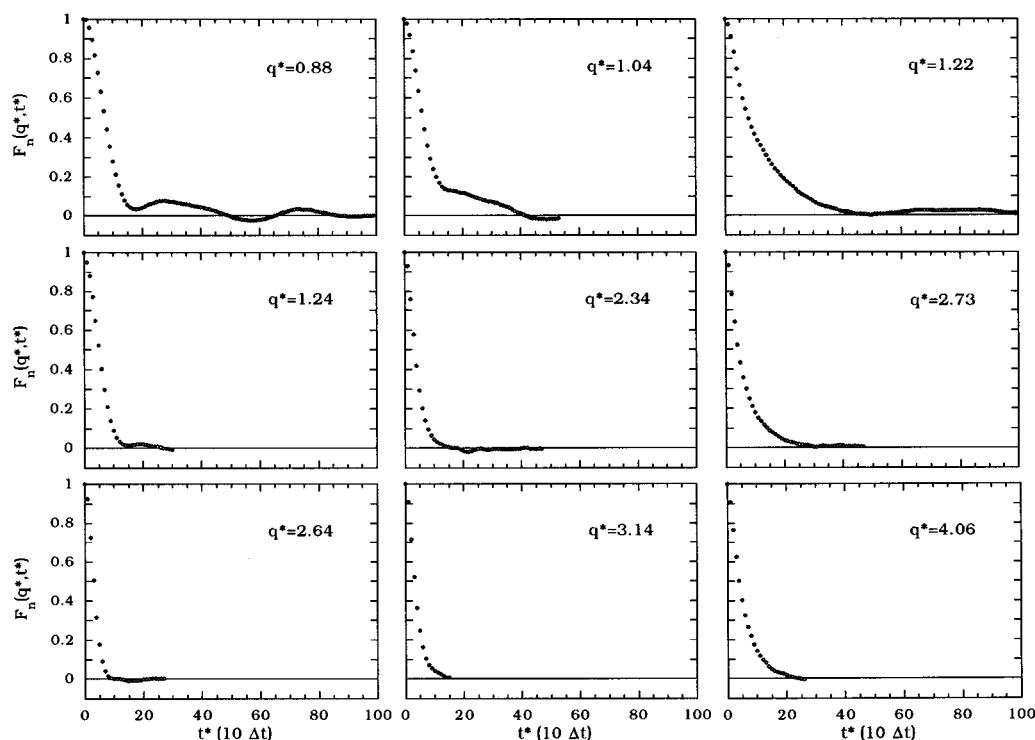
and

FIG. 1. Normalized intermediate scattering functions of the 108-particle HCY system for the states ($\rho^*=0.3$, $T^*=5.5$) (left), ($\rho^*=0.5$, $T^*=3.0$) (middle), and ($\rho^*=0.8$, $T^*=1.0$) (right), in each case for several wave numbers $q^*$.

$$C_t(q,t) = \frac{q^2}{N} \left\langle \sum_{m,n} v_m^x(0) v_n^x(t) \exp\{i\mathbf{q}\cdot[\mathbf{r}_m(0)-\mathbf{r}_n(t)]\} \right\rangle,$$

(6)

where $v_i^z$ and $v_i^x$ are the components of the velocity of particle $i$ respectively parallel and perpendicular to the wave vector $\mathbf{q}$, which is directed along the $z$ axis. The frequency spectrum of the longitudinal current correlation function, $C_l(q,\omega)$, was calculated using the FFT with an appropriate window function. Determination of the frequency spectrum $C_t(q\omega)$ is more difficult for the HCY fluid considered in this paper (see below).

The longitudinal current and density correlation functions are not independent, since the equation of continuity implies that[1,2]

$$C_l(q,t) = -\frac{d^2 F(q,t)}{dt^2},$$

(7)

or in frequency space

$$C_l(q,\omega) = \omega^2 S(q,\omega).$$

(8)

However, for all $q$ values the spectrum $C_l(q,\omega)$ has a well-defined maximum at some $\omega=\omega_{l,m}(q)>0$, while there may be $q$ values for which $S(q,\omega)$ has no such maximum (see, e.g., Refs. 1 and 17). Considered as functions of $q$, the frequencies $\omega_{l,m}(q)$ and $\omega_B(q)$ (the frequency of the maximum of $S(q,\omega)$, when it exists) are called dispersion relations.

The computed values of the time-dependent correlation functions of the HCY system are given in graphical form in the next section; the raw MD data are available on request.

## III. RESULTS AND DISCUSSION

For the sake of brevity we mainly report the results for only three states: ($\rho^*=0.3$, $T^*=5.5$), ($\rho^*=0.5$, $T^*=3.0$), and ($\rho^*=0.8$, $T^*=1.0$). Figure 1 shows, for each of these states, the normalized intermediate scattering magnitude $F_n(q^*,t^*)=F(q^*,t^*)/F(q^*,0)$ of the 108-particle HCY system for each of three reduced wave numbers $q^*=q\sigma$. In each case, this function decays in an oscillatory manner at the smallest $q^*$ value, which is indicative of collective, phononlike excitations in the HCY system. These oscillations are rapidly extinguished when $q^*$ is increased, so that above a certain $q^*$ value $F_n(q^*,t^*)$ becomes a simple, monotonically decreasing function of $t^*$. Our calculations show that oscillations disappear from $F_n(q^*,t^*)$ somewhere in the $q^*$ ranges 1.76–1.97, 1.81–2.09, and 1.73–2.12 for the states ($\rho^*=0.3$, $T^*=5.5$), ($\rho^*=0.5$, $T^*=3.0$), and ($\rho^*=0.8$, $T^*=1.0$), respectively. Hence, the maximum wave number for the propagation of these collective modes in the HCY system is practically the same at all densities, a behavior which is qualitatively similar to that of HS fluids[19] (we note, however, that for hard spheres, oscillations in the intermediate scattering function are completely damped for $q^*>1.52$; the absence of an attractive term in the intermolecular potential thus reduces the limiting wave number for sound wave propagation).

Figure 2 (bottom panel) shows that in the HCY system, at liquid densities, $F(q^*,t^*)$ decays very slowly at wave numbers near $q_p^*$, the position of the main peak in the static structure factor function $S(q)$. This effect (''de Gennes
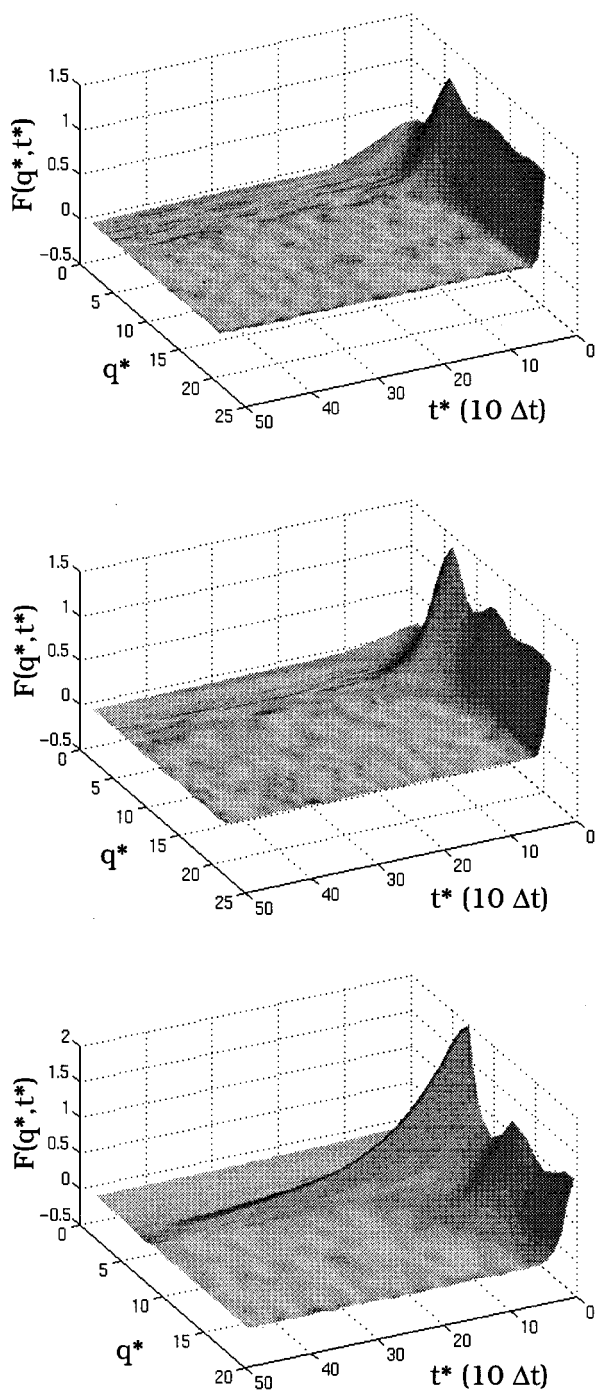
FIG. 3. Dynamic structure factors of the 108-particle HCY fluid in the states $(\rho^*=0.3, T^*=5.5)$ (upper panel) and $(\rho^*=0.3, T^*=7.0)$ (lower panel), in each case for two wave numbers. Lines joining data points are merely visual aids.



FIG. 2. Intermediate scattering functions of the 108-particle HCY system for the states $(\rho^*=0.3, T^*=5.5)$ (top), $(\rho^*=0.5, T^*=3.0)$ (middle), and $(\rho^*=0.8, T^*=1.0)$ (bottom) for the whole $q^*$-range investigated in each case.

narrowing''[32]) has been observed in both dense HS fluids[19] and systems with continuous interatomic potentials,[13,17,33] and has its origin in the strong spatial correlations that exist in the neighborhood of $q_p^*$.

Sound wave propagation at low $q^*$ is also shown by the appearance of a secondary (Brillouin) peak, as well as the central (Rayleigh) peak in the corresponding dynamic structure factor function. Figure 3 shows $S^*(q^*,\omega^*)$ for the 108-
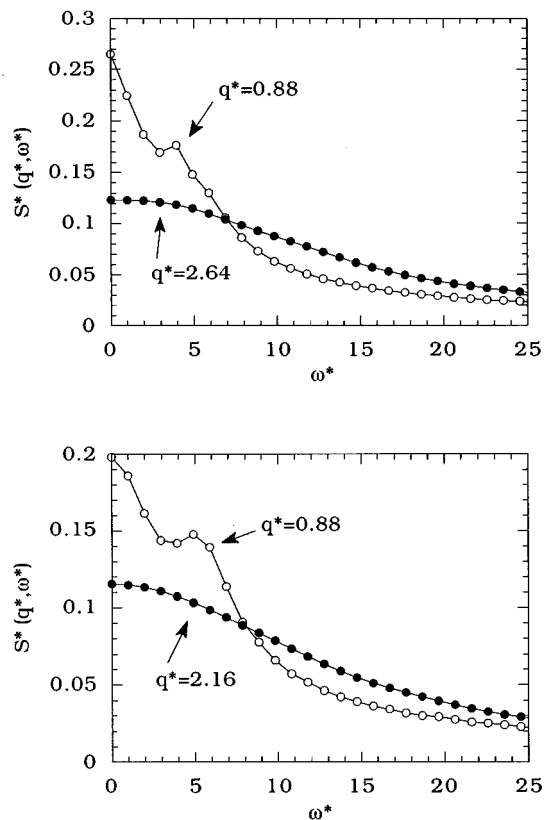
particle HCY fluid of $\rho^*=0.3$ at two different temperatures, $T^*=5.5$ and $T^*=7.0$, in each case for both a high value of $q^*$ and the lowest possible value for the 108-particle system.

The longitudinal current correlation function $C_l(q,t)$ always shows heavily damped oscillations. This is illustrated in Fig. 4, which shows the normalized correlation function $C_l^n(q^*,t^*) = C_l^*(q^*,t^*)/C_l^*(q^*,0)$ for the 108-particle HCY system in the state $(\rho^*=0.3, T^*=5.5)$ at $q^*=0.88$ and $q^*=2.64$. Figure 5 displays the frequency spectra $C_l^*(q^*,\omega^*)$ for the same states and wave numbers as those of Fig. 3. Unlike $S^*(q^*,\omega^*)$, $C_l^*(q^*,\omega^*)$ presents at all $q^*$ values a well-defined peak at some $\omega^*>0$. Comparison of Figs. 3 and 5 also shows that for the smaller $q^*$ value the frequency of the $C_l^*(q^*,\omega^*)$ peak is close to the frequency of the Brillouin peak in $S^*(q^*,\omega^*)$, in compliance with the general prediction that in the low-q region $\omega_{l,m}(q)\approx\omega_B(q)$.[1]

Figure 6 shows the dispersion relation $\omega_{l,m}^*(q^*)$ for the same states as those of Figs. 1 and 2. For the high density state in the liquid region $(\rho^*=0.8, T^*=1.0)$ we present results for both 108 and 256 particles (the latter system allows smaller $q^*$ values to be used in the MD simulations). The results for the two system sizes agree very well; in particular, both show a pronounced minimum near $q_p^*$, an effect which has also been found in liquefied noble gases[34] and liquid rubidium[17] and is closely related to the de Gennes narrowing
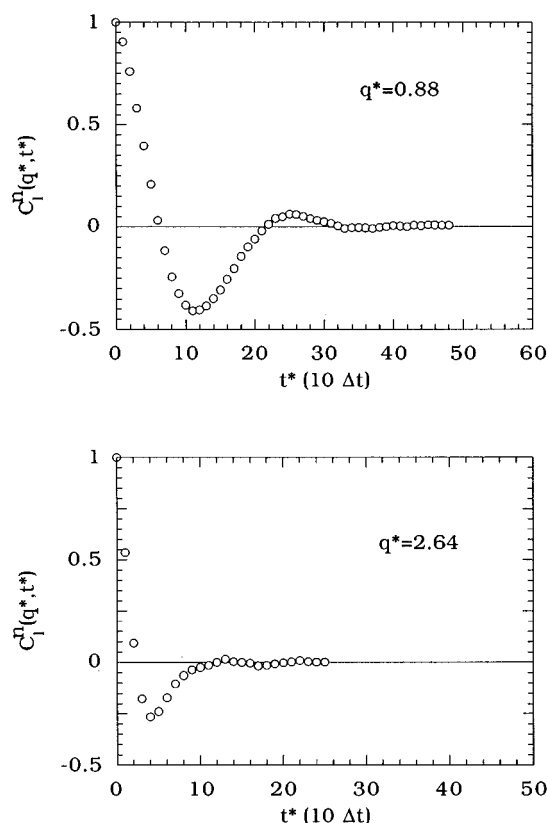
FIG. 4. Normalized longitudinal current correlation function of the 108-particle HCY fluid in the state ($\rho^*=0.3$, $T^*=5.5$) for two wave numbers.
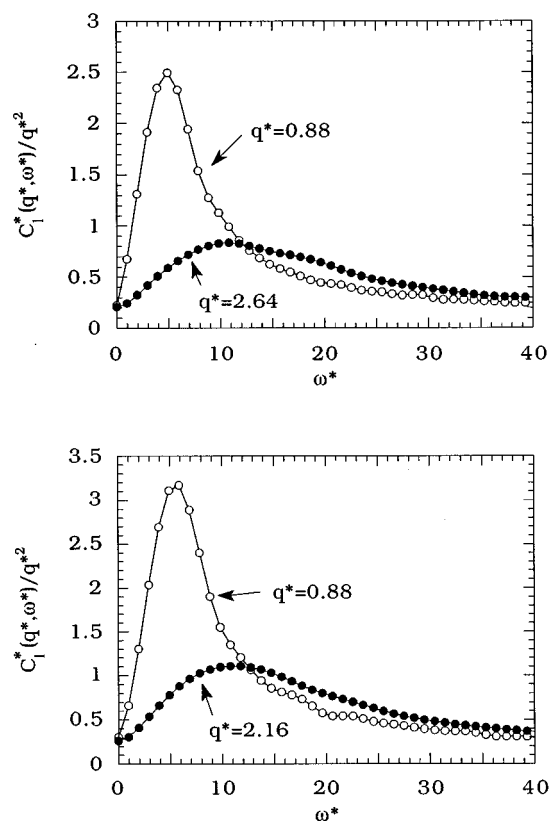


FIG. 5. Frequency spectra of the longitudinal current correlation functions of the 108-particle HCY fluid in the states ($\rho^*=0.3$, $T^*=5.5$) (upper panel) and ($\rho^*=0.3$, $T^*=7.0$) (lower panel), in each case for two wave numbers. Lines joining data points are merely visual aids.

observed in $F(q,t)$.[33] The minimum is smeared out as density decreases.

To estimate the reduced adiabatic speed of sound $c_s^*$ we fitted $\omega_{l,m}(q)$ data with the mode-coupling expression[13,17]

$$\omega_{l,m}(q) \approx \omega_B(q) \approx c_s q + \alpha_s q^{5/2}, \qquad (9)$$

which is strictly valid in the hydrodynamic region (i.e., for small $q$'s and small $\omega$'s). The "anomalous dispersion" term $\alpha_s q^{5/2}$ is associated with shear relaxation effects;[13] for several liquid alkali metals[11,13,15,16] it has been found that the coefficient $\alpha_s$ is positive. The values of $c_s^*$ for several states of the HCY system are listed in Table I. At fixed density, $c_s^*$ increases with temperature, and at fixed temperature $c_s^*$ increases with density. The statistical uncertainty of the value for the state ($\rho^*=0.8$, $T^*=1.0$) is smaller for $N=256$ than for $N=108$ because, as indicated above, the larger system allows better exploration of the low-$q$ region in the MD simulations. The values of the coefficient $\alpha_s$ (not shown) are negative for all the states of Table I. Negative values were also found by Alley *et al.*[19] in their MD study of an HS fluid with 4000 particles. It is presumably possible that positive values might be obtained if still larger systems were studied at very small wave numbers, i.e., in regions closer to the hydrodynamic limit.

For comparison, Table I also lists $c_{s,\text{HS}}^*$ values, i.e., $c_s^*$ values for the HS fluid. These values were obtained by taking data obtained using the Carnahan–Starling equation of state[2] (no MD $c_s$ data are available for the HS fluid) and reducing them by the same factor $\tau/\sigma = (m/\epsilon)^{1/2}$ as used for the HCY system. For $\rho^*=0.3$ and $\rho^*=0.5$, $c_{s,\text{HS}}^*$ and $c_{s,\text{HCY}}^*$ differ at the lowest temperatures, but $c_{s,\text{HCY}}^*$ approaches $c_{s,\text{HS}}^*$ as temperature rises. This was to be expected, of course, because, as indicated in Sec. II, at high temperature the attractive part of the HCY potential is negligible.

The transverse current correlation function $C_t(q,t)$ is not experimentally measurable but can be computed by MD simulation. Figure 7 shows the normalized function $C_t^n(q^*,t^*) = C_t^*(q^*,t^*)/C_t^*(q^*,0)$ of the 108-particle HCY system in the liquid state ($\rho^*=0.8$, $T^*=1.0$) for two wave numbers. For the smaller $q^*$ value, 1.22, $C_t^*(q^*,t^*)$ decays monotonically to zero with increasing $t^*$. However, for $q^*=2.12$ (which corresponds to the region where sound wave propagation ceases) there is a time interval in which the transverse current correlation function is slightly negative. This behavior, which is indicative of shear wave excitations, persists for wave numbers up to $q^*\approx 5$. For the lower density, fluid states ($\rho^*=0.3$ and 0.5) we found no evidence of shear wave propagation. Calculations carried out with 256 particles confirmed these findings, which are qualitatively similar to those found for an HS fluid[19] (although in dense HS fluids negative values of the transverse current correlation function do not occur for $q^*<1.52$). By contrast, studies
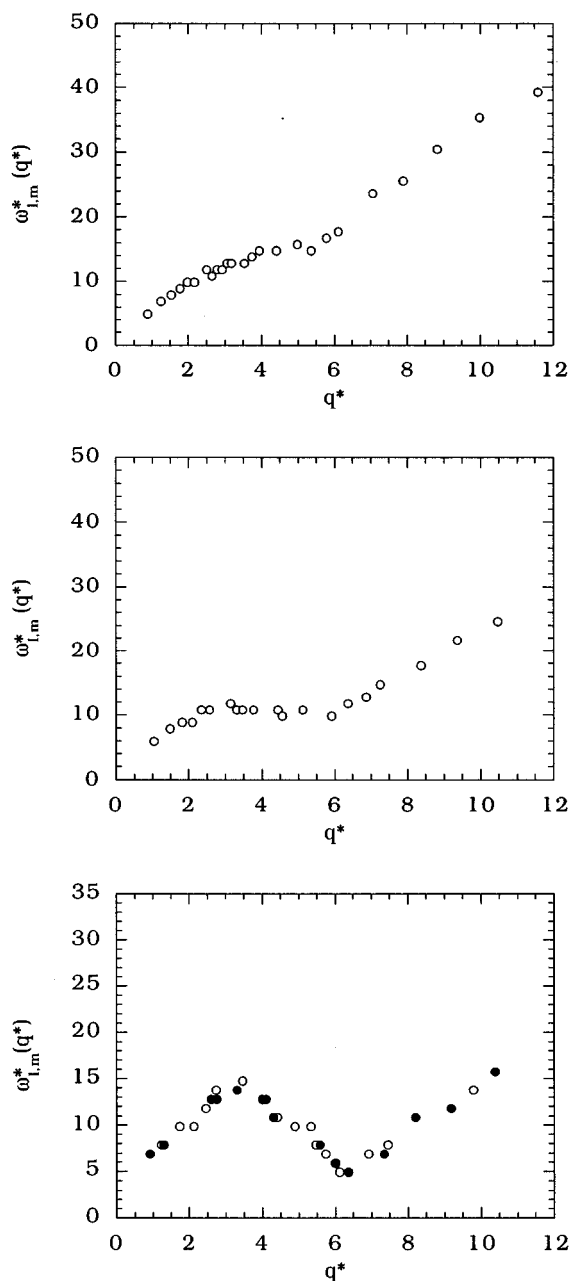
FIG. 6. Dispersion relations $\omega_{l,m}^*(q^*)$ of the longitudinal current correlation functions of the HCY system in the states ($\rho^*=0.3$, $T^*=5.5$) (top), ($\rho^*=0.5$, $T^*=3.0$) (middle), and ($\rho^*=0.8$, $T^*=1.0$) (bottom). Open circles are results for 108 particles; the solid dots in the lower panel are results for 256 particles.

of liquid alkali metals have shown that the regions where sound and shear waves are supported overlap.[13,16,17,35] The existence of a wide range of $q$ values for which liquid metals can support the propagation of both sound waves and shear waves shows that atomic motion in these systems has a much stronger collective character than for simple liquids, as has been pointed out by Copley and Lovesey[36] and Jacucci and McDonald.[35]

Our results for the transverse current correlation function were used to estimate the kinetic shear viscosity $\nu$ of the

TABLE I. Adiabatic speed of sound $c_s^*$ in the HCY system ($c_{s,\mathrm{HCY}}^*$) for several thermodynamic states. The result in parentheses for the state ($\rho^*=0.8$, $T^*=1.0$) is for 256 particles; all others are for 108 particles. For comparison, values for the HS reference system (reduced by the same factor as used for the $c_{s,\mathrm{HCY}}^*$ data) are also shown ($c_{s,\mathrm{HS}}^*$).

| $\rho^*$ | $T^*$ | $c_{s,\mathrm{HCY}}^*$ | $c_{s,\mathrm{HS}}^*$ |
|---|---|---|---|
| 0.3 | 1.5 | 2.4±0.2 | 2.99 |
| | 2.0 | 2.9±0.3 | 3.45 |
| | 4.0 | 4.5±0.4 | 4.88 |
| | 5.5 | 5.5±0.3 | 5.73 |
| | 7.0 | 6.7±0.4 | 6.46 |
| 0.5 | 1.5 | 4.3±0.2 | 4.69 |
| | 2.0 | 4.9±0.4 | 5.41 |
| | 2.5 | 6.0±0.5 | 6.05 |
| | 3.0 | 6.4±0.4 | 6.63 |
| | 4.0 | 7.3±0.4 | 7.66 |
| 0.8 | 1.0 | 6.7±0.5 | 8.20 |
| | 1.0 | (7.2±0.3) | |

HCY system from the hydrodynamic expression[1,2]

$$C_t(q,t) = C_t(q,0)e^{-\nu q^2 t}. \tag{10}$$

The results for several thermodynamic states are listed (in reduced units) in Table II. In each case, $\nu$ was evaluated by a least-squares fit of Eq. (10) to $C_t(q,t)$ for the smallest wave number $q$ accessible in our MD simulations. Table II also shows, for certain states, values of the ratio $D^*\nu^*\rho^*/T^*$ derived using values of the self-diffusion constant $D^*$ that were calculated in a previous study of the properties of HCY fluids.[20] The finding that $D^*\nu^*\rho^*/T^*$ is almost constant confirms the applicability of Stokes' law[2] to this kind of system.

## IV. SUMMARY AND CONCLUSION

In this work we performed an MD simulation study of the collective correlation functions of systems composed of particles interacting through a pairwise HCY potential. Several thermodynamic states in the fluid and liquid regions of the phase diagram were examined.

The low-$q$ behavior of the intermediate scattering function $F(q,t)$ shows indications of collective, phononlike ex-
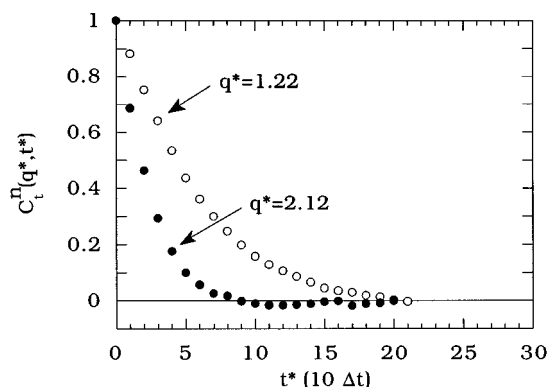


FIG. 7. Normalized transverse current correlation functions of the 108-particle HCY system in the state ($\rho^*=0.8$, $T^*=1.0$) for two wave numbers.

TABLE II. Kinetic shear viscosity $\nu^*$ of the HCY system for several thermodynamic states. The result in parentheses for the state ($\rho^*=0.8$, $T^*=1.0$) is for 256 particles; all others are for 108 particles. Also shown are values of the ratio $D^*\nu^*\rho^*/T^*$ calculated using values of the self-diffusion constant $D^*$ obtained in a previous MD study (Ref. 20).

| $\rho^*$ | $T^*$ | $\nu^*$ | $D^*\nu^*\rho^*/T^*$ |
|---|---|---|---|
| 0.3 | 1.5 | 0.99±0.09 | 0.11 |
|  | 2.0 | 1.05±0.09 | 0.11 |
|  | 4.0 | 1.43±0.08 |  |
|  | 5.5 | 1.79±0.09 |  |
|  | 7.0 | 2.1 ±0.1 |  |
| 0.5 | 1.5 | 1.23±0.07 | 0.11 |
|  | 2.0 | 1.32±0.08 | 0.11 |
|  | 2.5 | 1.61±0.05 |  |
|  | 3.0 | 1.69±0.08 |  |
|  | 4.0 | 2.0 ±0.2 |  |
| 0.8 | 1.0 | 2.6 ±0.1 | 0.12 |
|  | 1.0 | (2.8 ±0.2) |  |

citations in the HCY system. Within the range studied in this paper, the upper limit of $q$ for these collective modes is practically independent of the thermodynamic state. At liquid densities, $F(q,t)$ exhibits marked slowing as $q$ approaches $q_p$ ("de Gennes narrowing"[32,33]).

The longitudinal current correlation function $C_l(q,t)$ always exhibits heavily damped oscillatory behavior. At liquid densities, a deep minimum is observed in $\omega_{l,m}(q)$ near $q_p$, an effect which is closely related to the de Gennes slowing of $F(q,t)$.[17,33] At high temperature, the adiabatic speeds of sound of the HCY fluid are close to the corresponding values for hard spheres.

Our results for the transverse current correlation function $C_t(q,t)$ show the difficulty of propagating shear waves in the HCY fluid. Only at high density, in the liquid region, are small oscillations in this function observed in a $q$ region that begins near the upper limit for sound waves. The computed values of the kinetic shear viscosity of the HCY fluid, taken in conjunction with self-diffusion constant data reported elsewhere,[20] show the applicability of Stokes' law to this kind of system.

The computations reported in this paper, which supplement previous studies of the properties of HCY fluids,[20–22] show that the main qualitative features of the dynamical behavior of this kind of system are already present in the HS reference system. However, significant quantitative differences between HS and HCY fluids reflect the influence of the attractive tail of the HCY potential. Our "experimental" results may therefore be useful for theoretical studies of the dynamical behavior of HCY systems.

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