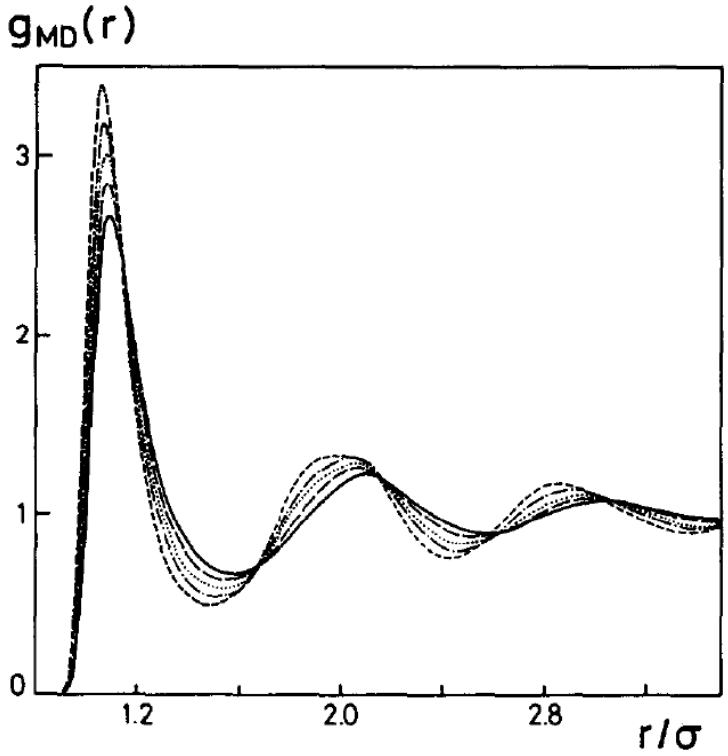
Radial distribution functions for a L-J liquid



ρ*=0.764

ρ*=0.813

ρ*=0.862

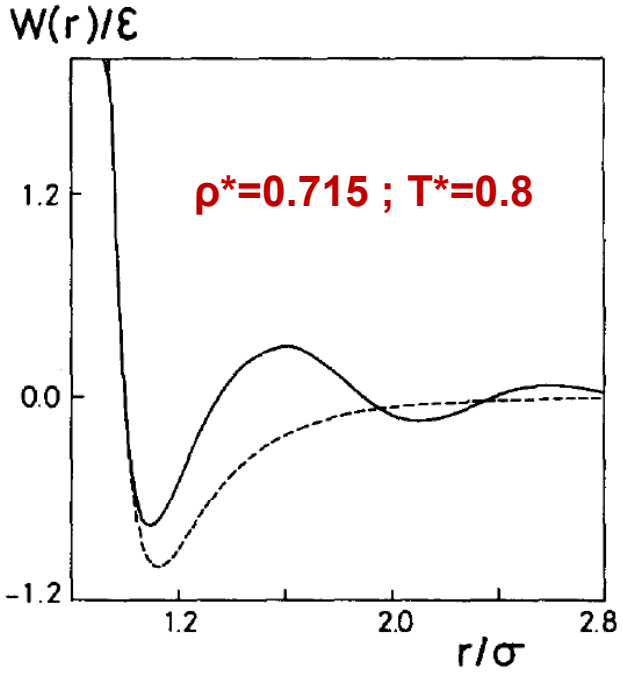
ρ*=0.910

ρ*=0.959

T*=0.8

E. Guàrdia et al., J. Chem.Phys. 84, 4569 (1986)

Interaction potentials for a L-J liquid



$$U_{LJ}(r) = 4\varepsilon\left\{\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right\}$$

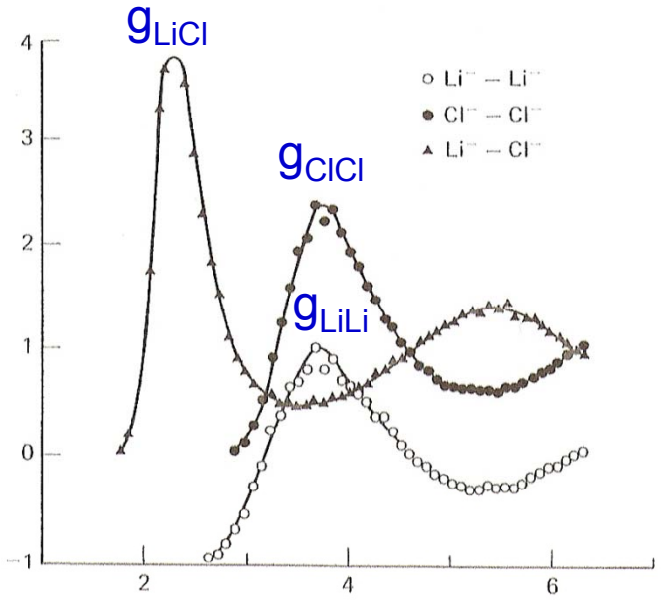
$$W(r) = -k_B T \ln g(r)$$

– – – – – Lennard-Jones potential

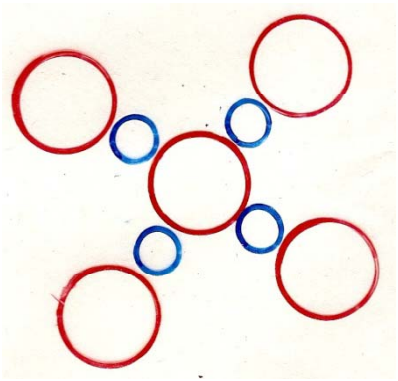
——— Mean Force potential

FUNCIONS DE DISTRIBUCIÓ RADIAL PER A LA SAL FOSA LiCl a T=883K , V=28.3cm^{-3}

obtingudes per Monte Carlo amb un potencial d'esferes dures carregades



La posició dels màxims i mínims indica una estructura de capes:

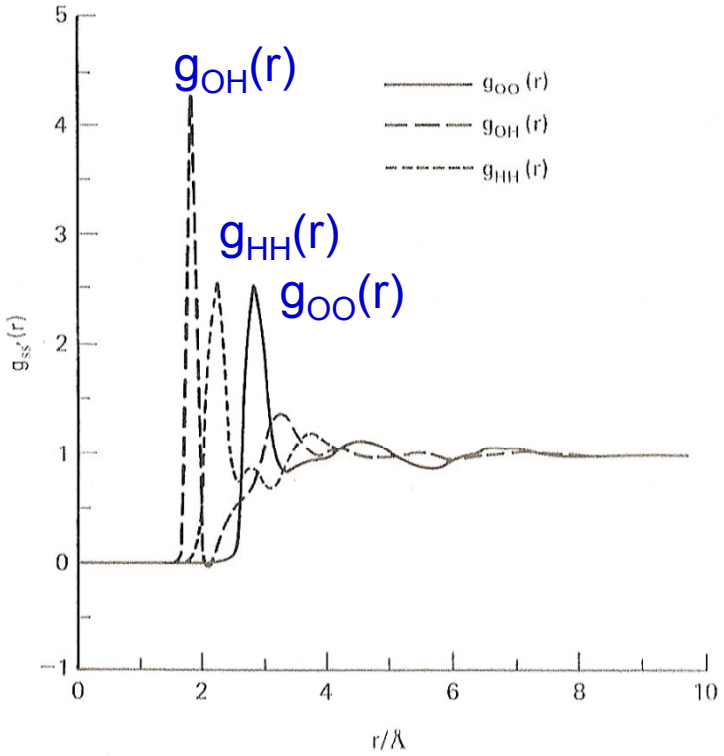


Integrant les $g_{\mu\nu}(r)$ es pot calcular els nombres de coordinació:

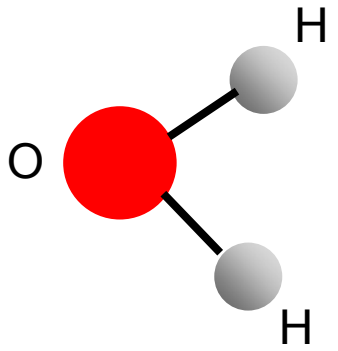
$$n_\nu = x_\nu \int_0^\infty \rho g_{\mu\nu}(r) 4\pi r^2 dr$$

H.L.Friedman, "A Course in Statistical Mechanics", pag.81

FUNCIONS DE DISTRIBUCIÓ RADIAL ÀTOM-ÀTOM DE L'AIGUA A T=25K, P=1atm



Molècula d'aigua:



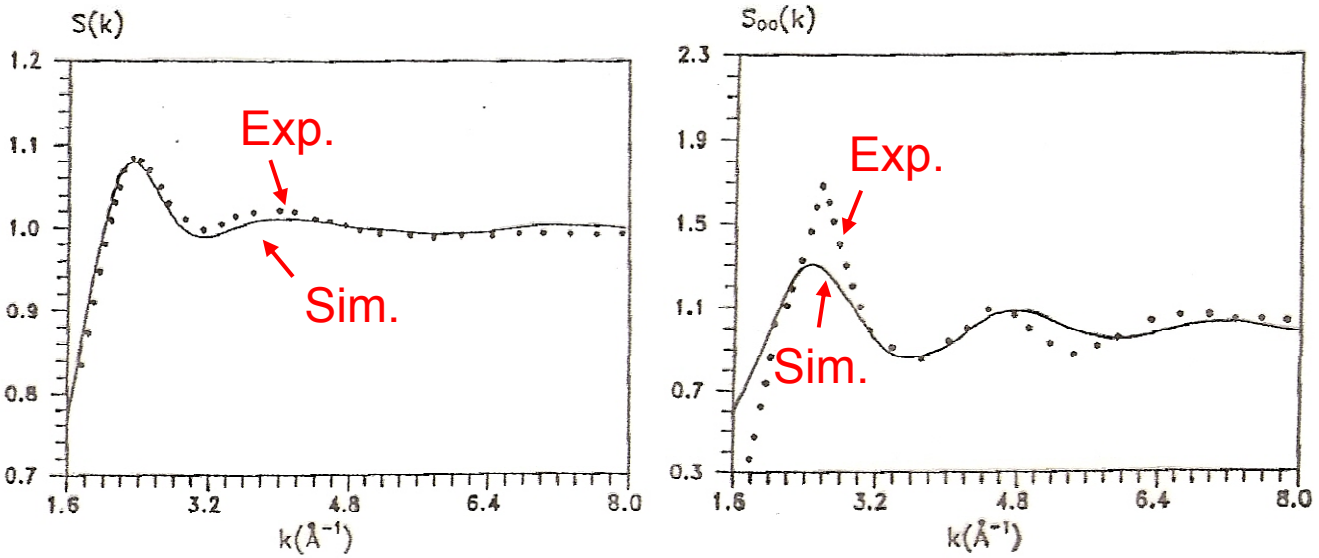
H.L.Friedman, "A Course in Statistical Mechanics", pag.81

lObtingudes per difracció de neutrons a partir de la g(r) total:

$$g(r) = 0.092 g_{oo}(r) + 0.422 g_{OH}(r) + 0.486 g_{HH}(r)$$

FACTORS D'ESTRUCTURA DE L'AIGUA A T=523K, ρ=0.75gcm^{-3}

comparació experimets/simulació



□ □ □ □ *U. Buontempo et al., Europhys.Lett. 19, 385(1982)*

——— *J. A. Padró, J. Martí, E. Guàrdia, J.Phys.Condens.Matter 6, 2283 (1994)*

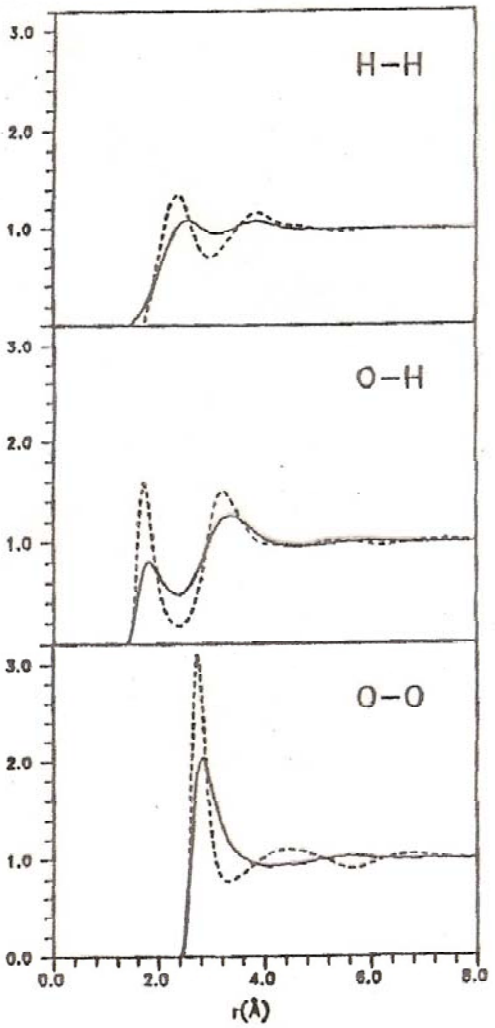
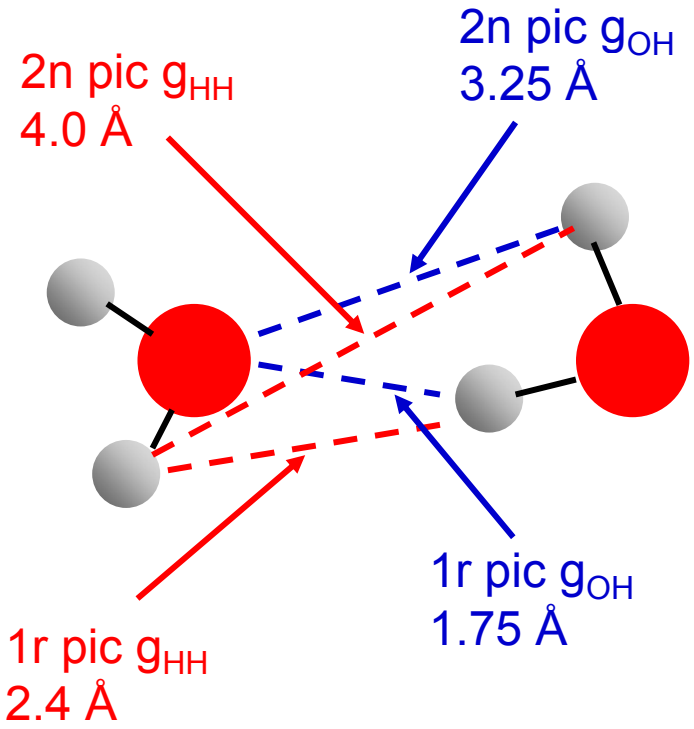


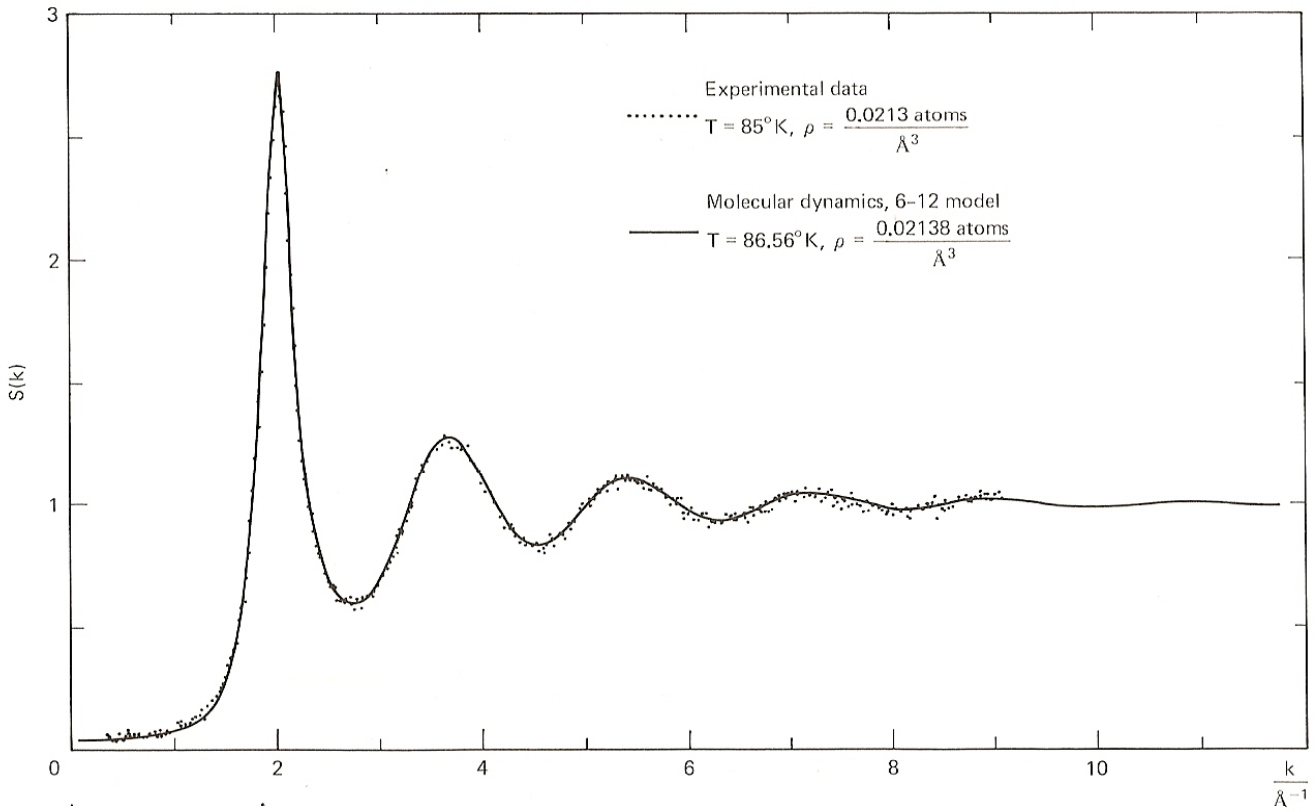
Figure 2. Partial radial distribution functions resulting from the MD simulations at 523 K (——) and 298 K (– – –).

Les posicion dels màxims es permeten deduir l'orientació de les molècules :



J. A. Padró, J. Martí, E. Guàrdia, J.Phys.Condens.Matter 6, 2283 (1994)

FACTOR D'ESTRUCTURA ESTÀTIC Ar LÍQUID



H.L.Friedman, "A Course in Statistical Mechanics", Cap. 5

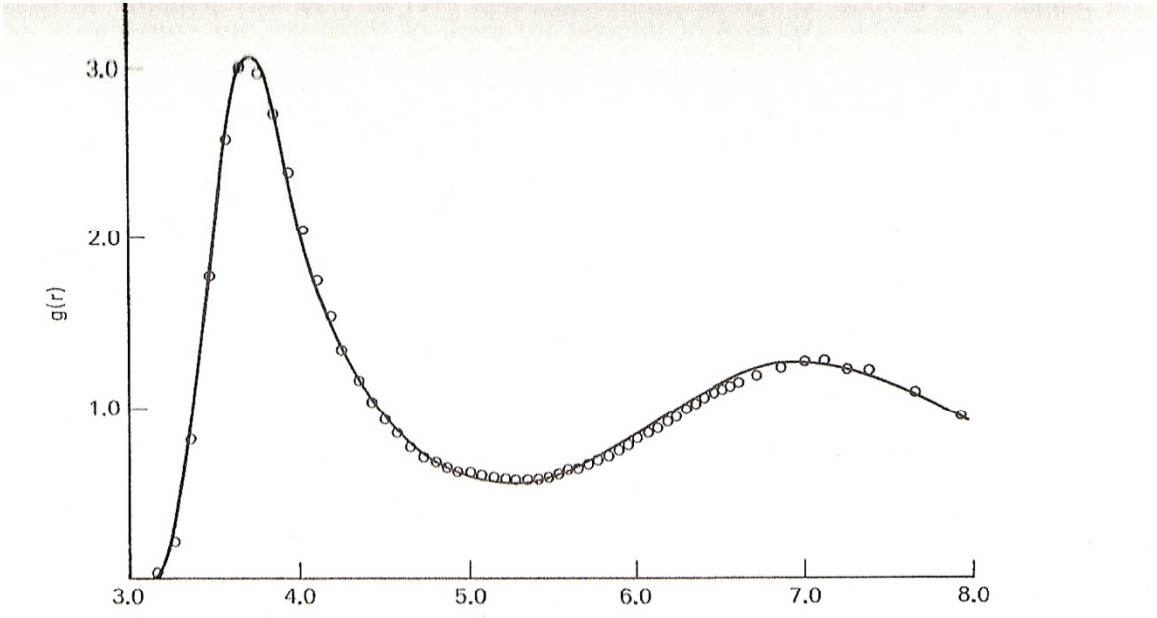
Factor d'estructura i funció de distribució radial

$$S(\vec{k}) = 1 + \rho \int \exp(-i\vec{k}.\vec{r}) g(\vec{r}) d\vec{r}$$

Relació inversa:

$$\rho g(\vec{r}) = \frac{1}{(2\pi)^3} \int \exp(i\vec{k}.\vec{r}) \left[s(\vec{k}) - 1 \right] d\vec{k}$$

FUNCIÓ DE DISTRIBUCIÓ RADIAL Ar LÍQUID



o o o o o : resultats experimentals

——— : resultats de simulació

FUNCIONS D'AUTOCORRELACIÓ DE VELOCITATS Ar LÍQUID

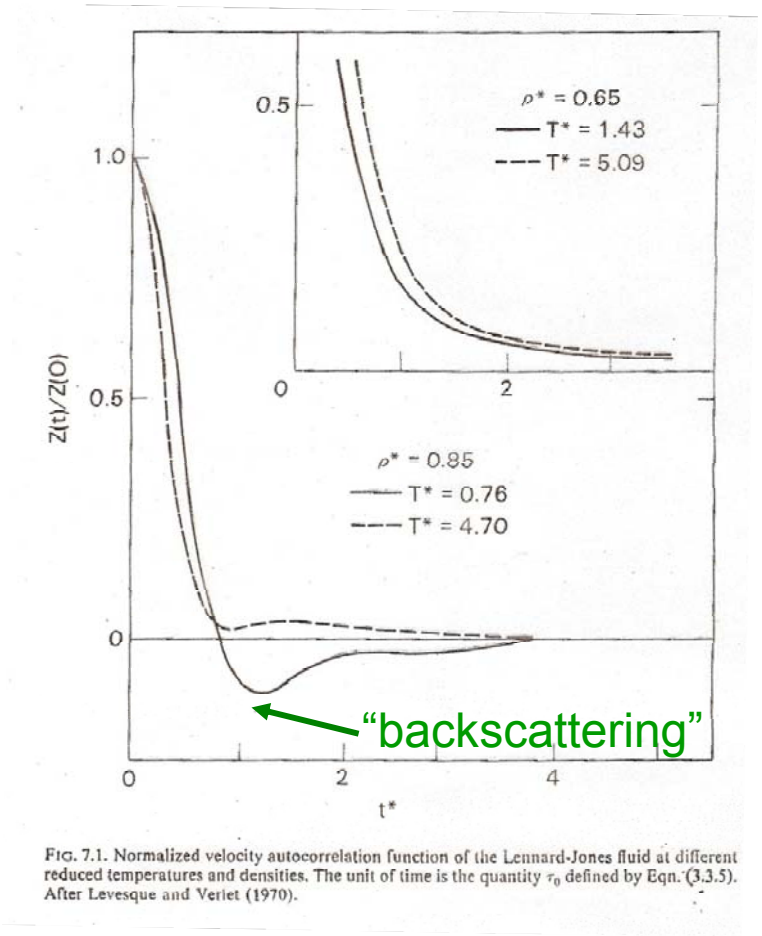


FIG. 7.1. Normalized velocity autocorrelation function of the Lennard-Jones fluid at different reduced temperatures and densities. The unit of time is the quantity τ_0 defined by Eqn. (3.3.5). After Levesque and Verlet (1970).

Unitats reduïdes:

$\rho^* = \rho/\sigma^3$

$T^* = K_B T/\varepsilon$

Hansen&McDonald, "Theory of Simple Liquids", Cap. 5

ESPECTRE DE FREQÜENCIES DE LA FUNCIO D'AUTOCORRELACIÓ DE VELOCITATS Ar LÍQUID

"Hindered translations"

Líquid molt dens

Líquid poc dens

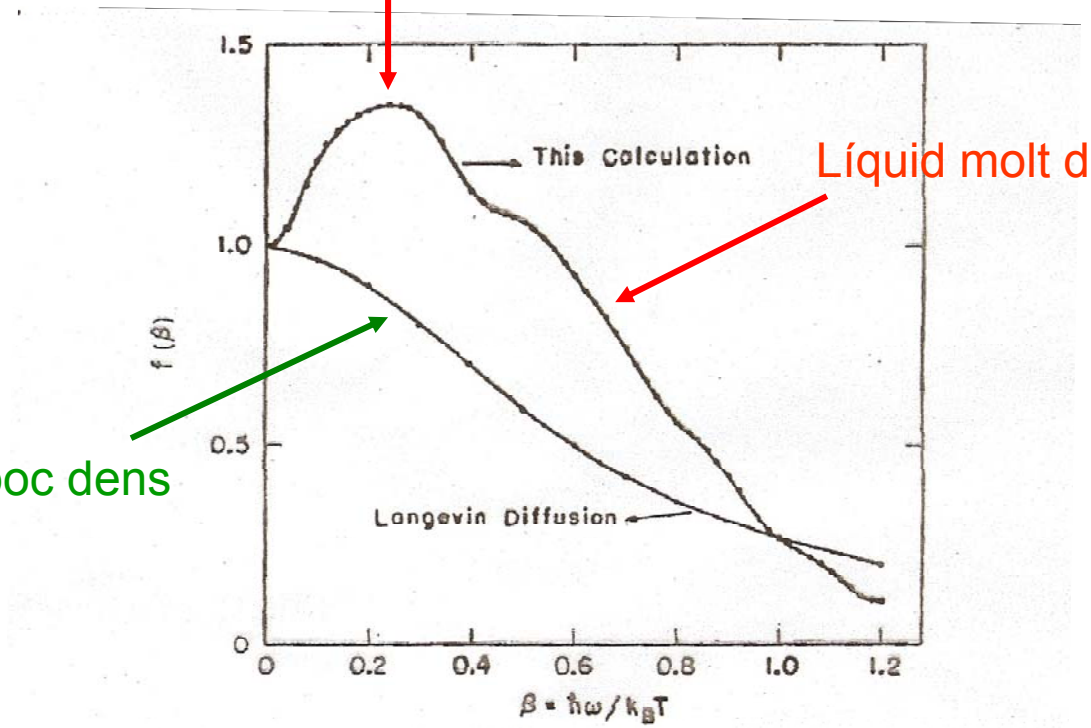
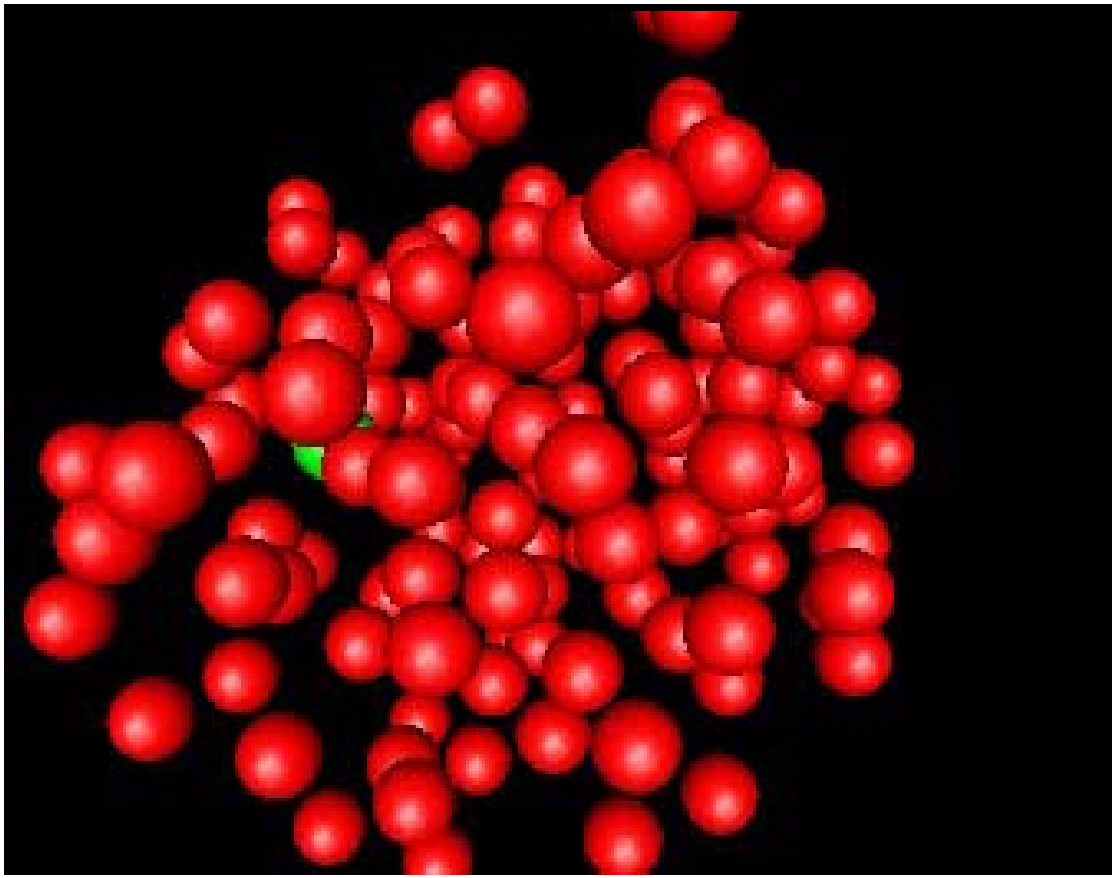


FIG. 5. Spectrum of the velocity autocorrelation function. The Lorentzian spectrum of a Langevin-type correlation is also shown.

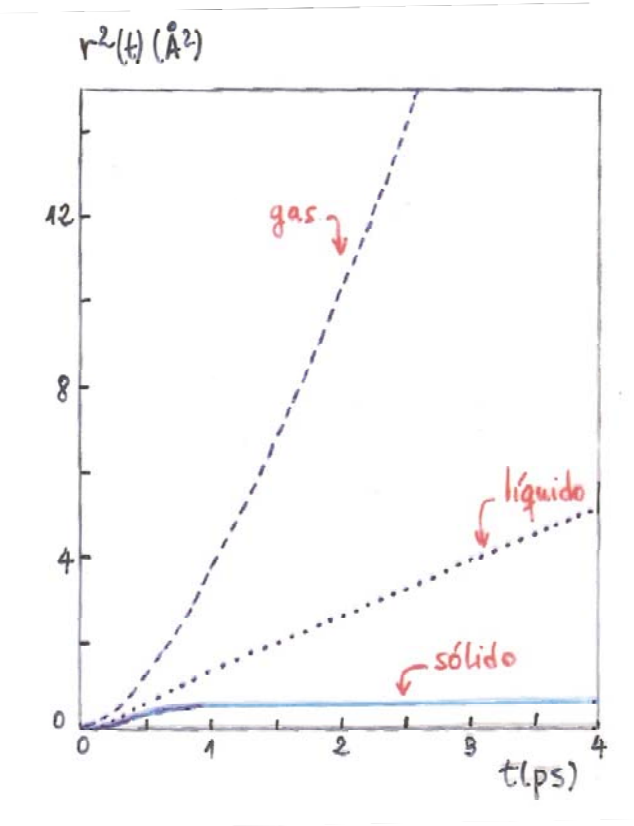
McQuarrie, "A Course in Statistical Mechanics", Cap. 22

Dense liquids: Snapshot of a typical MD configuration



DESPLAÇAMENT QUADRÀTIC MITJÀ Ar

$$r^2(t) = < (\vec{r}(t) - \vec{r}(0))^2 >$$



Líquid:

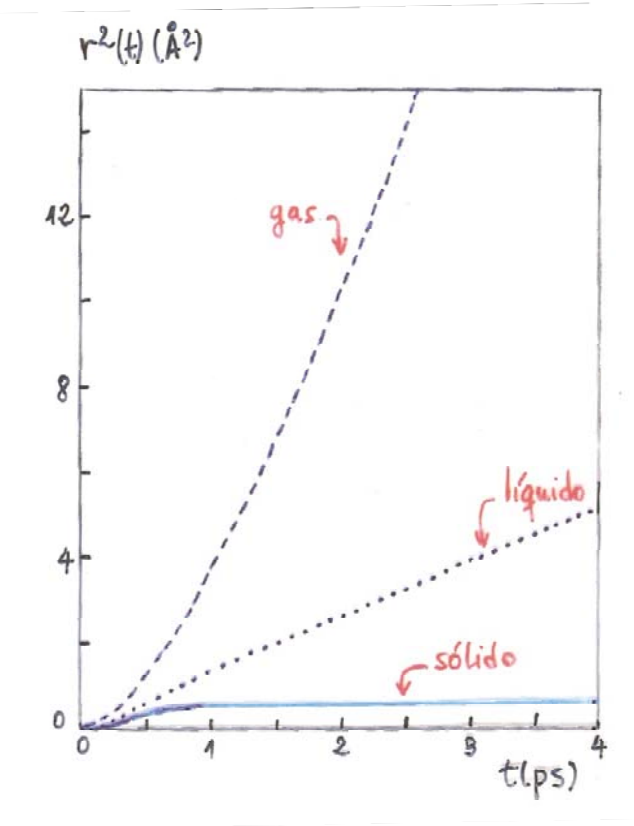
- Comportament asimptòtic:

$$r^2(t) \to 6Dt$$

D: Coeficient d'autodifusió

DESPLAÇAMENT QUADRÀTIC MITJÀ Ar

$$r^2(t) = < (\vec{r}(t) - \vec{r}(0))^2 >$$



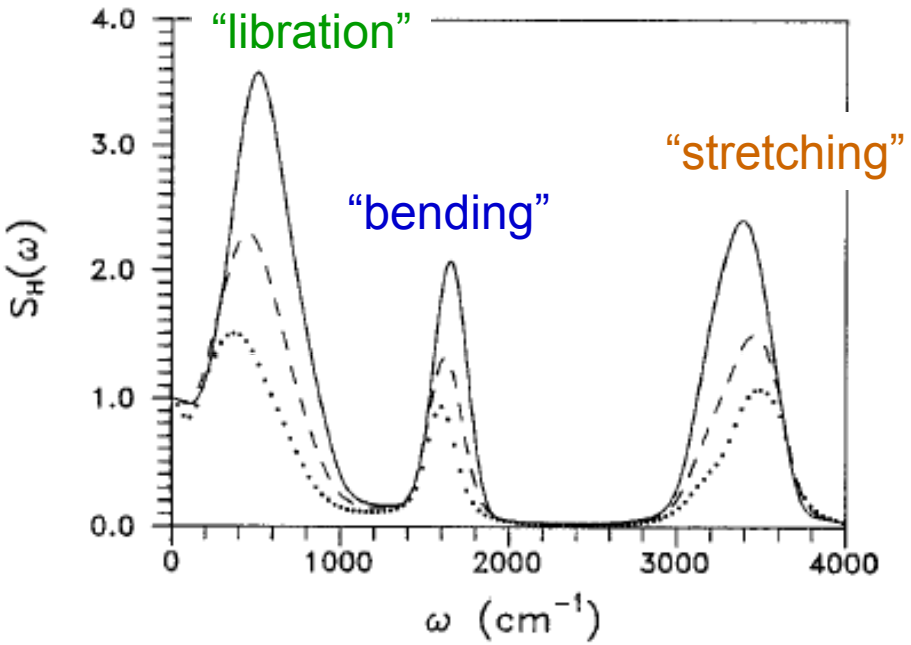
Líquid:

- Comportament asimptòtic:

$$r^2(t) \to 6Dt$$

D: Coeficient d'autodifusió

ESPECTRES DE FREQÜENCIES PER A L'AIGUA LÍQUIDA
ÁTOMS D'HIDROGEN



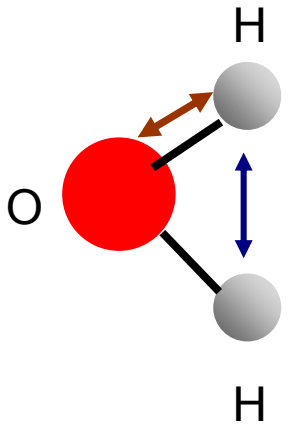
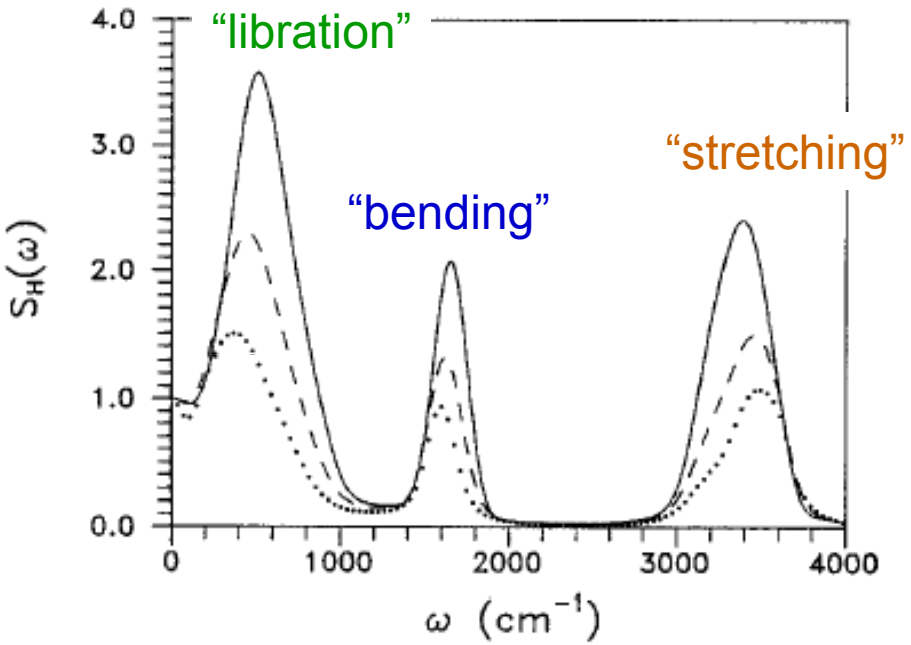


FIG. 11. Normalized hydrogen power spectra for water along the coexistence curve: T=298 K (—), T=403 K (– – –), and T=523 K (· · · ·).

J. Martí, J.A.Padró, E. Guàrdia, J. Chem. Phys. 105, 639 (1996)

ESPECTRES DE FREQÜENCIES PER A L'AIGUA LÍQUIDA
ÁTOMS D'HIDROGEN



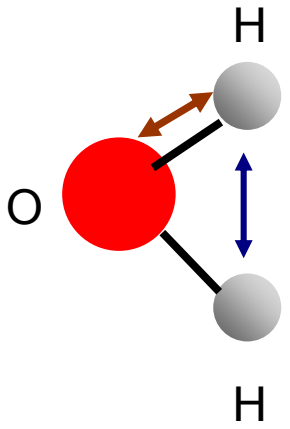


FIG. 11. Normalized hydrogen power spectra for water along the coexistence curve: T=298 K (—), T=403 K (– – –), and T=523 K (· · · ·).

J. Martí, J.A.Padró, E. Guàrdia, J. Chem. Phys. 105, 639 (1996)

ESPECTRES DE FREQÜENCIES PER A L'AIGUA LÍQUIDA
ÁTOMS D'OXíGEN

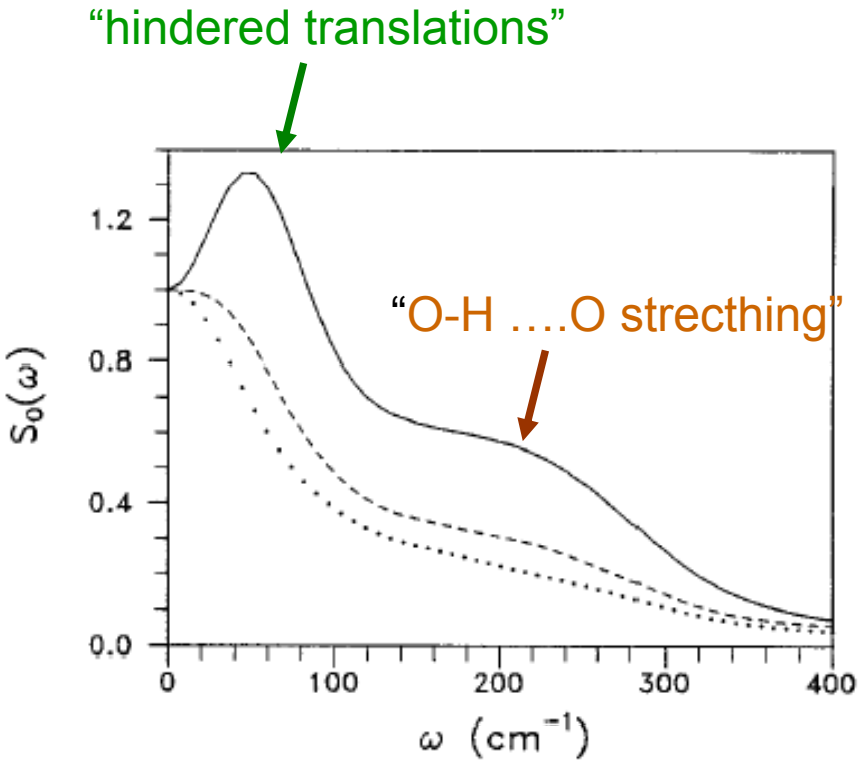
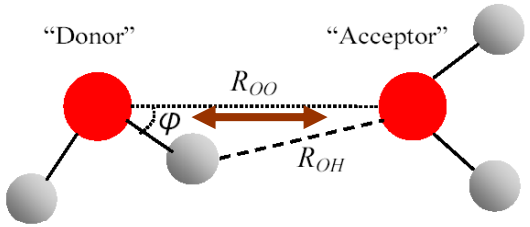


FIG. 8. Normalized $S_O(\omega)$ for water at ρ=0.91 g/cm^3 and T=298 K (—), T=403 K (----), and T=523 K (····).

Definición geométrica de un puente de hidrógeno



J. Martí, J.A.Padró, E. Guàrdia, J. Chem. Phys. 105, 639 (1996)

FACTOR D'ESTRUCTURA DINÀMIC: COMPORTAMENT QUALITATIU PER A DIFERENTS k

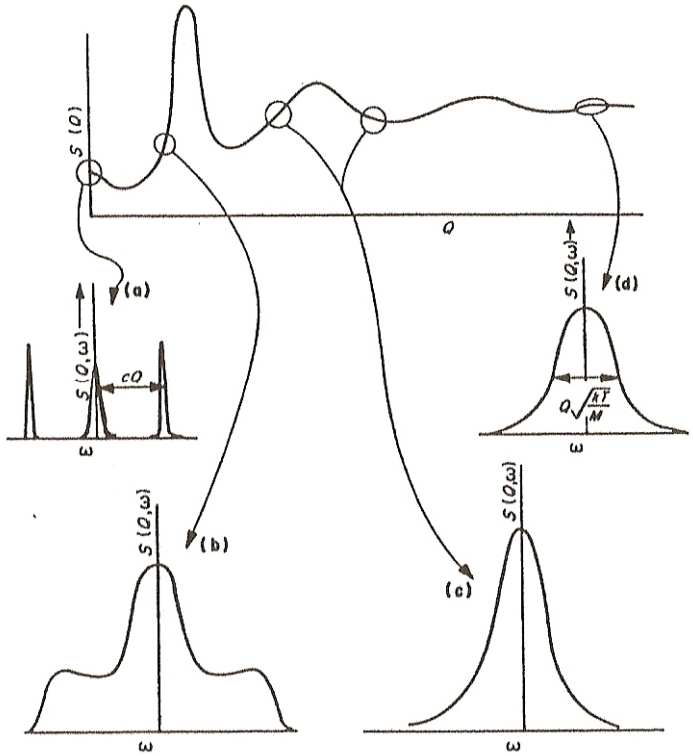


Fig. 16.1 Qualitative behaviour of $S(Q, \omega)$ for several values of Q in the case of a compressible fluid. The upper curve is the function $S(Q)$, and the remaining curves (a) to (d) show the spectral shape at fixed values of Q marked by circles on $S(Q)$. At low and high values of Q, the width can be calculated from simple considerations.

P.A.Egelstaff, "An Introduction to the Liquid State", Clarendon Press 1992

FACTOR D'ESTRUCTURA DINÀMIC
LÍMIT HIDRODINÀMIC K, ω →0

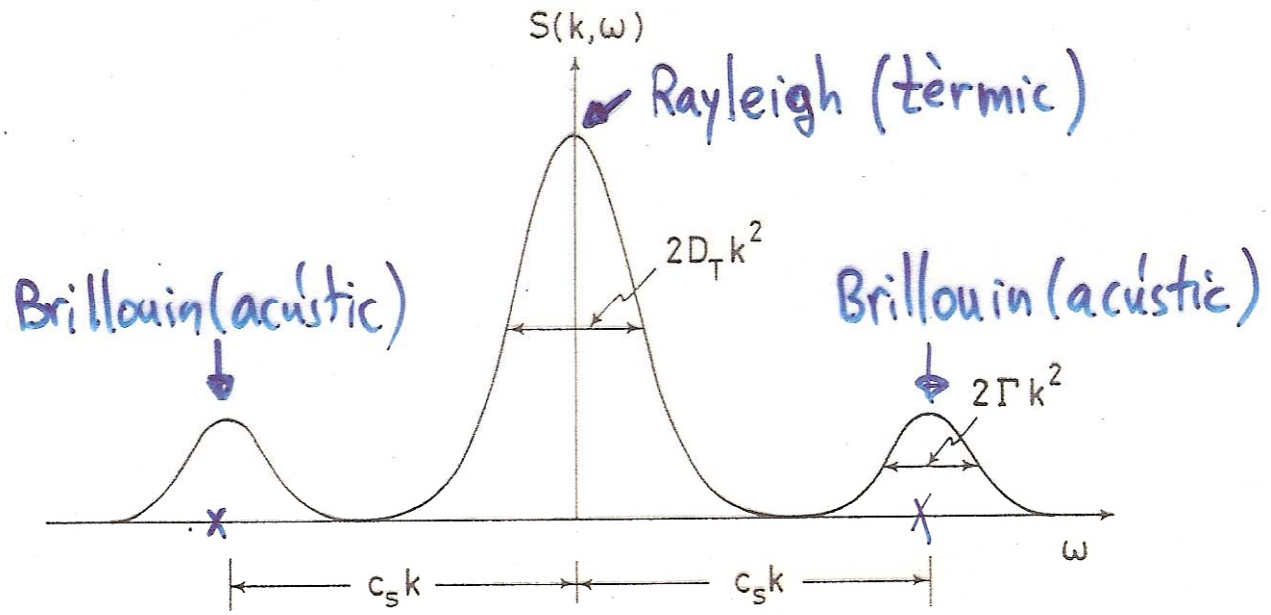


FIG. 8.4. Dynamic structure factor in the hydrodynamic limit; D_T is the thermal diffusivity, Γ is the sound-attenuation coefficient and c_s is the adiabatic speed of sound.

Hanse&McDonald, "Theory of Simple Liquids", Cap. 8

PHYSICAL REVIEW E VOLUME 50, NUMBER 5 NOVEMBER 1994

Computer simulation study of liquid lithium at 470 and 843 K

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(Received 20 January 1994)

Both structural and dynamical properties of ^{7}Li at 470 and 843 K are studied by molecular dynamics simulation and the results are compared with the available experimental data. Two effective interatomic potentials are used, i.e., a potential derived from the Ashcroft pseudopotential [Phys. Lett. **23**, 48 (1966)] and a recently proposed potential deduced from the neutral pseudoatom method [J. Phys. Condens. Matter **5**, 4283 (1993)]. Although the shape of the two potential functions is very different, the majority of the properties calculated from them are very similar. The differences among the results using the two interaction models are carefully discussed.

PACS number(s): 61.20.Ja, 61.20.Lc, 61.20.Ne

FACTOR DE SCATTERING INTERMEDIO

$$F(\vec{k},t) = \frac{1}{N} < \rho_{\vec{k}}(t)\rho_{-\vec{k}}(0) >$$

$$\rho_{\vec{k}}(t) = \sum_{i=1}^{N} \exp(-i\vec{k}.\vec{r}_i(t))$$

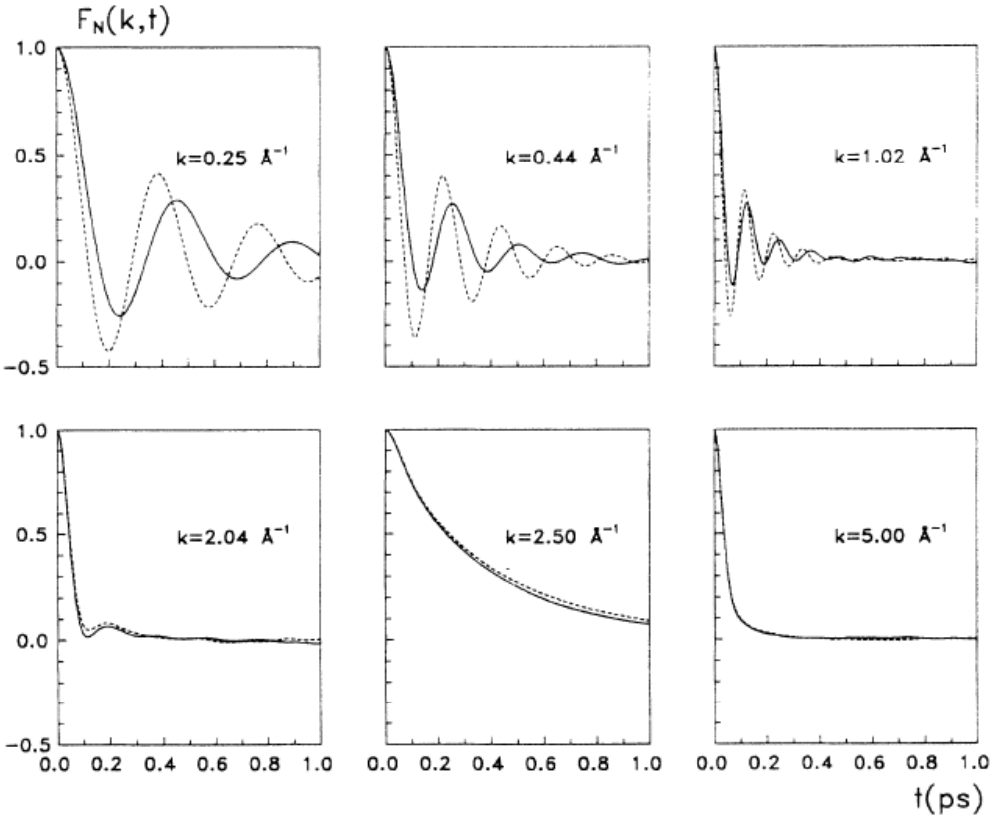

FIG. 7. Normalized intermediate scattering functions at 470 K [redacted]. Solid line, NPA potential; dashed line, Ashcroft potential.

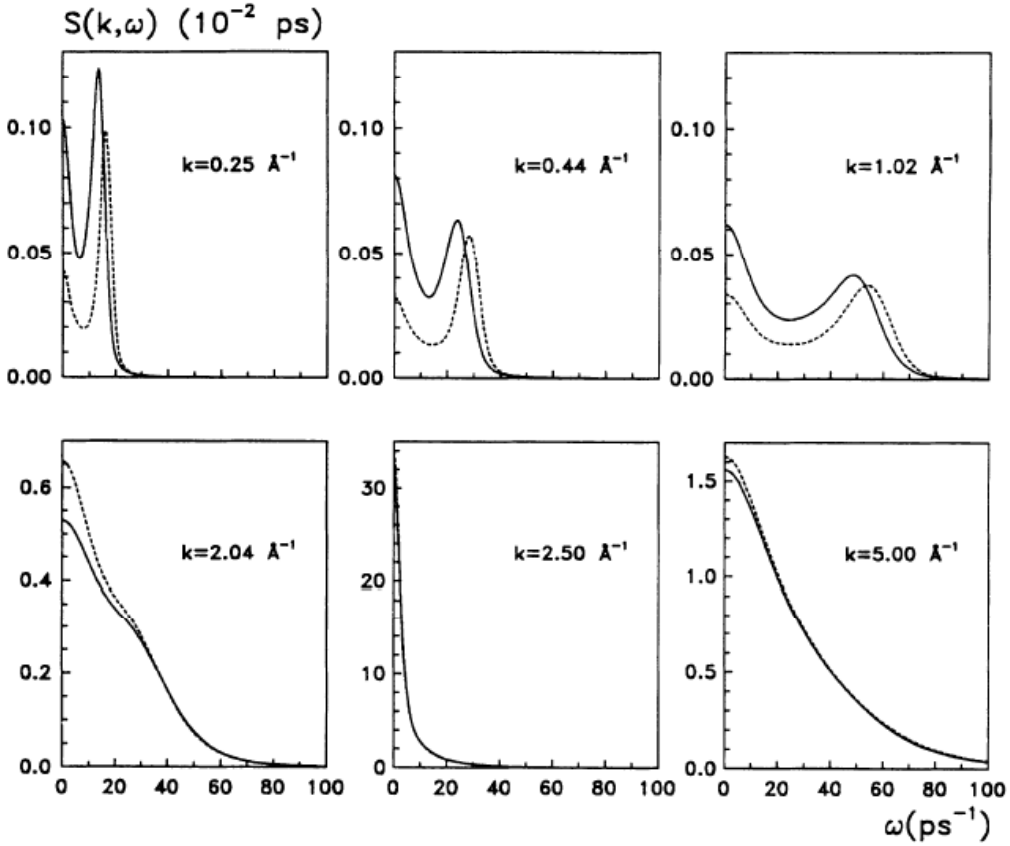

FIG. 11. Dynamic structure factors for different k values at 470 K. Solid line, NPA potential; dashed line, Ashcroft potential.

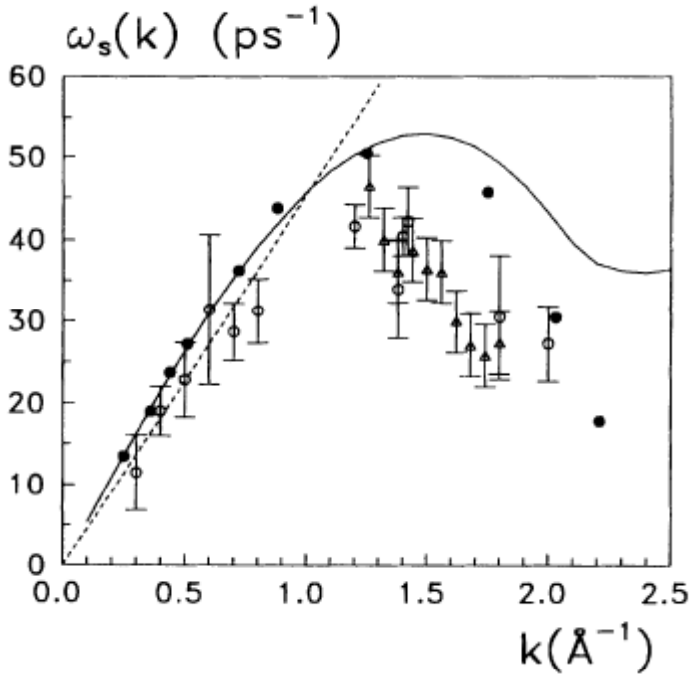

FIG. 14. Sound dispersion relation at 470 K. Solid line, Lovesey viscoelastic model [36]; dashed line, hydrodynamic sound dispersion curve; open circles with error bars, x-ray data [11]; triangles with error bars, neutron scattering data [10]; solid circles, MD results using the NPA potential.

Límite hidrodinámico: $\omega_s = c_s k$