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## Size effects and quasilocalized vibrations

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### ABSTRACT

The existence of localized vibrations at low frequencies in glasses and the notion and the properties of quasilocalized vibrations (QLVs) in glasses have been debated in the recent literature. By clarifying the main features of the QLVs and of the low-frequency vibration in model systems (a defect lattice and a Lennard-Jones glass in the harmonic approximation) we reach the conclusions, firstly, that truly localized modes are confined to the very-high-frequency tail and to gaps of the vibrational spectrum, secondly, that the QLVs are actually present at low frequencies in glasses, thirdly, that the QLVs are modes that involve all the atoms of the system (they are *extended*) but that they have few nearby atoms that carry a large fraction of the vibrational energy and, fourthly, that they are not a trivial mixing of extended and localized harmonic eigenmodes but rather appear to be an independent *species* of modes.

### §1. INTRODUCTION

The characterization of the vibrational modes of glasses or, more generally, of disordered structures and their classification is a long-lasting problem in condensed-matter physics. Even in the simple approximation of purely harmonic vibrations, where all the mathematical properties of the quadratic Hamiltonians can be exploited and the vibrational properties are encompassed in the eigenvalues and eigenvectors of the dynamic matrix, the matter is far from settled. In a recent attempt to rationalize the different kinds of vibration in disordered systems, Fabian and Allen (1996) introduced concepts such as ‘propagons’, ‘diffusons’ and ‘locons’ to characterize the modes. However, apart from the attempt to assign a name to modes with given properties (e.g. ‘locons’ are modes localized in the Anderson sense) a general agreement on which modes exist in disordered systems (in a given frequency region) is still lacking. It is also not clear whether the Fabian–Allen classification is complete. The present contribution aims to shed light on the characteristics of a small subset of vibrational modes of the disordered structure: the so-called quasilocalized vibrations (QLVs). The need for such a clarification emerges from recent studies that seem to lead to contradictory results.

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In the framework of the dynamics of defect crystals, QLVs (also called resonance modes) were first discussed by Brout and Visscher (1962) and by Kagan and Iosilevskii (1962) and have been treated in a number of reviews (for example Maradudin *et al.* (1971) and Dederichs and Zeller (1980)). They are distinct from the better-known true localized vibrations (LVs). Both types of vibration can be understood as the result of a weak bilinear interaction of a harmonic oscillator ('defect') with the vibrations of a harmonic lattice ('host'). A LV results if the frequency of the oscillator lies well above (or in a gap of) the band of frequencies of the lattice. The LV is an eigenstate of the combined harmonic system with a frequency above the band of host frequencies. The vibrational amplitude is centred on the defect and decays exponentially in the host. A QLV is produced if the frequency of the defect oscillator is in a frequency range where the host's density of states (DOS)  $Z(\omega)$  is low. Because  $Z(\omega) \propto \omega^2$  for low frequencies, QLVs are typically found at low frequencies. The exact eigenvectors are formed by hybridization of the host vibrations with the additional oscillator. The vibrational motion of the defect can be described by a damped low-frequency vibration, the QLV, and a residue of host vibrations. The damping  $\gamma_{\text{QLV}}$  of the QLV is given by the value of the host DOS at the QLV frequency  $Z(\omega_{\text{QLV}})$ , and  $\gamma_{\text{QLV}} \rightarrow 0$  for  $\omega_{\text{QLV}} \rightarrow 0$ . Also the amplitude of this vibration is centred on the defect but drops now only by a power law with distance in the host lattice. In the considered harmonic system, damping is equivalent to energy broadening of the added oscillator vibrational mode. The exact harmonic eigenvectors of the combined system will be extended but show an enhanced amplitude at the defect and the DOS will show the added degree of freedom due to the defect. For finite systems the spread of the QLVs over the exact eigenvectors changes with size, which has led to some confusion. This is a consequence of the fact that LVs are exact eigenmodes whereas QLVs are not.

Turning our attention to the glass case; one of the present authors and co-worker concluded from computer simulations of a soft-sphere glass that the low-frequency dynamics of glasses exhibits a number of QLVs (Laird and Schober 1991, Schober and Laird 1991). These QLVs were centred on ten or more atoms, in agreement with calculations using the soft-potential model (Buchenau *et al.* 1991, 1992). Similar observations were made subsequently in simulations by different researchers for a number of materials. As indicator for the QLV the participation ratio  $P_\lambda$  of the eigenvectors was used. In particular, it was found that for the lowest frequencies the participation ratios scale with the system size  $N$  as  $P_\lambda \propto 1/N$  which is the signature of *localized modes*. For finite frequencies this scaling was found to vanish owing to interaction between modes (Schober and Oligschleger 1996).

The existence of localized modes at low frequency in glasses was challenged by Mazzacurati *et al.* (1996) who numerically calculated the low-frequency eigenvectors in a Lennard-Jones (LJ) glass for different system sizes up to  $N=32\,000$ . These workers found that for large system sizes the participation ratios of the high-frequency localized modes scale with  $1/N$ . The low-frequency modes showed no such scaling. From this they concluded that the exact low-frequency eigenmodes are extended and argued that this is in contradiction to the work of Laird and Schober (1991), Schober and Laird (1991) and Buchenau *et al.* (1991, 1992).

In this contribution we shall show that the so-called QLVs present a *mixed* character, showing features of both *localized* modes (a large part of the atomic

motion concentrated in a small spatial region) and *extended* modes (the atomic motion actually extended over the whole system). To reach this conclusion, we shall study the spatial distribution of the local atomic energy associated with a given eigenmode and draw a parallel between the behaviours of the participation ratio in glasses and in a defect lattice. We find that the observed behaviour of the participation ratio is actually in agreement with that expected for QLVs. Furthermore, it does not indicate a disappearance of QLVs with system size, and it reflects the localization of QLVs for small system sizes when their frequency is smaller than the smallest frequency of the sound-wave-like modes. This property was used by Laird and Schober (1991) and Schober and Laird (1991).

In the following, we shall first study the effect of system size for the most simple QLVs, a heavy mass defect in a fcc lattice. In the light of these findings we shall then inspect the eigenvectors of the LJ glass.

## § 2. QUASILocalized MODES IN CRYSTALS

In harmonic approximation the vibrations of a lattice can be described by the eigenmodes and eigenfrequencies of the dynamic matrix. From the eigenfrequencies, one derives the vibrational DOS. In an ideal infinite crystal the eigenmodes are plane waves, acoustic phonons and optical phonons. They extend throughout the lattice. Using the translational symmetry of the lattice they can be classified according to their  $\mathbf{q}$  vector and polarization. In defect crystals the situation is more complex but at least for point defects still analytically tractable and it has been studied extensively in the past (for reviews see for example Maradudin *et al.* (1971) and Dederichs and Zeller (1980)). The lack of translational symmetry implies that the  $\mathbf{q}$  vector no longer characterizes the eigenmodes exactly. However, in many cases a description in terms of broadened phonon modes still holds (Schober *et al.* 1975, Zinken *et al.* 1977). The broadening can be seen as an admixture of the defect modes plus a mixing of phonon modes by the defect.

Apart from this broadening of the extended phonons, defects can also cause strong local effects. The defect and/or its neighbours might vibrate with frequencies outside the band of host frequencies. The eigenvector of these LVs decay exponentially with distance from the defect. Defects can show strongly enhanced vibrational amplitudes also at frequencies where there is a low DOS of the host: QLVs or resonant vibrations. Both types of vibration can be seen as a defect vibration which is weakly bilinearly coupled to the host vibrations. In the case of localized modes, diagonalization of the dynamic matrix leads to an exact isolated eigenmode above the band of host modes, or in a frequency gap. In the second case, diagonalization gives eigenmodes which are a mixture of the 'defect vibration' and the host modes: the well-known hybridization effect. The QLV is seen as a sharp peak in the vibrational DOS of the defect atoms. Counting the modes at the resonance frequency, one finds an extra mode, over and above the number of extended modes corresponding to the resonance frequency. The eigenmodes are maximal at the defect and decrease with a power law of distance to the level of the extended modes.

As discussed above, QLVs are soft local vibrations inside the frequency band of extended sound-wave-like vibrations, quasipplane waves (QPWs), to which they are bilinearly coupled. QLVs are not eigenmodes; they hybridize with the plane waves. The harmonic eigenmodes have contributions from the local vibration and the plane

waves. QLVs are characterized by a large amplitude of a few atoms which shows as a peak in the local spectrum of these atoms

$$Z^i(\omega) = \frac{1}{3} \sum_{\lambda=1}^{3N} \sum_{\alpha=1}^3 e_{i,\alpha}(\lambda) e_{i,\alpha}(\lambda) \delta(\omega - \omega_\lambda), \quad (1)$$

where  $\omega_\lambda$  is the frequency of eigenmode  $\lambda$  and  $e_{i,\alpha}(\lambda)$  the component of the eigenvector in direction  $\alpha$  on atom  $i$ . The eigenvectors obey orthonormality and closure relations, and  $\int Z^i(\omega) d\omega = 1$ . In an ideal monatomic lattice, all local spectra  $Z^i(\omega)$  are identical and equal to the total spectral density  $Z(\omega)$ .

Such local spectra have been calculated in the past for a multitude of different defects in crystals: heavy masses, force constant defects and geometrical defects. One observes the low-frequency resonances in the local spectrum as narrow peaks with a finite frequency-dependent width (Zeller and Dederichs 1976, Dederichs and Zeller 1980). This originates from the general  $\omega$  dependence of the vibrational Green's function and, therefore, also holds in the glass. For large systems this implies that a number of modes  $N_r = \Delta N$  contribute with similar amplitude to the peak in  $Z^i(\omega)$  with  $\Delta$  a finite size-independent number. From equation (1) it then follows that  $e_{i,\alpha}(\lambda) \propto 1/N^{1/2}$ , which is the same scaling with size as for ideal lattice phonons. Inserting this scaling into the equation for the participation ratio

$$P_\lambda = \frac{1}{N} \left( \sum_{i=1}^N [\mathbf{e}_i(\lambda) \cdot \mathbf{e}_i(\lambda)]^2 \right)^{-1}, \quad (2)$$

one finds that there is no scaling with  $1/N$  for quasilocalized modes.

When the simulated systems are so small that some QLV frequencies fall below the lowest frequency  $\omega_{\min}$  of a plane wave, which fits into the periodicity volume, the QLVs are artificially localized and  $P_\lambda$  scales with  $1/N$  for  $\omega_{\text{QLV}} < \omega_{\min}$ . This scaling was used by Laird and Schober (1991) and Schober and Laird (1991) as a characteristic sign of the lowest-frequency QLV. For higher but still low frequencies, the scaling vanished.

This effect can also be observed for the well-studied mass defect in a fcc lattice where one atom of host mass  $m$  is replaced by an otherwise equal atom of mass  $m_d$ .  $Z^i(\omega)$  can easily be written in terms of the host Green's function (for example Dederichs and Zeller (1980)). Figure 1 shows the local vibrational spectrum of the heavy substitutional mass defect for two mass ratios in an infinite lattice. The resonance frequency scales as  $\omega_r \propto (m/m_d)^{1/2}$ . The width of the resonance scales as  $\Gamma \propto \omega_r^2$ . If one excites a vibration of the defect atom with frequency  $\omega_r$ , the vibration decays slowly and the energy of the vibration is dissipated to the lattice. The lower the resonance frequency, the less is the energy dissipation and the more the resonance vibration resembles an eigenstate.

Figure 2 shows the effect of size for the same mass defect in a finite system of  $N$  atoms with periodic boundary conditions. In figure 2(a) the minimal participation ratio found by diagonalizing the dynamic matrix is depicted. It clearly shows that after an initial drop with  $1/N$  the minimal value of  $P_\lambda$  saturates. The average  $P_\lambda$  for a given frequency band (sufficiently wide to span the gaps in the phonon spectrum of the finite system) correspondingly increases (not shown). Figure 2(b) shows that the levelling off of the participation ratio occurs when the resonance frequency becomes comparable with the lowest frequency of a QPW.

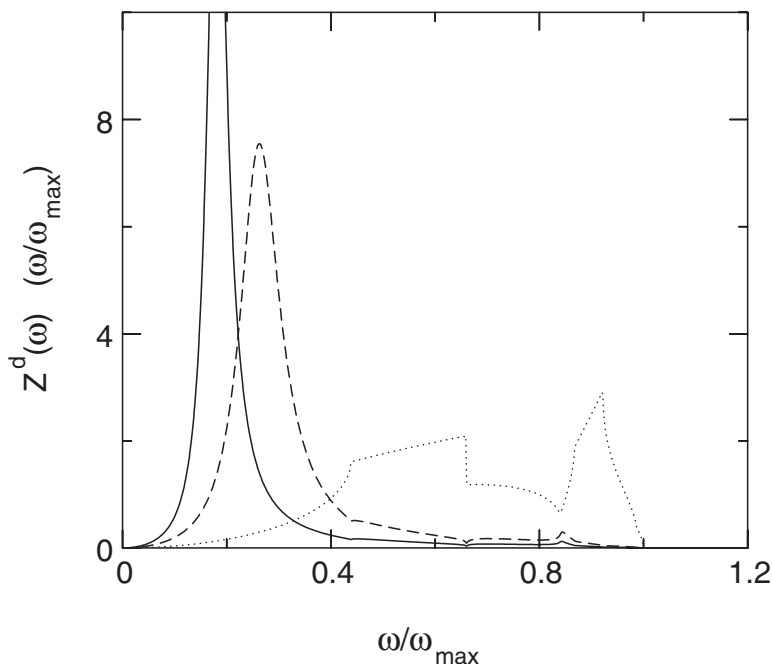


Figure 1. Exact local spectrum for a mass defect in a fcc lattice: (—),  $m_d/m = 8$ ; (---),  $m_d/m = 4$ ; (.....), ideal lattice.

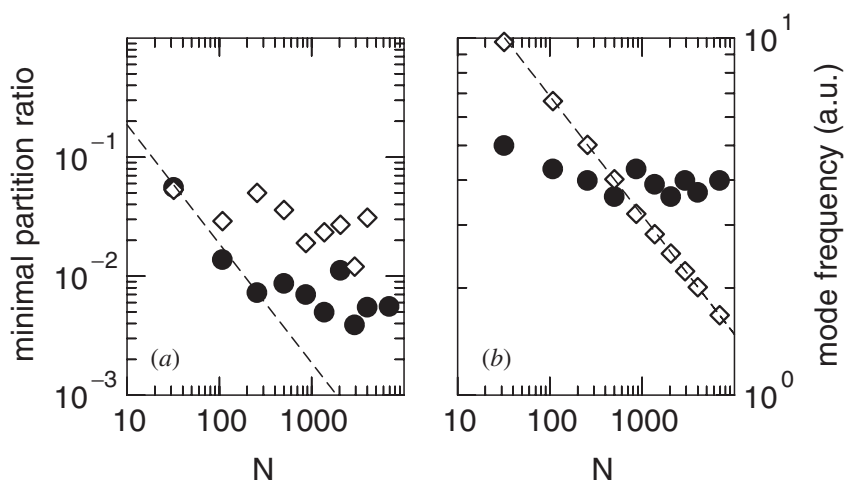


Figure 2. (a) log-log plot of the minimal participation ratio as function of system size: (●),  $m_d/m = 8$ ; (◇),  $m_d/m = 4$ ; (---),  $1/N$  scaling. (b) log-log plot of resonance frequency (●) and lowest frequency of extended mode (◇) versus system size ( $m_d/m = 8$ ) (a.u., arbitrary units); (---), scaling with  $1/N^{1/3}$ .

For a finite defect concentration, coupling between the QLVs additionally destroys the  $1/N$  scaling by similar effects (Schober and Oligschleger 1996). Schober and Oligschleger also showed how, at low frequencies, the exact eigenvectors can be decomposed into a basis of extended modes and approximate localized modes with a weak bilinear coupling. The latter are the basis of the

soft-potential model (Karpov *et al.* 1983, Il'in *et al.* 1987). The bilinear coupling is the source of sound attenuation in that model (Buchenau *et al.* 1992). Following Laird and Schober (1991), Schober and Laird (1991) and Buchenau *et al.* (1991, 1992), we expect in glasses a spectrum of resonant modes, each centred on ten or more atoms. Owing to orthonormality of the eigenvectors, this reduces the amplitudes  $e_{i,\alpha}(\lambda)$  on the resonant atoms even before interaction. The amplitudes are then further reduced by interaction as discussed above. A single eigenvector will then have weak contributions of many QLVs. This will, for large systems, look like ‘random noise’.

### §3. LENNARD-JONES GLASS

We shall use the outcome of previous investigations (Mazzacurati *et al.* 1996) to study the QLVs. Therefore, we shall only briefly recall the details of the molecular dynamics (MD) simulation. The investigated systems consist of  $N = 256, 864, 2048, 10976$  and  $32000$  particles interacting via a (6–12) LJ potential (the constants have been chosen to represent argon atoms;  $\epsilon = 125.2$  K;  $\sigma = 3.405$  Å). A standard NVE (constant number of atoms, volume and energy) MD simulation is performed at different temperatures in the normal liquid phase. The glass is obtained by a fast quench ( $\dot{T} \approx 10^{12}$  K s<sup>-1</sup>) of the equilibrated liquid at  $T = 60$  K (very close to the mode-coupling theory temperature  $T_{\text{MCT}}$  for this system (Angelani *et al.* 2000b)) down to about 5 K. Starting from the glass configuration at  $T = 5$  K, we calculated by a steepest-descent method the ‘inherent’ configuration (Stillinger and Weber 1983), that is the  $T = 0$  K configuration of the system. The dynamics of the atoms in the glass around the inherent configuration are then studied in the harmonic approximation (normal mode analysis). This procedure consists in retaining only the quadratic terms of the interatomic interaction potential, and in calculating the dynamic matrix  $\bar{\mathbf{D}}$ . This method was also used in the calculations for the soft-sphere glass (Laird and Schober 1991). From the dynamic matrix the eigenvalues and eigenvectors are obtained from the direct diagonalization or, bypassing the explicit knowledge of the eigenmodes, by the spectral moments method (Benoit *et al.* 1992, Viliani *et al.* 1995). For large samples (where direct diagonalization of the dynamic matrix is not easily accessible) the DOS and the dynamic structure factor are obtained with the spectral moments method, while low- and high-frequency eigenvectors (used for the study of spatial patterns of eigenmodes) are calculated by a modified Lanczos method.

In figure 3 we report the vibrational DOS for three different system sizes ( $N = 2048, 10976$  and  $32000$ ). In this case, for comparison, the DOS for the two larger systems are calculated by Fourier transforming the velocity self-correlation function obtained by the true MD at  $T = 5$  K:

$$Z^{\text{MD}}(\omega) = \frac{1}{3N} \frac{m}{k_{\text{B}}T} \int dt \exp(i\omega t) \sum_i \langle \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle, \quad (3)$$

where  $\mathbf{v}_i(t)$  is the instantaneous velocity of the  $i$ th atom and  $m$  the atomic mass. For the  $N = 2048$  system the DOS is calculated in the harmonic approximation from the complete set of eigenvalues  $\omega_\lambda$  obtained via direct diagonalization, that is

$$Z^{\text{DD}}(\omega) = \frac{1}{3N} \sum_\lambda \delta(\omega - \omega_\lambda). \quad (4)$$

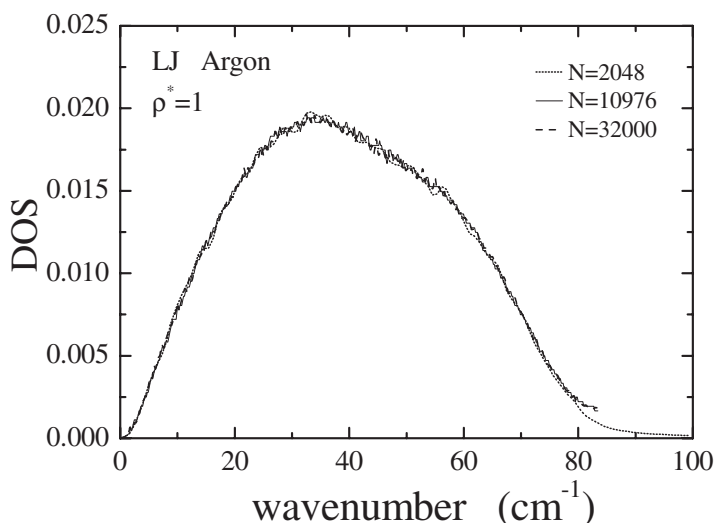


Figure 3. Vibrational DOS for LJ glass at a density  $\rho = 42 \text{ mol l}^{-1}$  (corresponding to a reduced density  $\rho^* = \rho\sigma^3 = 1$ ) calculated from different system sizes: ( $\cdots$ ),  $N = 2048$ ; ( $\text{—}$ ),  $N = 10976$ ; ( $-\text{--}$ ),  $N = 32000$ . The DOS for  $N = 2048$  is the histogram of the eigenvalues that have been obtained by direct diagonalization of the dynamic matrix; those for  $N = 10976$  and  $N = 32000$  are derived from the Fourier transform of the velocity-velocity correlation function.

Figure 3 shows the equivalence of the two ('real' and approximated) DOSs, which indicates that the low-temperature dynamics are basically harmonic in the investigated frequency range and that no evidence is found of more subtle effects, such as two-level systems (TLSs), responsible for the very-low-temperature anomaly of the specific heat, or their crossover to highly anharmonic vibrations predicted by the soft-potential model. Both of these are expected to be too rare to be observable in the MD box. Since our calculation is classical, tunnelling in TLSs would only be observed as an anharmonicity and/or jump process. The small deviation at high frequencies is due to the aliasing effect in the numerical Fourier transformation.

Of central interest here is the behaviour of the participation ratio, defined in equation (2), which is reported as a function of frequency in figures 4 and 5. In figure 4 the participation ratio is averaged over a frequency bin  $0.5 \text{ cm}^{-1}$  wide and plotted in the whole frequency range. In contrast, figure 5 reports the individual mode participation ratios for different system sizes in the low-frequency part of the spectrum, where localized and quasilocalized modes are expected to be found. The participation ratio is well below unity at the lowest and highest frequencies. As shown by Mazzacurati *et al.* (1996), the participation ratio at high frequencies scales with the system size, indicating that the modes are truly localized. In contrast, in the low-frequency part of the spectrum, despite its low value,  $P_\lambda$  does not show any scaling, so excluding the existence of localized modes at low frequencies. However, the value of the participation ratio is definitively much smaller than unity, which hints at a qualitative difference between these low  $P_\lambda$  modes and the extended modes of the central frequency region. The size independence of the position of the 'dip' (about  $2.5 \text{ cm}^{-1}$ ) suggests that this is a real feature of the glass, and not a phenomenon induced by the quantization of the low-frequency modes in the MD boxes.



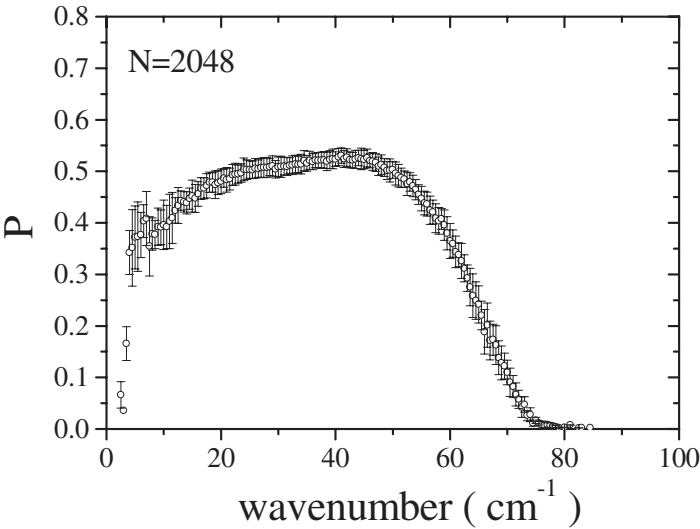


Figure 4. Participation ratio for the investigated LJ glass with  $N=2048$ . Each point (error bar) is the average (standard deviation  $\pm \sigma$ ) of  $P_\lambda$  of all the modes belonging to a bin of  $0.5 \text{ cm}^{-1}$  width.

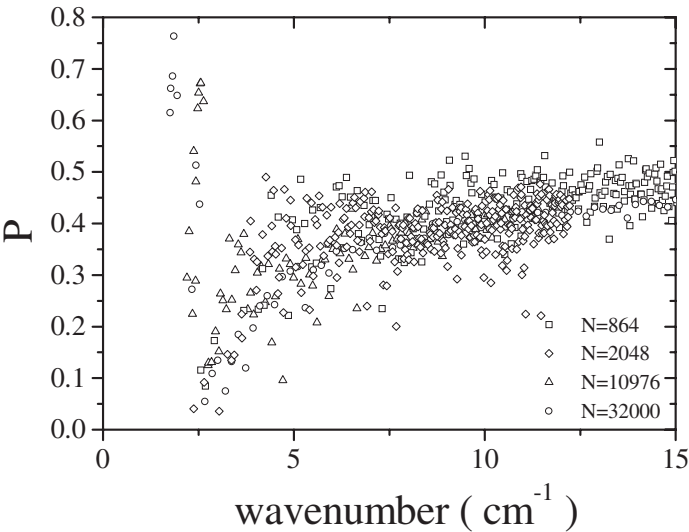


Figure 5. Similar to figure 4, but each point represents the value of an individual  $P_\lambda$ , for different system sizes: ( $\square$ ),  $N=864$ ; ( $\diamond$ ),  $N=2048$ ; ( $\triangle$ ),  $N=10976$ ; ( $\circ$ ),  $N=32000$ .

As discussed in the case of defect lattices, the behaviour observed for the modes around  $2.5 \text{ cm}^{-1}$  ( $P_\lambda$  is small and is size independent) is typical for what is called QLV or resonant mode. To understand better whether or not these modes can actually be classified as QLVs and to study their features, we have introduced the spatial correlation function of the local (atomic) energy content associated with each mode. Given a mode (index  $\lambda$  and frequency  $\omega_\lambda$ ), and the pattern of atomic

displacements induced by this mode (i.e. the eigenvector  $\mathbf{e}_i(\lambda)$ ), similarly to (Angelani *et al.* 2000a), we define the total energy associated to each atom  $i$  as

$$\mathcal{E}_i(\lambda) = \frac{M\omega_\lambda^2 a^2}{2} |\mathbf{e}_i(\lambda)|^2 - \frac{Ma^2}{4} \sum_{\alpha\beta} \sum_j [e_{i,\alpha}(\lambda) - e_{j,\alpha}(\lambda)] D_{ij}^{\alpha\beta} [e_{i,\beta}(\lambda) - e_{j,\beta}(\lambda)], \quad (5)$$

that is the kinetic energy plus the potential energy acquired by atom  $i$  under the action of a normal mode  $\lambda$ , whose amplitude  $a$  acts here as an irrelevant factor<sup>†</sup>. The potential energy of each atom is obtained by summing over all the springs connected to the atom and taking half the potential energy stored in the spring stretched by the normal mode.  $\mathcal{E}_i(\lambda)$  tells us the energy stored in a given spatial position  $\mathbf{r}_i$  when the mode  $\lambda$  is switched on. Information on the localized or extended character of this mode can be obtained by studying the correlation function

$$C_\lambda(R) = \frac{1}{Ng(R)} \sum_{ij} \mathcal{E}_i(\lambda) \mathcal{E}_j(\lambda) \delta(R - |\mathbf{r}_i - \mathbf{r}_j|), \quad (6)$$

where  $g(R)$  is the usual pair correlation function. For truly localized modes, we expect  $C(R)$  to decay rapidly as a function of  $R$  while, for extended modes,  $C(R)$  is expected to be almost constant. An example of  $C(R)$  for a mode on the high-energy side of the spectrum, above the localization edge, is reported in figure 6. We observe an exponential decay of  $C(R)$  on a very short length scale, a clear indication of localization that parallels the  $1/N$  scaling of  $P_\lambda$ . In the intermediate-frequency range (figure 7),  $C(R)$  is actually constant.

The behaviour of  $C(R)$  for a mode belonging to the low-frequency region is more interesting; figure 8 also shows the size independence of the result.  $C(R)$  shows two distinct regions. At short distances we observe the exponential decay typical of localized modes, but this decay does not continue to very large distances. Rather it ends at about 25 Å and then becomes constant. This behaviour, together with the behaviour of  $P_\lambda$  already discussed, indicates that the modes with low values of  $P_\lambda$ , in the low-frequency spectral region, are actually *extended* (which explain the  $N$  independence of  $P_\lambda$ ) but also contain a few neighbouring atoms that move with increased amplitudes (which is reflected in the low values of  $P_\lambda$ ).

These modes are the QLVs in disordered systems; they are different from the extended modes (although they are extended according to the definition of Anderson localization) and they are not truly localized. They can be considered as a superposition of extended and localized modes created by hybridization.

However, this claim can be misleading. In order to consider the QLVs as a superposition of eigenvectors, we should find a new basis of eigenvectors where truly extended and truly localized modes are separated. This is possible only if, for a given frequency interval which goes to zero in the thermodynamic limit, we have a finite number of degenerate QLVs. In this case, owing to energy degeneracy, we have the freedom to choose a new basis, and we can hopefully separate extended and localized modes. This does not seem to be the case. Indeed, an analysis of the

<sup>†</sup> In fact, as each individual spring is not in equilibrium when the whole system is in equilibrium, equation (5) should have a term linear in  $a$ . However, for values of  $a$  typical in the dynamics at  $T = 5$  K, this linear term in  $a$  turns out to be negligible in the investigated system.

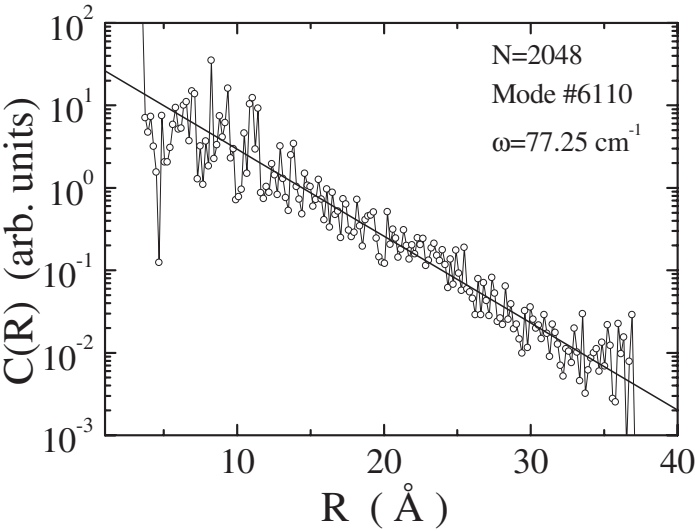


Figure 6. Local energy correlation function (○) (see text) as a function of distance for a mode ( $\omega_\lambda = 77.25 \text{ cm}^{-1}$ ) in the high-frequency spectral region of the  $N=2048$  system: (—), best fit to an exponential decay law, where the localization length is  $\xi = 3.5 \text{ Å}$  ( $\xi^* = \xi/\sigma \approx 1$ ).

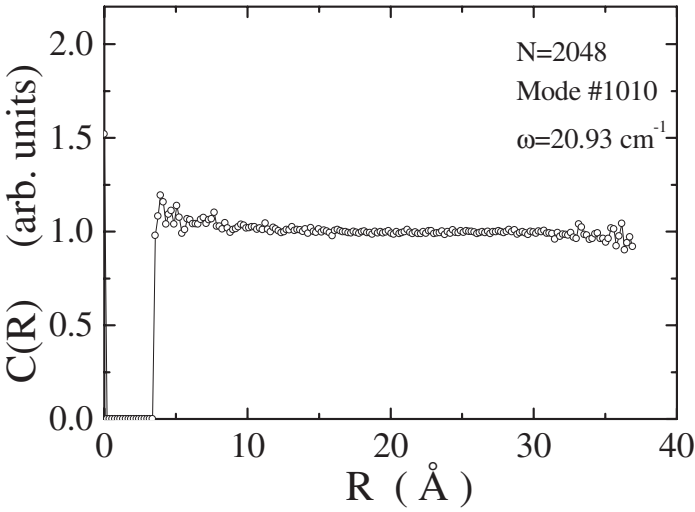


Figure 7. Local energy correlation function (○) as a function of distance for a mode ( $\omega_\lambda=20.93 \text{ cm}^{-1}$ ) in the central frequency spectral region of the  $N=2048$  system. The selected mode is extended and has a value of  $P_\lambda$  close to one.

frequency distance between successive modes shows that for disordered systems the degeneracy is removed and, in the thermodynamic limit, the probability of finding degenerate modes goes to zero (figure 9). We conclude that a change in eigenvector basis is not possible and that the QLVs are genuine modes of the disordered structures. However, this does not exclude an approach where the harmonic system is

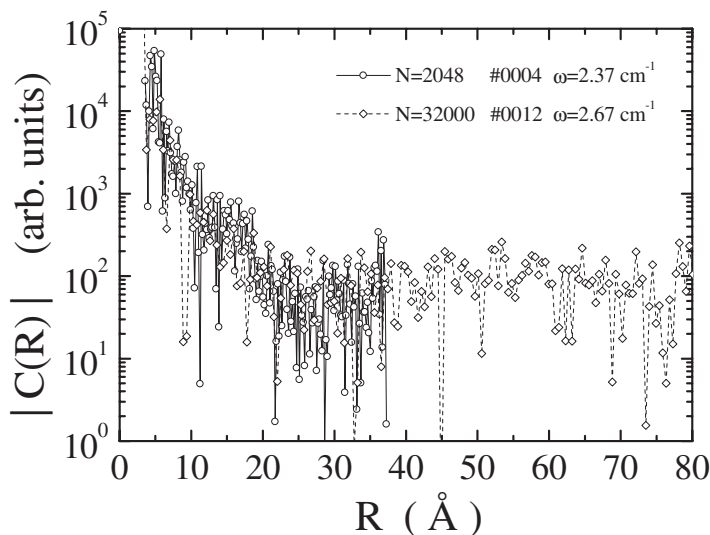


Figure 8. Absolute value of the local energy correlation function as a function of distance for two modes in systems of different sizes ( $\circ$ ),  $N=2048$ ,  $\omega_\lambda=2.37\text{ cm}^{-1}$ ; ( $\diamond$ ),  $N=32\,000$ ,  $\omega_\lambda=2.67\text{ cm}^{-1}$ ) in the low end of the spectral region. The selected modes have low (about 0.1) values of  $P_\lambda$ , which do not scale with  $N$ .

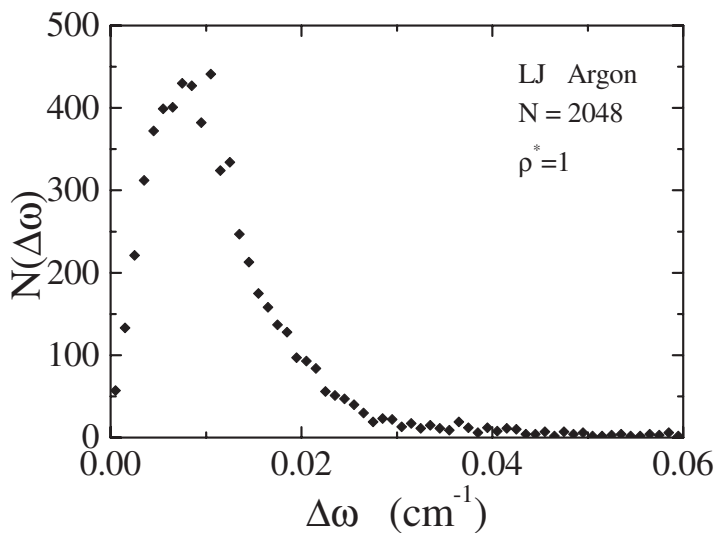


Figure 9. Distribution of the level spacing  $\Delta\omega$  for the  $N=2048$  system.

split into harmonic subsystems which interact bilinearly. This is formally exact and, as long as the interaction between the subsystems is sufficiently small, can be used to employ the methods developed for the lattice dynamics of defects. Such an approach is used in the soft-potential model where one subsystem consists of low-frequency extended modes and the other subsystem consists of localized modes which by the bilinear interaction are transformed to QLVs. Numerically such a splitting was done for the soft-sphere glass (Schober and Oligschleger 1996).

## §4. CONCLUSION

In conclusion, we have tried to clarify an existing controversy on the existence of the QLVs in disordered harmonic systems. The QLVs do actually exist, they are situated in the low-frequency side of the frequency spectrum, and, at variance with their name that can be misleading, they are *not localized* modes. The QLVs are extended, that is all the atoms are involved in the vibrations, but few nearby atoms move much more than the others, thus exhibiting properties of the truly localized modes as well. As the distribution of the level spacing in disordered systems shows absence of degeneracy, the QLVs cannot be considered to result from a mixing of degenerate extended and localized eigenmodes; rather they are a genuine pattern of atomic displacements in glasses and, most probably, they represent an independent entry in the Fabian–Allen classification scheme.

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