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Vibrational spectra in glasses

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ABSTRACT

The findings of X-ray and neutron scattering experiments on amorphous systems are interpreted within the framework of the theory of Euclidean random matrices. This allows us to take into account the topological nature of the disorder, a key ingredient which strongly affects the vibrational spectra of those systems. We present a resummation scheme for a perturbative expansion in the inverse particle density, allowing an accurate analytical computation of the dynamic structure factor within the range of densities encountered in real systems.

§ 1. INTRODUCTION

Propagating density fluctuation of macroscopic size (hydrodynamic limit) are known to exist both in ordered and in disordered materials. Whereas in the ordered materials those excitations (phonons) persist up to momenta of about one tenth of the Debye momentum, the fate of excitations of macroscopic size in disordered systems is still quite a puzzling issue, from both the theoretical and the experimental point of view.

Recently, much experimental attention (Buchenau *et al*. 1996, Benassi *et al*. 1996, Foret *et al*. 1996, Masciovecchio *et al*. 1996, 1997, 1998, Monaco *et al*. 1998, Sette *et al*. 1998, Fioretto *et al* 1999, Ruocco *et al*. 1999, Sokolov *et al*. 1999) has been paid to the high-frequency dynamics of disordered systems such as glasses. In fact, high-resolution inelastic X-ray scattering and neutron scattering techniques have made accessible to experiment the region where the exchanged external momentum p is comparable with p_0, namely the momentum where the static structure factor has its first maximum:

$$0.1p_0 < p < p_0. \tag{1}$$

The typical momentum p_0 can be thought of as the generalization of the Debye momentum to the case of disordered systems. With these data available for the study of excitations of microscopic size, one is naturally led to ask which of the

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well-known features of phonons survive even in disordered systems. A number of facts have emerged from the experiment.

(i) The dynamic structure factor $S(p, \omega)$ has a Brillouin-like peak for momenta up to $p/p_0 \approx 0.5$. This inelastic peak is due to the interaction of the external photon (or neutron) with some excitation of the system. A very controversial issue is the propagating nature of the excitations within that range of momenta. As a guideline, one could say that, as long as the dispersion relation between the position of the peak (in the frequency domain) and the external momentum $\omega_p(p)$ is nearly linear, the excitations are probably propagating. Of course, the study of Anderson localization (for example Parisi (1994)) shows that, strictly speaking, this condition is neither necessary nor sufficient; so care should be taken.

(ii) The peak has a width Γ, whose dependence on the momentum p within the range (1) has been described by means of the scaling law (for a large variety of materials):

$$\Gamma \propto p^{\alpha}. \tag{2}$$

It should be noted that, while there seems to be quite general agreement about the fact that Γ is not affected by changes in the temperature, there is still some debate about the actual value of the exponent α. More precisely, at sufficiently low momenta (e.g. light scattering), α is undoubtedly approximately 2, while at higher momenta (e.g. X-ray scattering) neither the value of $\alpha \approx 2$, nor the value $\alpha \approx 4$, describing instead a Rayleigh scattering regime, can be ruled out on experimental grounds.

(iii) The density of states (DOS) exhibits an excess with respect to the Debye behaviour ($g(\omega) \propto \omega^2$), known as the *boson peak*. This feature is particularly pronounded for strong glasses. Generally speaking, the typical frequencies of the boson peak are in the region where the relation between the frequency ω_p of the Brillouin peak and the momentum p is still linear.

(iv) A secondary peak at frequencies smaller than the Brillouin frequency develops for large momenta, becoming dominant for $p/p_0 \approx 0.5$.

A number of basic insights on the spectral properties of glasses have been obtained by means of molecular dynamics simulations (Mazzacurati *et al* 1996, Dell'Anna *et al*. 1998, Horbach *et al*. 1998, Ribeiro *et al*. 1998, Sampoli *et al* 1998, Allen *et al*. 1999, Feldman *et al*. 1999, Taraskin and Elliott 1999) on systems such as argon, silica and water. It should be pointed out that, in the glass phase, the high-frequency dynamics are very well described in the framework of the *harmonic approximation*. Both dynamic quantities such as the dynamic structure factor (Ruocco *et al* 2000) and thermodynamic observables such as the specific heat (Horbach *et al*. 1999) have been shown to be correctly described by models where only vibrations around quenched positions are taken into account. In figure 1 the numerical results obtained by Ruocco *et al*. (2000) are shown, which illustrate the above-mentioned spectral features.

On the theoretical side, the study of the short-time properties of glasses has been attempted from two different (and somewhat complementary) points of view.

On the one hand, it has been shown (Götze and Mayr 2000) that the mode coupling theory (MCT), which usually describes the long-time limit of the time correlators, can be modified in the glassy phase so as to describe only the excitations

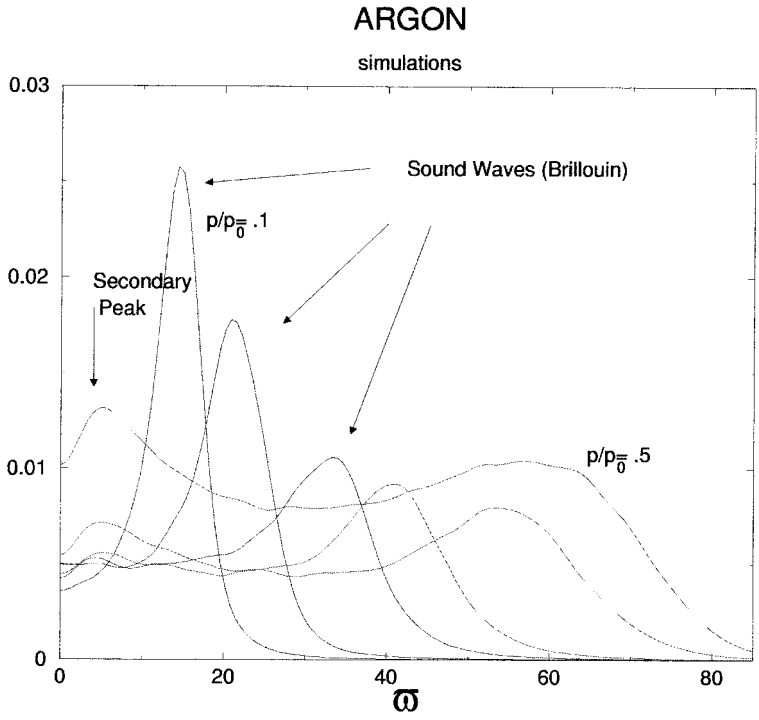

Figure 1. Dynamic structure factor for argon, obtained numerically by Ruocco *et al.* (2000) at a low temperature (approximately 10 K). The Brillouin-like peak and the secondary peak appear quite clearly.

around the quenched structure. Within such an approach, $S(p, \omega)$ was computed for a hard-sphere glass by means of a *generalized hydrodynamics approximation*. In this framework, a Brillouin peak with a linear dispersion relation (propagating excitations) is obtained up to $p/p_0 \approx 0.5$, as well as a secondary peak for higher values. Interestingly, the peak width Γ was shown to follow the simple scaling law

$$\Gamma_{\mathrm{MCT}} \propto p^2 \tag{3}$$

only in the very-low-momenta regime $p/p_0 < 0.1$, whereas a different law applies to the range of momenta comparable with the experimental and simulation values (see Götze and Mayr (2000, figure 8)) which seems hard to reduce to the simple form (2). Moreover, it has been shown (Ruocco *et al.* 2000) that, resorting to the harmonic approximation, the memory function can be simply obtained by means of the eigenvalues and eigenvectors of the Hessian matrix.

A second approach relies on the study of the statistical properties of random matrices (Metha 1991), since within the harmonic approxmation the whole dynamic features are encoded in the system's Hessian matrix. A crucial point is to distinguish between two different classes of systems:

(i) vibrational systems whose disorder has a topological origin, as in glasses (Elliott 1983);
(ii) vibrational systems on a lattice, where random coupling constants

(Schirmacher *et al.* 1998, Montagna *et al.* 1999, Martin-Mayor *et al.* 2000, Kantelhardt *et al.* 2001, Taraskin *et al.* 2001) are introduced in order to mimic the behaviour of real glasses.

The latter class has recently been studied in some detail (Schirmacher *et al.* 1998, Taraskin *et al.* 2001) in order to give an insight into the spectral properties, in particular into the boson peak. It turns out (Martin-Mayor *et al.* 2000), however, that these models definitely miss the p^2 behaviour of the peak width. Because of the long-range order due to the underlying lattice, the general behaviour is given instead by

$$\Gamma_{\mathrm{CPA}} \propto p^4, \tag{4}$$

even at very low momenta. The above result can be easily obtained within the coherent-potential approximation and can be checked by the direct inspection of the eigenvectors. As the discrepancy with the low-momenta behaviour of glasses is due precisely to the lack of topological disorder in lattice models, it seems reasonable to address the study of the former class. The problem turns out to reduce to the study of a very special class of random matrices, which have been called *Euclidean random matrices* (Mèzard *et al.* 1999). It is worthwhile to note that this approach would allow us to address, besides the study of the high-frequency regime of glasses, even the problem of instantaneous normal modes, that is the statistical properties of the Hessian matrix of a liquid at equilibrium (Wu and Loring 1992, Wan and Stratt 1994, Keyes 1997, Biroli and Monasson 1999), the framework being very similar (Cavagna *et al.* 1999). Nevertheless, in the following we shall focus only on the former. Recently (Martin-Mayor *et al.* 2001), the dynamic structure factor $S(p,\omega)$ was analytically computed. The computation relies on a perturbative expansion, the expansion parameter being the inverse particle density $1/\rho$. Let us recall what those perturbative results undoubtedly have shown.

(i) At $\rho \to \infty$, the dynamic structure factor is composed of a single delta function, whose position changes linearly with the external momentum p at low momenta, representing the undamped propagation of a sound wave in an elastic medium. This can be easily understood by considering the infinite number of particles per waveguide in that limit

(ii) For high but finite densities, the disorder of the position of the particles involved in the propagation causes a broadening of the Brillouin peak. In other words, the plane waves are no longer eigenstates of the Hessian; hence a finite spreading of the eigenfrequencies involved arises. In principle, no analogy with the Rayleigh scattering should be expected. In fact, the perturbative computation, performed up to $1/\rho^2$ order, shows that at sufficiently low momenta the general behaviour is instead given by

$$\Gamma_{\mathrm{ERM}} \propto \left(\frac{1}{\rho}\right)^2 p^2. \tag{5}$$

Yet at density $\rho = 1$ a significant deviation from that behaviour is seen as p/p_0 becomes greater than approximately 0.1, in good qualitative agreement with the results of the MCT approach.

The perturbative calculation has the problem that both the structure factor and the DOS end abruptly at a cut-off frequency. Moreover, the experimental densities are of the order $\rho \approx 1$ or less (in reduced units); hence the ability of perturbation theory to catch the features of real systems is at least questionable.

In order to overcome those difficulties, we present a resummation scheme for the perturbative results (Grigera *et al.* 2001) which includes terms at all orders in $1/\rho$. Within this scheme, very good agreement with numerical results, even at high frequencies, is found for values of $\rho > 0.3$ (reduced units)

§ 2. Harmonic approximation

We shall assume that the particles of our system in the glass phase can only oscillate around their equilibrium position, claiming that this is enough to predict the high-frequency properties. Here by 'equilibrium' we do not mean thermodynamic equilibrium (the thermodynamics of glasses are an entirely different issue from that addressed here), but rather mechanical equilibrium (i.e. a position where the forces on all particles are zero). For simplicity, let us consider displacements only along a given direction $\mathbf{u}$:

$$\mathbf{x}_j(t) = \mathbf{x}_j^{\mathrm{eq}} + \mathbf{u}\varphi_j(t). \tag{6}$$

Since the number of equilibrium positions $\{\mathbf{x}_j^{\mathrm{eq}}\}$ available to the system is actually infinite, growing exponentially with the number N of particles, one can ask which position should be taken in order to compute the vibrational spectra. The answer lies in the so-called self-averaging hypothesis, which has proved to be correct for many observables in disordered systems. Hence, we shall assume that, in the thermodynamic limit, the spectra obtained for the different realizations of disorder are equal to those computed by considering the average over the disorder. This statistical approach leads to a tremendous simplification of our task, as shown in the following, because the model is defined simply by the probability distribution of the random variables $\{\mathbf{x}_j^{\mathrm{eq}}\}$, $j = 1, \ldots, N$.

Within that harmonic framework, the energy of the system is (m is the mass of the particles and Ω is a frequency scale)

$$V(\{\varphi_i\}) = \frac{m\Omega^2}{2} \sum_{i,j} f(\mathbf{x}_i^{\mathrm{eq}} - \mathbf{x}_j^{\mathrm{eq}})(\varphi_i - \varphi_j)^2. \tag{7}$$

We choose units such that $m = 1$ and $\Omega = 1$. Thus the Hessian matrix

$$M_{ij} = \delta_{ij} \sum_{k=1}^{N} f(\mathbf{x}_i^{\mathrm{eq}} - \mathbf{x}_k^{\mathrm{eq}}) - f(\mathbf{x}_i^{\mathrm{eq}} - \mathbf{x}_j^{\mathrm{eq}}) \tag{8}$$

is a Euclidean random matrix, whose spectral properties we are studying.

In particular, we are interested both in the dynamic structure factor and in the DOS.

(i) The dynamic structure factor $S(p, \omega)$, roughly speaking, gives the spectrum of states 'excited' by a plane wave with a given momentum p. It can be obtained from the Hessian matrix of the potential (7) in the classical limit and in the one-excitation approximation (see for instance Martin-Mayor *et al.* (2001) for a detailed discussion):

$$S^{(1)}(p,\omega) = \frac{k_B T p^2}{\omega^2} \overline{\sum_n |\langle n|\mathbf{p}\rangle|^2 \delta(\omega - \omega_n)}, \tag{9}$$

where $|n\rangle$ are the eigenvectors of the Hessian matrix (8), the eigenfrequencies ω_n are the square root of the eigenvalues (which are all positive; see equation (7)), T is the temperature, the overbar indicates the average of the equilibrium positions $\{\mathbf{x}_i^{\mathrm{eq}}\}$, while $|\mathbf{p}\rangle$ stands for a momentum plane wave ($\langle j|\mathbf{p}\rangle = \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{x}_j^{\mathrm{eq}})/N^{1/2}$, where $|j\rangle$ represents the vector where the jth particle has displacement $\mathbf{u}$ and the other particles do not move).

(ii) The DOS describes instead the density of 'all' the vibrational states existing within the system. Interestingly, at the level of the one-excitation approximation, the DOS can be obtained from

$$g(\omega) = \frac{\omega^2}{k_B T p^2} S^{(1)}(p \to \infty, \omega). \tag{10}$$

The above theoretical result has been pointed out only very recently (Martin-Mayor *et al*. 2001). Athough it can be checked very easily by means of numerical simulations, we believe it would be also very interesting to check it on real systems, using experimental data at large momenta which are now available. On the other hand, at very high frequencies the one-excitation approximation does not hold, and many-excitation contributions should be taken into account; hence equation (10) is obviously only an approximation, whose reliability in describing real systems is very interesting. Moreover, we shall see in the following that equation (10) is crucial in obtaining a model-independent derivation of the actual small-p behaviour of the width of the Brillouin peak, holding only for topologically disordered systems. In fact, the same argument cannot be applied to lattice models, because equation (10) is not true in topologically ordered models.

As mentioned, the Hessian is averaged over the disorder, that is over all the allowed equilibrium positions. Those are clearly distributed in a highly correlated manner, owing to the hard-core repulsion and long-range attraction of the potential. It was shown (Martin-Mayor *et al*. 2001) that, at the level of the superposition approximation, the correlations can be taken into account by determining an uncorrelated average while at the same time suitably renormalizing the interaction f; if the k point static correlation function is written as

$$g(r_1, \ldots, r_k) = g(r_1) \cdots g(r_k), \tag{11}$$

then the inverse-density expansion for the dynamic structure factor of a system with correlation function $g(r)$ and force $F(r)$ can be obtained from the expansion of a fully uncorrelated system defining a *dressed* interaction:

$$f(r) \equiv g(r)F(r), \tag{12}$$

where the value of the 'spring' constant $F(r)$ is weighted by the probability of finding two centres of oscillations at the relative distance r.

§ 3. Non-perturbative results

Let $\hat{f}(p)$ be the Fourier transform of $f(r)$. The main 'object' to compute is the resolvent of the Hessian matrix (8), whch depends on the complex variable $z = \omega^2 + \mathrm{i}\eta$. It can be written in the following way:

$$G(p,z) = \frac{1}{z - \epsilon(p) - \Sigma(p,z)}, \tag{13}$$

$$\epsilon(p) = \rho[\hat{f}(0) - \hat{f}(p)]. \tag{14}$$

where the complex self-energy $\Sigma(p,z)$ has been introduced. Exploiting the well-known relation between resolvent and dynamical structure factor (ignoring the pre-factor $k_{\mathrm{B}}Tp^2$, which is inessential for the ω dependence), given by

$$S^{(1)}(p,\omega) = -\frac{1}{\omega\pi} \lim_{\eta \to 0} \mathrm{Im}\,[G(p,\omega^2 + \mathrm{i}\eta)], \tag{15}$$

the following connections between the main features of the dynamic structure factor and the self-energy are established:

(i) The 'bare' dispersion relation $\epsilon(p)$, which would give the position of the peak in the elastic medium limit, is renormalized by the real part of the self-energy $\Sigma'(p,z)$. This gives $\omega^{\mathrm{renorm}}(p)$, the position of the maximum of the structure factor in the frequency domain. Note that $\omega^{\mathrm{renorm}}(p)$ is certainly linear for small p, as expected.

(ii) The imaginary part $\Sigma''(p,z)$ computed at the position of the peak $\omega = \omega^{\mathrm{renorm}}(p)$ gives the width $\Gamma(p)$ of $S^{(1)}(p,\omega)$ by means of

$$\Sigma''(p, \omega^{\mathrm{renorm}}(p)) = \omega^{\mathrm{renorm}}(p)\Gamma(p). \tag{16}$$

The self-energy can be obtained as a series in $1/\rho$: the kth-order corresponds to k particle-label repetitions when calculating the moments of $S^{(1)}(p,\omega)$ (the details have been given by Martin-Mayor *et al.* (2001)). It is easy to show that the sum of all the *cactus diagrams* (figure 2) is given by the solution of the following integral equation:

$$\Sigma(p,z) = \frac{1}{\rho} \int \frac{\mathrm{d}^D q}{(2\pi)^D} \frac{\{\rho[\hat{f}(\mathbf{q}) - \hat{f}(\mathbf{p}-\mathbf{q})]\}^2}{z - \epsilon(q) - \Sigma(q,z)}. \tag{17}$$

Interestingly, equation (17) provides a model-independent derivation of the p^2 scaling of width of the peak of $S^{(1)}(p,\omega)$. Indeed, the large-q contribution to the imaginary part of the integral in equation (17) is, because of equation (10),

$$\Sigma''_{\infty}(p,z) = -\pi\rho g_{\lambda}(\lambda) \int \frac{\mathrm{d}^D q}{(2\pi)^D} [\hat{f}(\mathbf{q}) - \hat{f}(\mathbf{p}-\mathbf{q})]^2. \tag{18}$$

where $g_{\lambda}(\lambda)$ is the density of states in the domain of eigenvalues ($\lambda = \omega^2, q_{\lambda}(\omega^2) = g(\omega)/2\omega$). If the spectrum is Debye like, we have $g_{\lambda}(\lambda) \propto \lambda^{0.5}$, and it is straightforward to show that equation (18) is proportional to $\omega^{\mathrm{renorm}}(p)p^2$. Then equation (16) implies the scaling

$$\Gamma(p) \propto p^2, \tag{19}$$

irrespective of the function $f(r)$. Clearly this is only the large-q contribution to the integral, but it has been shown (Grigera *et al.* 2001) that is indeed controls the peak width at small p.

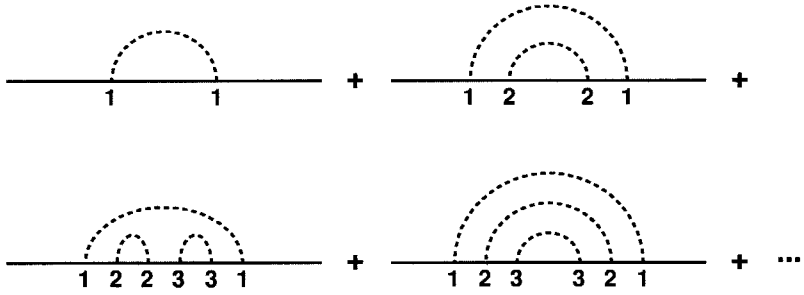

Figure 2. Cactus diagrams of the $1/\rho$ expansion. The numbers correspond to the particle-label repetitions.

§4. The Gaussian case

In the following we shall study the simple case

$$f(r) = \exp\left(-\frac{r^2}{2\sigma^2}\right). \tag{20}$$

This may seem an oversimplification, too distant from any realistic case. However, it is not actually the case, at least for small momenta. For comparison we can see in figure 3 the Fourier transform of the function $g(r)F(r)$ for argon at very low temperature (about 10 K) together with that of equation (20). We thus expect our results to be reasonable for momenta smaller than the first zero of the Fourier transform of $g(r)F(r)$, which in general is close to the maximum of the static structure factor p_0. Since the Fourier transform of our force decreases by an order of magnitude by

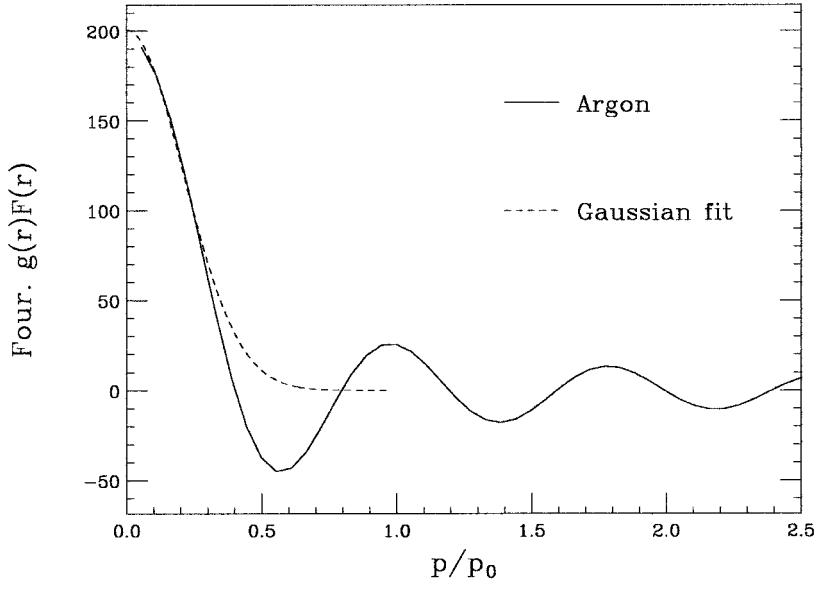

Figure 3. The Gaussian choice for $f(q)$ compared with the Fourier transform of $g(r)F(r)$ at approximately 10 K, $F(r)$ being the second derivative of the Lennard-Jones pair potential which is assumed to model the argon pair interactions.

$p_0 = 2/\sigma$, we shall take this as *our* p_0 during the following discussion, and σ will be our unit of length.

We have numerically solved equation (17) to find the self-energy for several values of ρ with the Gaussian choice (20), thus obtaining the structure factor and the density of states, in the eigenvalue domain. In figure 4 we show $S^{(1)}(p, \lambda)$ for several values of the momentum as obtained from equation (17) for $\rho = 1$. We also plot the structure factor obtained numerically by the method of moments (Turchi *et al.* 1982, Benoit 1989, Benoit *et al.* 1992) (for lower momenta, the comparison with the method of moments cannot be made owing to finite-volume effects (Martin-Mayor *et al.* 2001)). Very good agreement with the numerical data is achieved. Note the absence of the secondary peak in this model (see below).

We found that, for densities down to $\rho \approx 0.6$, the agreement is good for all momenta; in fact good results are also obtained for the density of states (figure 5). For lower densities, the DOS starts to deviate from Debye behaviour at small λ, in contradiction with the numerical results. Moreover, below $\rho \approx 0.31$ the approximation gives a DOS with an unphysical negative spectrum. The negative spectrum develops continuously as a function of ρ. Also included in figure 5 is the one-loop result. Note that, even for $\rho = 1$, the cactus resummation fails to reproduce the exponential decay of the DOS. This is not unexpected, however, owing to the non-perturbative nature (in $1/\rho$) of this tail (Zee and Affleck 2000).

It is interesting to consider the small-λ limit of $g_\lambda(\lambda)$. As seen in figure 5(*a*) the behaviour is very nearly of a Debye type (i.e. $\lambda^{1/2}$). An excess of states relative to the Debye case develops for higher λ, but in a region of eigenstates well beyond the

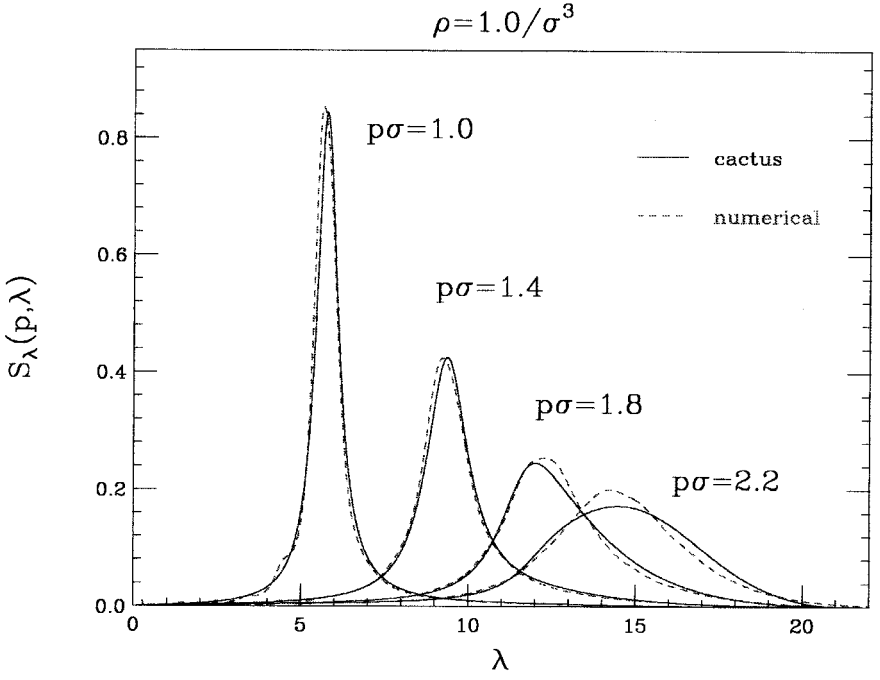

Figure 4. Dynamic structure factor in the eigenvalues domain for several values of the momentum at $\rho = 1$.

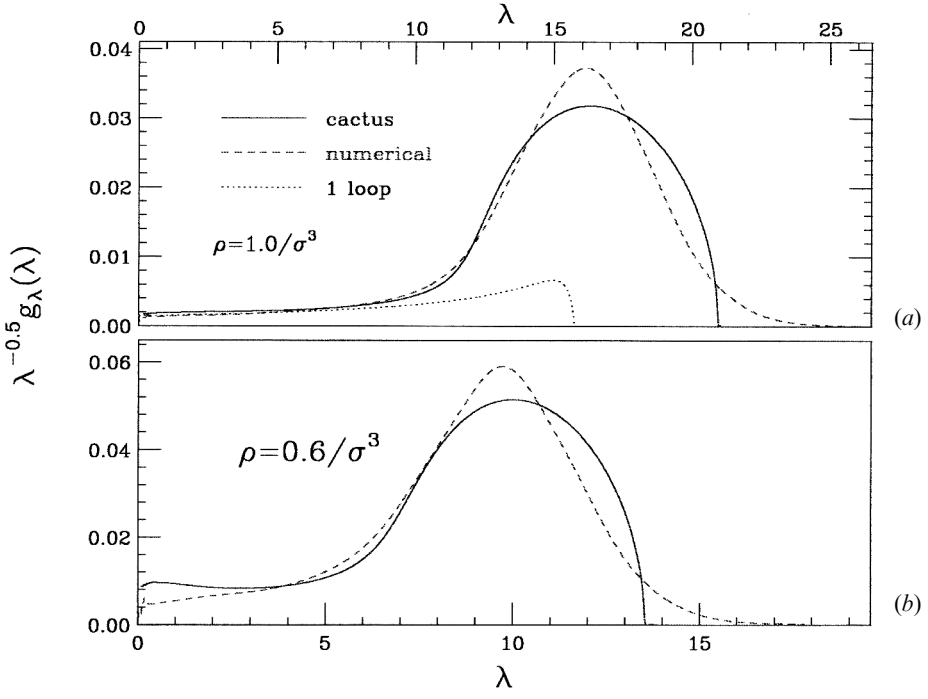

Figure 5. (*a*) DOS in the eigenvalues domain divided by $\lambda^{1/2}$ (Debye behaviour) for $\rho = 1$. (*b*) DOS for $\rho = 0.6$.

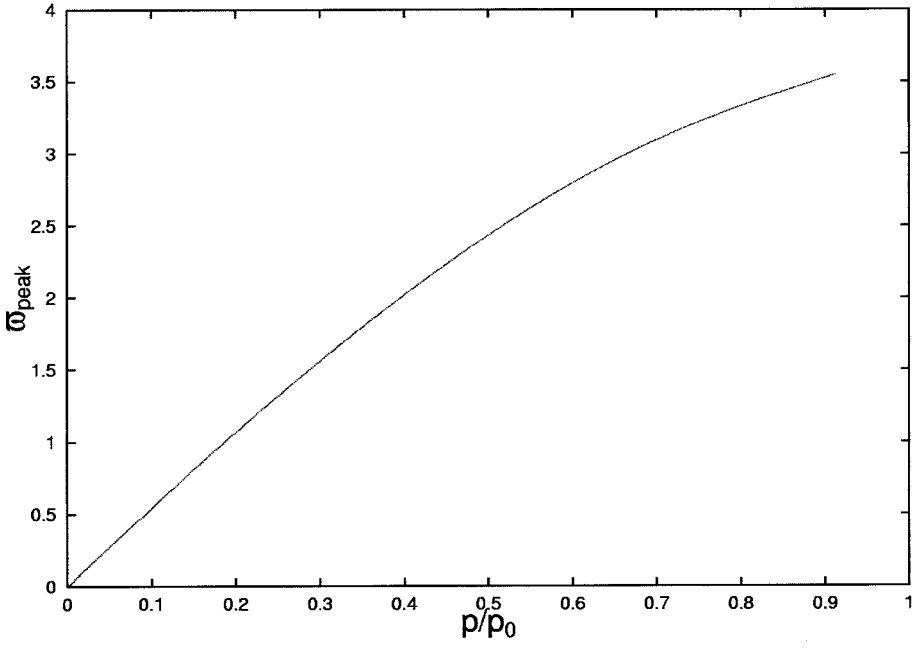

Figure 6. Scaling behaviour of the position of the peak, in the frequency domain, for $\rho = 1$.

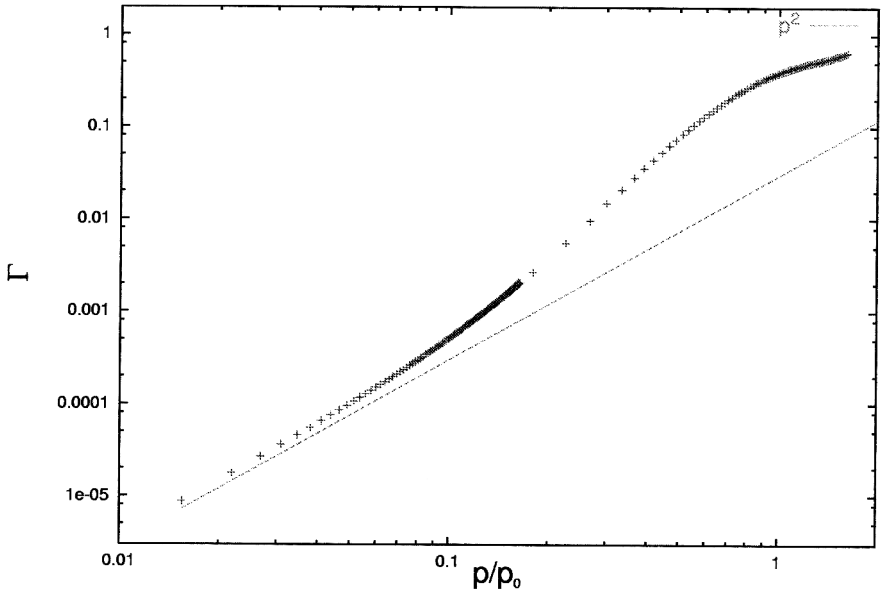

Figure 7. Scaling behaviour of the peak width at a function of p, in the frequency domain, for $\rho = 1$

linear dispersion regime (see figure 5 (*b*)). Thus this peak, similar to that found by Schirmacher *et al.* (1998), should not be regarded as a boson peak.

Finally, let us look at the scaling of the position and the width of the peak in the frequency domain. In figure 6 we show the frequency corresponding to the Brillouin peak as a function of the external momentum p. Let us note that a nearly linear dependence (indicating probably a propagating excitation) persists up to $p/p_0 \approx 0.6$–0.7. In figure 7, instead we plot $\Gamma(p)$, obtained by means of equation (16). As expected, the p^2 scaling is found for very small momenta, which crosses over to a region where a simple law such as equation (2) is not suitable for describing the real behaviour of the system.

Note that the region where the p^2 scaling is actually found, that is $p/p_0 < 0.1$ is quite different from the region explored by X-ray and neutron scattering experiments, which rather span the momenta $0.1 < p/p_0 < 0.5$. It is worthwhile to note that the same conclusion can be drawn from the results of Götze and Mayr (2000) using the MCT for hard spheres.

§ 5. Conclusions and outlook

In summary, we have applied the random-matrix approach to the study of the high-frequency excitations of glassy systems. We have presented a resummation scheme (Grigera *et al.* 2001) that greatly enhances the predictive power of the $1/\rho$ expansion previously obtained (Martin-Mayor *et al.* 2001). We have compared our analytical calculation with numerical results, finding that for not too low densities the only failure of the resummation scheme is its inability to reproduce the exponential decay of the DOS.

Our calculations have been performed by choosing a Gaussian force, in order to model the interparticle force dressed with the pair correlation function, and only

collinear displacements have been considered. We believe that our results are relevant for realistic glasses, at least in the regime $p/p_0 < 1$. The basic equation (17) shows that, in the general case, the position of the spectral peak is linear at small momenta, and the numerical solution of the integral equation in the Gaussian case shows that the linearity persists up to $p/p_0 \approx 0.6$–0.7.

Moreover, the width of the spectral peak turns out to be proportional to p^2 in the limit of $p \to 0$ (see equation (18)) irrespective of the potential function $f(x)$. Interestingly, in the Gaussian case the scaling law holds for a momentum range one order of magnitude smaller than the experimental range. At larger momenta, the law is more complicated (see figure 7). As this result is quite similar to the MCT result for a hard-spheres system (Götze and Mayr 2000), we believe that it could have a certain degree of universality.

This model lacks an important feature of the experimental spectra, namely the secondary peak of $S(q, \omega)$ (which some workers have interpreted as the boson peak (Horbach *et al.* 1998)). We believe this to be related to two important ingredients missing in our model: the vectorial nature of the vibration, and a detailed consideration of the particle correlations. The latter should not affect our results for momenta much smaller than the first maximum of the static structure factor p_0. Since the secondary peak appears for $p \approx p_0$, we should not really expect to describe it; in this momentum range the dispersion relation is no longer monotonic in real glasses. Furthermore, Dell'Anna *et al.* (1998) have suggested that transverse excitations may play a prominent role in the increase in the secondary peak. Our approach can be extended to include transverse displacements, however, and work in this direction is in progress.

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