Dynamical structure factor in disordered systems

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We study the spectral width as a function of the external momentum for the dynamical structure factor of a disordered harmonic solid, considered as a toy model for supercooled liquids and glasses. In the contexts of both the single-link coherent potential approximation and a single-defect approximation, two different regimes are clearly identified: if the density of states at zero energy is zero, the usual p^4 law is recovered for small momentum. On the contrary, if the disorder induces a nonvanishing density of states at zero energy, a linear behavior is obtained. The dynamical structure factor is numerically calculated in lattices as large as 96^3 and satisfactorily agrees with the analytical computations.

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I. INTRODUCTION

The spectrum of vibrational excitations of supercooled liquids and glasses is attracting a great deal of attention from the experimental side [1], in numerical simulations [2], and also from the analytical point of view [3–5]. The recent development of high-resolution inelastic x-ray scattering facilities has allowed study of the dynamical structure factors of glasses and liquids up to mesoscopic exchanged moments. It has become clear that the spectra of excitations of both *fragile* and *strong* glass formers present interesting features in the >0.1 THz frequency range, namely, the boson peak and high-frequency sound. In the dynamical structure factor, a peak is observed at frequencies $\Omega(p)$ linear in the exchanged momentum up to $0.1p_0-0.5p_0$, p_0 being the position of the first maximum in the static structure factor. The slope of the almost linear dispersion relation $\Omega(p)$, if extrapolated to zero exchanged momentum, yields the macroscopic sound velocity (thus the name ''high-frequency sound''). This peak located at $\Omega(p)$ has a very mildly temperature-dependent width, which grows with the square of the external momentum. This independence of the spectral width on temperature makes it very plausible that the microscopic origin of this broadening is to be found in disorder. At higher exchanged momenta, however, the peak position ceases to depend on the external momentum, and stabilizes at a frequency still small if compared to the Debye frequency. This boson peak is reflected in the low-temperature anomalies of the specific heat, and appears in instantaneous normal mode analysis as an excess in the density of states compared to the ω^2 Debye spectrum.

The above mentioned spectral properties have recently been recovered in the context of the mode-coupling theory, properly adapted to describe the glassy phase [5]. Yet it would also be very interesting to obtain the high-frequency sound properties microscopically, using a very simplified model, in order to understand which are the essential ingredients. An appealingly simple model was proposed in Ref. [6]: it is a model of a disordered three-dimensional harmonic solid, where the disorder is put on the values of the spring constants, in order to mimic the topological disorder [7] existing in supercooled liquids. Interestingly enough, the model shares qualitatively with the supercooled liquids some relevant spectral properties: the existence of high-frequency sound and a boson peak. The dynamical structure factor of the disordered-solid model was also studied in Ref. [6], but, in the context of the well known coherent potential approximation (CPA) [8], the broadening of the peak corresponding to the high-frequency sound turned out to be proportional to p^4, very different from supercooled liquids, where it is proportional to p^2. It was noticed, however, that a rather different scaling appeared at the characteristic frequencies of the boson peak, and it was argued that the boson peak develops when some spring constants are allowed to have a small negative value. On the other hand, in Ref. [9], it was also suggested that if an extensive number of negative spring constants is present in three-dimensional disordered-solid-like systems, the p^2 broadening will appear. In this paper, we want to investigate the problem of the peak broadening, by both numerical and analytical means. By focusing on the high-frequency sound, our main finding will be that the p^4 broadening *always* holds, unless the solid becomes *unstable*. That is, if the dynamical matrix, to be defined later, has an extensive number of negative eigenvalues, the system does present soundlike peaks in its dynamical structure factor, but with a width proportional to p, not p^2. Otherwise, the standard p^4 behavior is to be expected. Furthermore, this $\propto p$ behavior of disordered lattice models is closely linked to the fact that the disorder concerns the strengths of the interactions and not the geometry of the system. Hence there is no reason to expect a similar connection between negative eigenvalues and deviations from the p^4 scaling in supercooled liquids.

The layout of the rest of this paper is as follows. In Sec. II we present the model that we shall study, and we introduce our notation. In Sec. III we present our analytical calculations for the dynamical structure factor. The results are compared with a numerical computation in Sec. IV. In Sec. V, we discuss our results and the outlook for this work.

II. MODEL

A disorderd harmonic solid [6] consists of a set of particles of mass m, placed on the nodes of a simple cubic

lattice in D dimensions, with lattice spacing a, connected with their nearest neighbors through random springs. The potential energy of such a system is given in terms of the displacement of the particles from the lattice nodes:

$$H=\frac{m\Omega^2 a^2}{2}\sum_x \sum_{\mu=1}^{D} (1+\alpha_{x,\mu})\left(\frac{\phi_x-\phi_{x+\hat{\mu}}}{a}\right)^2. \quad (1)$$

In the above expression, Ω is a characteristic frequency and $\hat{\mu}$ is the lattice unit vector in the μ direction. Periodic boundary conditions are assumed in a finite lattice, and we have also introduced the notation $\alpha_{x,\mu}$ for the random part of the spring constant of the spring connecting sites x and $x+\hat{\mu}$. Notice that, for the sake of simplicity, the displacement field ϕ_x is a scalar rather than a vector [6], so that we will not be able to separate the longitudinal and transverse modes. Let us now choose units such that $m=a=\Omega=1$, and write the energy as a quadratic form, whose asociated matrix will be called the dynamical matrix of the problem:

$$H=\frac{1}{2}\sum_{xy}\phi_x \mathcal{H}_{xy}\phi_y, \quad (2)$$

$$\mathcal{H}_{xy}=\sum_{\mu=1}^{D}\frac{1+\alpha_{y,\mu}}{2}(\delta_{xy}-\delta_{x,y+\hat{\mu}}) + \frac{1+\alpha_{y-\hat{\mu},\mu}}{2}(\delta_{xy}-\delta_{x,y-\hat{\mu}}), \quad (3)$$

Since the potential energy (1) is translationally invariant, the dynamical matrix, satisfies the constraint related to translational symmetry: the vector of all equal components (ϕ_x = const) is an eigenvector with zero eigenvalue.

Notice that if all $\alpha_{x,\mu}=0$ the dynamical matrix turns out to be that of a perfect crystal (hence we call a *defect* a nonvanishing α), which has plane-waves as eigenvectors:

$$\mathcal{H}^0|p\rangle=E_0(p)|p\rangle, \quad \langle x|p\rangle=\frac{e^{ipx}}{\sqrt{N}}, \quad (4)$$

$$E_0(p)=\sum_\nu (1-\cos p_\nu)=\frac{p^2}{2}+O(p^4). \quad (5)$$

In the above equation, we have used the bra-ket notation and we have denoted the total number of lattice points as N. We shall study the case where the $\alpha_{y,\mu}$ are uncorrelated, random variables whose probability distribution is

$$p(\alpha)=(1-\rho)\delta(\alpha)+\rho h(\alpha), \quad 0\leqslant\rho\leqslant 1. \quad (6)$$

In the above equation, ρ is the probability of finding one defect, while h is a continuous probability function, which we take flat between λ and 0 ($\lambda<0$). Notice that the disorder of Ref. [6] is recovered by taking $\rho=1$ and h Gaussian. The rationale for choosing this kind of distribution is that we need somehow to go beyond the perturbative calculations that yield a broadening proportional to p^4 for the peak of the dynamical structure factor. This will be achieved by allowing the random part of the springs to take large negative values, but only for a small fraction ρ of them: we will study an expansion in the density of defects. Our nonperturbative effect will be a level crossing (the only possible source of nonanalyticity in such a simple model). Indeed, if all the α's are greater than -1, it is evident from Eq. (1) that no negative eigenvalue may arise, and so the plane wave of zero momentum is the ground state of the dynamical matrix, with zero eigenvalue. On the other hand, we shall now sketch a variational estimate of the ground state that shows that if there is only *one* defect on the lattice, but this is negative enough, the ground state of the dynamical matrix is no longer zero, but negative. Let us first keep in Eq. (3) only the spring connecting sites 1 and 2, corresponding to the large negative defect. The eigenvectors are easily shown to be $\phi_x=(\delta_{x,1}+\delta_{x,2})/\sqrt{2}$ and $(\delta_{x,1}-\delta_{x,2})/\sqrt{2}$. The first one is the restriction of the zero-momentum plane wave to this trivial two-site problem, while the second is our variational candidate:

$$|V\rangle, \quad \langle x|V\rangle=\frac{\delta_{x,1}-\delta_{x,2}}{\sqrt{2}}. \quad (7)$$

Using Eq. (1) it is easy to check that

$$\langle V|\mathcal{H}^{1defect}|V\rangle<0 \quad \text{if} \quad \alpha<-\left(D+\frac{1}{2}\right). \quad (8)$$

Therefore, if $\alpha<-(D+1/2)$ (we shall see in the next section that the true threshold is actually $-D$), the ground state of the dynamical matrix will certainly have a negative eigenvalue. Since the plane wave of zero momentum is *always* an eigenvector of zero eigenvalue [see Eq. (1)], our level crossing has taken place. Moreover, the trial vector $|V\rangle$ is strongly localized on the defect (the real ground-state eigenvector is also localized; see Sec. III). One can thus expect a contribution of order ρ to the density of states over the negative spectrum, if the function h in Eq. (6) is such that the probability of having $\alpha<-D$ is nonvanishing. However, in the previous arguments, we have assumed that the defect was isolated. Under the hypothesis of uncorrelated spring constants, this will not be the generic case, unless ρ is exceedingly small (the probability of having k defects in touch is proportional to ρ^k). One can repeat the above variational argument assuming that some of the surrounding springs have very small positive values. It turns out that a contribution of higher order in ρ to the density of states at negative eigenvalues is generated, no matter how small is the negative value of the spring constant $\alpha+1$. Therefore, if the probability of $\alpha<-1.0$ is nonvanishing, the hybridization of the localized field configuration described above with the plane-wave eigenstates will nontrivially modify the eigenvectors of $\mathcal{H}$.

Let us now present our notation for the quantity under study, namely, the dynamical structure factor. It can be obtained through the Fourier transform of the intermediate scattering function [10]:

$$F(p,t)=\frac{1}{N}\left\langle \exp\left(i\vec{p}\cdot\sum_{x=1}^{N}[\vec{r}_x(t)-\vec{r}_x(0)]\right)\right\rangle. \quad (9)$$

In the above expression, $\vec{r}_x(t)$ is the time-dependent position of the particle labeled by the lattice site x. Assuming that all the eigenvalues of the dynamical matrix are positive, in the classical limit, the one-excitation approximation to the dynamical structure factor turns out to be

$$\mathcal{S}^{(1)}(q,\omega)=\frac{k_B T p^2}{m\omega^2}\overline{\sum_{n=1}^{N}|\langle q\,|\,n\rangle|^2\,\delta(\omega-\omega_n)}, \qquad (10)$$

where the overbar stands for the averages over the α's, the $|n\rangle$ are the eigenvectors of the dynamical matrix, $|p\rangle$ is the plane wave of momentum p, and the eigenfrequencies ω_n are obtained from the eigenvalues E_n by the simple relation $E_n=\omega_n^2$. Notice also that in our scalar model we have dropped all the complications related to the distinction between parallel and longitudinal excitations. Now, since the dynamical structure factor is strongly peaked at a frequency value linear in the momentum, the p^2/ω^2 prefactor is rather uninteresting, and we shall focus on the sum term. The quantity that we shall be interested in is $S(p,E)$ defined as

$$S(p,E)\equiv\overline{\sum_{n=1}^{N}|\langle q\,|\,n\rangle|^2\,\delta(E-E_n)}$$

$$=\frac{1}{2\omega}\overline{\sum_{n=1}^{N}|\langle q\,|\,n\rangle|^2\,\delta(\omega-\omega_n)}. \qquad (11)$$

The rationale for taking as our privileged variable the eigenvalue rather than the frequency is that negative eigenvalues will be important for our argument, as we have previously said, and therefore the transformation $\omega_n=\sqrt{E_n}$ introduces some problems. A drawback of this convention is that the peak broadening in the eigenvalue domain gets an extra factor p: the perturbative result is proportional to p^5 (p^4 in the frequency domain), while the physical glassy behavior is proportional to p^3 (p^2 in the frequency domain).

The representation of $S(p,E)$ that will be most convenient for us is based on the distribution identity $(x+i0)^{-1}=\mathcal{P}(1/x)-i\pi\delta(x)$, and on the resolvent $G(p,z)$:

$$G(p,z)\equiv\overline{\langle p|\frac{1}{z-\mathcal{H}}|p\rangle}, \qquad (12)$$

$$S(p,E)=-\frac{1}{\pi}\,\mathrm{Im}\lim_{\epsilon\to 0^+}G(p,E+i\epsilon). \qquad (13)$$

In other words, as a function of the complex variable z, the resolvent is an analytic function with a cut along the part of the real axis where the spectrum of the dynamical matrix lies. The discontinuity of the resolvent across the cut is precisely the $S(p,E)$. In the case of a crystal [all α's in Eq. (1) equal to zero], the cut degenerates into a point, and the resolvent has a pole,

$$G^0(p,z)=\frac{1}{z-E_0(p)}. \qquad (14)$$

For small momentum the pole is placed at a value of z linear in p^2, that is, at a frequency linear in p. It thus corresponds to an undamped sound wave propagating in the crystal. When some disorder is introduced in the system, however, the momentum is no longer a good ''quantum'' number. We have for the resolvent

$$G(p,z)=\frac{1}{z-E_0(p)-\Sigma(p,z)}. \qquad (15)$$

The function $\Sigma(p,z)$ is called the self-energy, and its real and imaginary parts have a nice physical interpretation. For small momentum and z close to $E_0(p)$, the real part $\Sigma'(p,z)$ is a slowly varying function of z times p^2. The maximum of $S(p,E)$ gets shifted roughly to $E_0(p)+\Sigma'(p,E_0(p))\propto p^2$, so that we have a renormalization of the speed of sound. If the behavior of Σ' was very different from that it would have a rather catastrophic meaning: there would be no sound propagation in the system. The value of the imaginary part of the self-energy $\Sigma''(p,z)$ at the peak position yields the width of the peak, which has a Breit-Wigner shape close to the maxima [the shape of the $S(p,E)$ distribution function far from the peak, depends strongly on the precise behavior of $\Sigma''(p,E+i\epsilon)$ along the spectrum].

III. ANALYTICAL CALCULATIONS

In this section we will sketch two approximate calculations, namely, the single-defect approximation and the single-link CPA [8] approximation. The first will yield the exact solution of the problem of a crystal with a single defect, and will motivate the more powerful CPA approximation that can also be used for large values of ρ. In this way, we learn that the order ρ threshold for the presence of negative eigenvalues is not $\alpha=-D-1/2$, as roughly shown in Sec. II, but $-D$. This threshold separates two well defined scaling limits for the width of $S(p,E)$ at small p.

(1) If the density of states is null at zero energy the imaginary part of the self-energy Σ'' is proportional to p^{D+2} (which yields a spectral width proportional to p^{D+2} in the eigenvalue domain and to p^{D+1} in the frequency domain).

(2) When an extensive number of negative eigenvalues is present, $\Sigma''\propto p^2$ (or p for the width in the frequency domain). Of course, the p^{D+2} contribution will still be present but it will be subdominant at low momentum. A crossover might be visible, depending on the strength of the disorder.

As an introduction let us first solve the problem of the crystal with a single defect. The dynamical matrix in the presence of a unique defect of amplitude α can be split into two terms:

$$\mathcal{H}_{xy}=\mathcal{H}^0_{xy}+\mathcal{R}_{xy}. \qquad (16)$$

The perturbation term $\mathcal{R}_{xy}$ hence connects the two sites y^0 and $y^0+\nu$, connected by the spring where the defect exists:

$$\mathcal{R}_{xy}\equiv\alpha^{y^0;\nu}|y^0;\nu\rangle\langle y^0;\nu|, \qquad (17)$$

$$\langle x|y^0;\nu\rangle\equiv\frac{\delta_{x,y^0}-\delta_{x,y^0+\nu}}{\sqrt{2}}. \qquad (18)$$

The propagator can be expanded in powers of the perturbation $\mathcal{R}$. Writing the exact propagator as

$$\frac{1}{z-\mathcal{H}}=\frac{1}{z-\mathcal{H}^0}+\frac{1}{z-\mathcal{H}^0}\mathcal{T}\frac{1}{z-\mathcal{H}^0}, \tag{19}$$

the resummation of the harmonic series yields

$$\mathcal{T}=|y^0;\nu\rangle\frac{\alpha}{1-\alpha a(z)}\langle y^0;\nu|. \tag{20}$$

The function $a(z)$ in Eq. (20) is given by

$$a(z)=\frac{1}{D}\int_{BZ}\frac{d^Dq}{(2\pi)^D}\frac{E_0(q)}{z-E_0(q)} \tag{21}$$

$$=\frac{1}{D}\int_0^{2D}dE g_0(E)\frac{E}{z-E}, \tag{22}$$

$$g_0(E)\equiv\int_{BZ}\frac{d^Dq}{(2\pi)^D}\delta(E-E_0(q)). \tag{23}$$

In the above expressions the lattice integrals are extended to the first Brillouin zone, and we have denoted by $g_0(E)$ the density of states of the pure crystal. From the small momentum result $E_0(p)=p^2/2+O(p^4)$, it is easy to get for small E the following approximate result [11]:

$$g_0(E)\sim\frac{E^{D/2-1}}{\Gamma(D/2)\pi^{D/2}2^{D/2}}. \tag{24}$$

Applying the decomposition $(x+i0)^{-1}=\mathcal{P}(1/x)-i\pi\delta(x)$ to Eq. (21) and using Eq. (24), we immediately get for small positive values of the eigenvalue the useful result

$$a(E+i0)\sim-\frac{1}{D}-i\frac{E^{D/2}}{2^{D/2}\pi^{D/2-1}\Gamma(D/2)}. \tag{25}$$

For negative values of E the function $a(E+i0)$ is real and monotonically decreasing: its value is zero at $-\infty$, and it tends to $-1/D$ when E tends to 0^-.

We are now ready to discuss our exact result given in Eq. (20). The correction term in Eq. (20) has a singularity for the value of the energy E_α satisfying $1-\alpha a(E_\alpha+i0)=0$. This singularity corresponds to an eigenstate of the system, induced by the defect, and the relation $1-\alpha a(E_\alpha+i0)=0$ is analogous to a quantum-mechanical gap equation. If $0<E<2D$, that is, over the crystal spectrum, then $a(E+i0)$ has a finite imaginary part, so that the gap equation has no solution. For negative E, if $\alpha>-D$, no solution can be found either since $|a(E+i0)|<|\alpha|^{-1}$ in this region. On the other hand, if $\alpha<-D$, a unique solution E_α appears. The position of the singularity decreases monotonically from $E_\alpha=0$ for $\alpha=-D$ to $E_\alpha=-\infty$ for $\alpha=-\infty$. In this situation, the propagator has a cut running from 0 to $2D$, plus an isolated singularity (a pole) that corresponds to the ground state of the dynamical matrix: the level crossing that we anticipated in Sec. II has taken place. The residue of this pole is $\Psi_F(x)\Psi_F^*(y)$. Therefore, one obtains the wave function for the ground state of the dynamical matrix,

$$\Psi_F(x)\propto\int_{BZ}\frac{d^Dq}{(2\pi)^D}\frac{1-e^{iq_\nu}}{E_\alpha-E_0(q)}e^{iq(x+y_0)}, \tag{26}$$

which has a localization length of order $|E_\alpha|^{-1/2}$. We thus see that unless α is exceedingly close to the critical value $-D$ the eigenvector is strongly localized around the defect.

The single-defect approximation to the self-energy, Eq. (27), amounts to considering that each defect contributes only to its own localized eigenvector, and that no other defect is within its localization length. Let us turn back to the original problem, with an extensive number of defects, and repeat the above calculation, neglecting all terms that contain two different defects. The matrix $\mathcal{T}$ is now a sum of terms like the one in Eq.(20). If we now perform the average over the α's and apply Dyson resummation, the self-energy part of the propagator turns out to be

$$\Sigma(p,z)=\rho E_0(p)\int d\alpha h(\alpha)\frac{\alpha}{1-\alpha a(z)}, \tag{27}$$

at first order in ρ (the defect interactions will generate the order ρ^2 and higher-order corrections to the single-defect result).

The width of $S(q,E)$ is simply given by the value of the imaginary part of the self-energy at the peak, whose position can be obtained from the real part of the self-energy, $E^{\max}(p)\approx E_0(p)+\mathrm{Re}\,\Sigma(p,E_0(p))$. Notice that our self-energy is proportional to $E_0(p)$ so that we are basically getting a finite renormalization of the speed of sound. We can estimate the imaginary part of the self-energy using Eq. (25). If the probability density $h(\alpha)$ does not allow α to be smaller than $-D$, the only imaginary term in Eq. (27) comes from $a(E+i0)$, and it is of order $p^2E^{D/2}$, yielding a value of order p^{2+D} at the peak. On the other hand, if α can be smaller than $-D$, an imaginary part of order $p^2h(-D)$ arises from the pole in Eq. (27).

Led by the functional form of the self-energy in Eq. (27), one can consider self-energies of the form of a function of energy multiplied by $E_0(p)$ also when ρ is not small and the single-defect approximation no longer holds. This is the idea underlying the well-known CPA approximation [8], where one sets $\Sigma(p,z)=[\Gamma(z)-1]E_0(p)$. A self-consistency equation can be readily written for $\Gamma(z)$:

$$\overline{\frac{1+\alpha-\Gamma(z)}{\Gamma(z)-a[z/\Gamma(z)][1+\alpha-\Gamma(z)]}}=0. \tag{28}$$

It is clear that the width of $S(q,E)$ critically depends on the value of $\Gamma(0+i\epsilon)$. For the flat distribution of α introduced in Eq. (6), one can solve Eq. (28) in the limit of small ρ, as $\Gamma(0)=1+b\rho+O(\rho^2)$, obtaining

$$b=D\left(1-D\ln\frac{D}{|\lambda+D|}+i\pi\frac{D}{\lambda}\theta(D+\lambda)\right), \tag{29}$$

where $\theta(x)=1$ for $x<0$ and zero otherwise. It is easy to check that the single-defect result is exactly the same as Eq. (29).

Fixing from now on $D=3$, Eq. (28) can be numerically solved in the general case. We choose to write it as a *fixed-point* equation, and solve it recursively. The evaluation of

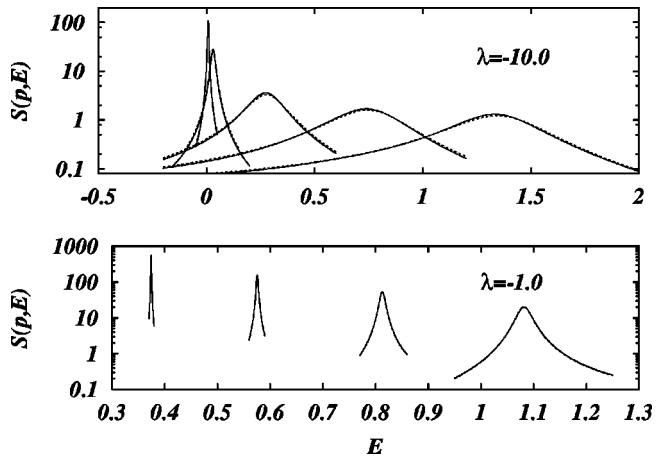

FIG. 1. Upper part: The $S(q,E)$ function, for $p=2\sqrt{3}\pi n/96$ for $n=1,2,6,10,14$, from left to right, both in the CPA (dashed lines) and in the numerical calculation (full lines), for $\rho=0.1$ and $\lambda=-10.0$. Lower part: The same for $\rho=0.1$ and $\lambda=-1.0$, and $p=2\sqrt{3}\pi n/96$ for $n=8,10,12,14$, from left to right.

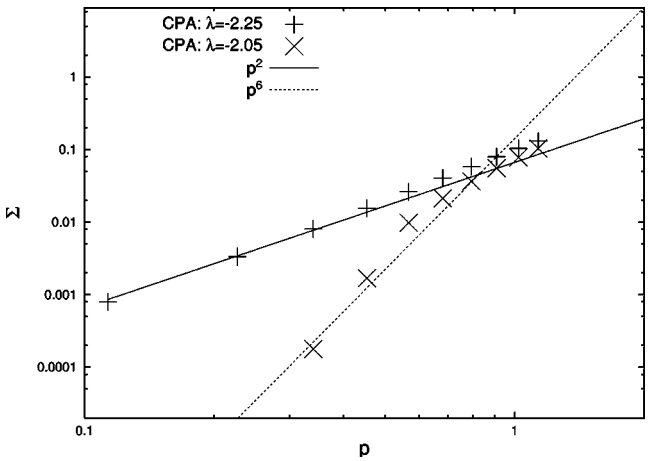

FIG. 2. The spectral width Σ [see Eq.(30)] as a function of the external momentum in the CPA, for a density of defects $\rho=0.1$.

$a(z)$ defined in Eq. (21) requires numerical calculation of the density of states for the pure crystal [11]. In this way, we are able to obtain estimates of $\Gamma(z)$ with an accuracy of 10^{-4}, which is roughly the smallest spectral broadening that we can accurately calculate with the CPA. We find that in the CPA there are the same two regimes as in the single-defect computation, separated by a critical line, that starts at $\lambda_c(\rho\to 0)=-3$ and ends at $\lambda_c(\rho=1)=-1.22$. The appearance of the p^5 regime coincides with, and is due to, the vanishing of the negative-energy spectrum. However, as explained in Sec. II, one rather expects that what vanishes is the order ρ contribution to the density of states in this region. In fact, we expect a nonvanishing density of states all the way down to $\lambda=-1$, where no negative spring exists. It is remarkable that when $\rho=1$ the CPA retains a nonvanishing fraction of negative eigenvalues up to $\lambda=-1.22$, quite close to the correct value $\lambda=-1$.

The agreement between the CPA and the results from numerical simulations for $S(p,E)$ turns out to be better than 5% in the two extreme cases (see Fig. 1). That is the one where there are no negative springs ($\lambda=-1$) and the one where the spring constant can be very negative ($\lambda=-10$). Close to the CPA critical line (on the unstable crystal side) the agreement is still quite good. On the (CPA) stable border side, a scaling between p^6 and p^5 is found, depending on the density of defects, ρ. For example, with the value of the density of defects $\rho=0.1$, in Fig. 2 the transition between the two regimes found by the CPA at $\lambda=-2.15$ is very evident.

IV. NUMERICAL COMPUTATIONS

We numerically computed the structure factor $S(E,q)$ for our model utilizing the method of moments [12], which allows study of the statistical properties of the eigenvalues and the eigenvectors of large dynamical matrices, avoiding their diagonalization. This method is a clever modification of the Lanczos method and it shares the same weakness, namely, the lack of orthogonality when too large a number of moments is computed. Another limitation is the necessity of setting a finite value of ϵ in Eq. (13). A reasonable value for ϵ is the mean distance between eigenstates, which is roughly given by $(2D-\lambda)/N$, where N is the lattice volume ($\epsilon\approx 10^{-5}$ in our 96^3 lattice). If the width of the peak is comparable with ϵ, the results will be definitely affected by finite-size effects. The limitation related to the number of moments is not serious for the central part of the $S(q,E)$ curve, but can be rather strong if one wants to calculate the tails of the distribution. In practice, we have used 30 moments for 10 different disorder realizations, and we have truncated the continuous fraction in a standard way [13], finding very satisfactory results, unless the peak height approaches values of order 10^5, when finite-size effects turn out to be important. We fit our results to the Breit-Wigner form

$$S(E,q)=\frac{\mathcal{N}}{(E-E_0)^2+\Sigma^2}, \tag{30}$$

which satisfactorily describes the peak in all cases, although it usually overestimates the tails of the distribution. The position of the peak E_0 is linear in p^2 as expected. More importantly, the results from numerical simulations (Fig. 3) show very clearly that the critical line previously discussed is

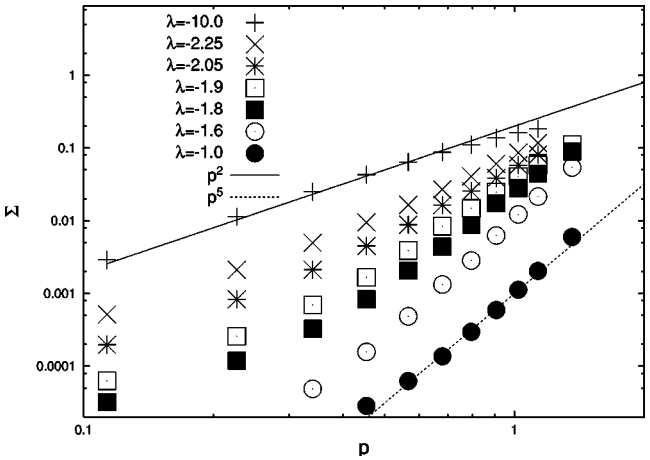

FIG. 3. Σ as a function of the external momentum in the numerical simulations, for a density of defects $\rho=0.1$. The errors are smaller than the data points.

an artifact of the CPA, the real behavior being rather a cross over. Let us finally stress that another source of finite-size effects is that a real system actually becomes unstable when there is an extensive number of negative springs, no matter how small their negative value, as follows from the simple analytic considerations sketched previously. If the probability of the spring-constant configurations giving rise to localized negative-energy eigenvectors is smaller than the inverse lattice volume, no negative-energy spectrum will be found and the spectral broadening will be too p^5-like. This is quite likely the case for $\lambda = -1.6$ in Fig. 3.

V. DISCUSSION AND OUTLOOK

In this work, we have studied the dynamical structure factor of a disordered harmonic solid, proposed as a simple model for the boson peak [6] found in the THz range of the vibrational excitations of supercooled liquids and glasses. We have shown that, under the hypothesis of uncorrelated random spring constants, an extensive number of negative springs always produces an extensive number of negative eigenvalues of the dynamical matrix of this model. Now, both the single-defect approximation and the CPA [8] allow us to write the self-energy of a disordered harmonic solid, for small E and p, as a function of energy times $E_0(p)$. An unavoidable consequence of this functional form is that, for the stable solid (no negative eigenvalues), the perturbative p^4 result holds (in frequency space). For the *unstable* solid, the broadening is proportional to p, rather than to p^2. Our numerical calculations on 96^3 disordered lattices confirm the above picture. For wavelengths in the range $[a,10a]$ (a being the lattice constant), a crossover regime may result, depending on the strength of the disorder, from the competition between the p and p^4 terms in the self-energy. Since the onset of slow dynamics in supercooled liquids is clearly correlated with a rather strong decrease of the density of negative states on their instantaneous normal modes [14], it is natural to conclude that the mechanism of Ref. [9] cannot be responsible for the physical p^2 broadening of the dynamical structure factor. Moreover, in Ref. [15], a Lennard-Jones model of a glass was studied, and the dynamical structure factor was obtained from the instantaneous normal modes calculated in the inherent structures of the glass phase. Since an inherent structure does not have negative eigenvalues, and yet displays the typical p^2 broadening, it seems clear that the presence of negative eigenvalues is not an essential microscopic ingredient for reproducing the features of high-frequency sound.

Further progress can be made only by recognizing which feature of the model is responsible for this failure. The fact that the model is scalar and so one cannot separate transverse and longitudinal excitations does not seem of major importance to us. The fact of dealing with quenched disorder does not seem crucial either. In fact, we believe that the principal suspect is the lattice. Indeed, an on-lattice system is topologically ordered, which produces a number of anomalous features if compared with an off-lattice system. For instance, the density of states is the integral over the Brillouin zone of $S(p,E)$, which is at the root of the close connection we have found between the presence of negative eigenvalues and the broadening of the peak of $S(p,E)$. Moreover, for a topologically disordered system, $S(p,E)$ and the density of states are very similar in the limit of large p, while for an on-lattice model $S(p,E)$ is a periodic function of the momentum. We therefore believe that it will be very interesting to study similar models where the particles are not constrained to oscillate around lattice points, like, for instance, the one in Ref. [4], and so do not have the peculiar lattice properties.

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lated the three-dimensional $g_0(E)$ function at intervals of 10^{-4} with the same level of accuracy, in a half-an-hour run on a desktop computer. This is the maximum level of accuracy that we can expect in the numerical integrations where we have used our tabulated $g_0(E)$.

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