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Local Oscillators vs. Elastic Disorder: A Comparison of Two Models for the Boson Peak*

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In order to study the vibrational properties of harmonic disordered solids we consider two models for disorder: Randomly fluctuating elastic constants (intrinsic disorder) and coupling to local oscillators (defects) with random eigen frequencies. The first model is treated in self-consistent Born approximation (SCBA), whereas the second can be solved exactly. This enables us to discuss the accuracy of the SCBA. In both models an enhancement of the low-frequency vibrational density of states over that predicted by Debye is obtained ("boson peak") as a result of the presence of the disorder. In the frequency regime above the boson peak an almost exponential decrease of the reduced density of states is obtained, which is widely observed in experiments. Whereas the gross features of the models are similar, the details can be different, depending on the model parameters chosen.

It is argued that models involving intrinsic disorder are suitable for structurally disordered solids, whereas defect models seem more adequate for disordered crystals.

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1. INTRODUCTION

The origin of the low-frequency vibrational anomalies of disordered solids and the associated low-temperature thermal ones have been intensively discussed in the past decades.[1–4] In particular the low frequency enhancement of the vibrational density of states (DOS) $g(\omega)$ with respect to Debye's ω^2 law - which appears as a peak if represented as $g(\omega)/\omega^2$ ("boson

*Dedicated to Siegfried Hunklinger on the occasion of his 65th birthday peak") - has been attributed to a lot of different microscopic origins.[4–17] The main controversy is between models with local defects (e. g. the two-level model[2,3] or the soft-potential model[7]) and models with randomly modified bulk properties (see, for example, refs.[8–10,12,13,16]). In the present contribution we compare two models of disorder in a harmonic Debye-like solid.[18]

In the first model an elastic continuum is considered in which the local elastic constant (square of the sound velocity) is assumed to vary randomly in space. Such a model can be treated by field theoretical techniques to derive a self-consistent Born approximation (SCBA).[14,15,19]

In the second model the Debye waves are supposed to interact with local oscillators the eigen frequencies of which are randomly distributed. It is well-known that such a model can be solved exactly.[20] Here the Green's function of the oscillators acts as the self energy of the Debye waves.

In both models the DOS exhibits a boson peak. The position is given by the frequency where the imaginary part of the complex sound velocity becomes comparable to its real part, or - in other words - where the disorder induced mean free path becomes comparable to the wavelength (Ioffe-Regel limit[21]). In both models the boson peak becomes stronger and shifted towards lower frequencies if the degree of disorder - as given by the variance of the fluctuating parameters - is increased. Beyond the boson peak the reduced DOS $g(\omega)/\omega^2$ exhibits an approximately exponential decrease as it is observed frequently experimentally.[16] We are able to explain this in terms of the spatial variation of the Green's function of the perturbed waves.

Both models produce an instability if the degree of disorder is increased beyond a critical value, and the boson peak can be interpreted as a precursor phenomenon of this instability. We conclude that from the DOS alone it is difficult to distinguish between the underlying microscopic mechanisms, but in the case of structurally disordered solids we favor the elastic constant model, because it appears to be more adequate and has less adjustable parameters. Defect models might be useful for disordered crystals.

2. ELASTIC CONSTANT DISORDER

We consider (longitudinal) waves in a random medium with an elastic constant

$$\frac{\lambda + 2\mu}{m_0} \equiv \tilde{K}(\mathbf{r}) = c^2(\mathbf{r}) = c_0^2 + \Delta(\mathbf{r}) \qquad , \qquad (1)$$

which is supposed to be varying randomly in space. λ and μ are Lamé's constants and m_0 is the mass density. $c(\mathbf{r})$ is the local sound velocity and c_0 is the average one. We assume Gaussian disorder with $\overline{\Delta} = 0$ and a correlation function

$$C(\mathbf{r}) = \overline{\Delta(\mathbf{r}_0)\Delta(\mathbf{r}_0+\mathbf{r})} = \gamma\, c_0^2\, \delta(\mathbf{r}) \tag{2}$$

Here γ is the variance of $\tilde{K}$, divided by its mean, times the cube of a correlation length (which is assumed to be smaller than the length scales of interest, e. g. the wavelength in the boson peak regime).

The equation of motion in frequency space ($z = \omega + i0$) for the matrix of Green's functions $G_{ij}(\mathbf{r}, \mathbf{r}', z)$ of the waves can be written as

$$\sum_{\ell=1}^{3} \left(z^2\delta_{i\ell} + \nabla_i \tilde{K}(\mathbf{r})\nabla_\ell\right) G_{\ell j}(\mathbf{r}, \mathbf{r}', z) = -\delta_{ij}\delta(\mathbf{r}-\mathbf{r}') \tag{3}$$

This model is equivalent to that for an electron moving in a random environment with energy $E = -\omega^2$. It therefore can be treated with the same field-theoretical techniques used for the electronic problem.[22]

The functional weight for calculating the configurational average is

$$P[\Delta(\mathbf{r})] = P_0\, e^{-\frac{1}{2\gamma}\int \mathrm{d}^3\mathbf{r}\Delta(\mathbf{r})^2} \tag{4}$$

Applying the replica trick,[23,24] the generating functional for calculating the Green's function takes the form

$$Z[\mathbf{J}(\mathbf{r})]^n = \int \mathcal{D}[u_i^\alpha(\mathbf{r})]\, e^{-\frac{1}{2} < \mathbf{u}|A(z)|\mathbf{u} >} e^{< \mathbf{J}|\mathbf{u} >} \tag{5}$$

(n is the number of replicas) where the matrix element is given by

$$\begin{aligned} < \mathbf{u}|A(z)|\mathbf{u} > &= \sum_{\alpha=1}^{n}\sum_{i,j=1}^{3}\int \mathrm{d}^3\mathbf{r}\, u_i^\alpha(\mathbf{r})\left[-z^2\delta_{ij} - \nabla_i\tilde{K}(\mathbf{r})\nabla_j\right] u_j^\alpha(\mathbf{r}) \\ &= \sum_{\alpha=1}^{n}\int \mathrm{d}^3\mathbf{r}\left[-z^2\mathbf{u}^\alpha(\mathbf{r})^2 + \tilde{K}(\mathbf{r})\left(\nabla\cdot\mathbf{u}^\alpha(\mathbf{r})\right)^2\right] \end{aligned} \tag{6}$$

The α are the replica indices[25] indices which run from 1 to n. The source is given by

$$< \mathbf{J}|\mathbf{u} >= \sum_{\alpha=1}^{n}\int \mathrm{d}^3\mathbf{r}\mathbf{J}^\alpha(\mathbf{r})\cdot\mathbf{u}^\alpha(\mathbf{r}) \qquad , \tag{7}$$

and we have

$$C_{lj}(\mathbf{r}, \mathbf{r}') = \lim_{n\to 0}\frac{1}{n}\frac{\partial^2}{\partial J_{l1}(\mathbf{r})\partial J_{j1}(\mathbf{r}')} Z^n[\mathbf{J}_\alpha(\mathbf{r})]\Big|_{\mathbf{J}(\mathbf{r})=0} \tag{8}$$

$$= \lim_{n\to 0} Z^{n-1}[\mathbf{J}=0]\frac{\partial^2}{\partial J_l(\mathbf{r})\partial J_j(\mathbf{r}')} Z[\mathbf{J}(\mathbf{r})]\Big|_{\mathbf{J}(\mathbf{r})=0} \tag{9}$$

We can now perform the configurational average explicitly to obtain

$$\left\langle e^{\frac{1}{2}\int \mathrm{d}^3\mathbf{r}\Delta(\mathbf{r})(\nabla\cdot\mathbf{u}^\alpha)^2}\right\rangle = \int \mathcal{D}[\Delta(\mathbf{r})]P_0\, e^{-\frac{1}{2\gamma}\int \mathrm{d}^3\mathbf{r}\Delta(\mathbf{r})^2}\, e^{\frac{1}{2}\int \mathrm{d}^3\mathbf{r}\Delta(\mathbf{r})(\nabla\cdot\mathbf{u}^\alpha)^2}$$
$$= e^{\frac{1}{8}\gamma\sum_{\alpha\alpha'}(\nabla\cdot\mathbf{u}^\alpha)^2(\nabla\cdot\mathbf{u}^{\alpha'})^2} \tag{10}$$

We now apply a Hubbard-Stratonovich transformation to the right-hand side of (10):

$$e^{\frac{1}{8}\gamma\sum_{\alpha\alpha'}(\nabla\cdot\mathbf{u}^\alpha)^2(\nabla\cdot\mathbf{u}^{\alpha'})^2}$$
$$= \tilde{C}\int \mathcal{D}[\Lambda_{\alpha\alpha'}(\mathbf{r},z)]\, e^{-\frac{1}{2\gamma}\sum_{\alpha\alpha'}\int \mathrm{d}^3\mathbf{r}\Lambda_{\alpha\alpha'}(\mathbf{r},z)^2}$$
$$e^{-\frac{1}{2}\sum_{\alpha\alpha'}\int \mathrm{d}^3\mathbf{r}\Lambda_{\alpha\alpha'}(\mathbf{r},z)(\nabla\cdot\mathbf{u}^\alpha)(\nabla\cdot\mathbf{u}^{\alpha'})} \tag{11}$$

The configurationally averaged generating functional for $\mathbf{J} = 0$ takes the form:

$$\langle Z^n\rangle \propto \int \mathcal{D}[\mathbf{u}^\alpha(\mathbf{r})]\int \mathcal{D}[\Lambda_{\alpha\alpha'}(\mathbf{r},z)]e^{-\frac{1}{2} < \mathbf{u}|A[\Lambda]|\mathbf{u} >}\, e^{-\frac{1}{2\gamma}\mathrm{Tr}\Lambda^2}$$
$$\propto \int \mathcal{D}[\Lambda_{\alpha\alpha'}(\mathbf{r},z)]e^{-\frac{1}{2}\mathrm{Tr}\ln A[\Lambda]}\, e^{-\frac{1}{2\gamma}\mathrm{Tr}\Lambda^2} \tag{12}$$

Here the trace operation implies a summation over all internal indices and an integral over the continuous variables. The matrix element $< \mathbf{u}|A[\Lambda]|\mathbf{u} >$ is given by

$$< \mathbf{u}|A[\Lambda]|\mathbf{u} >= \int \mathrm{d}^3\mathbf{r}\sum_{ij}\sum_{\alpha\alpha'}\mathbf{u}_i^\alpha < \mathbf{r}|A[\Lambda]|\mathbf{r} >_{ij}^{\alpha\alpha'}\mathbf{u}_j^{\alpha'} \tag{13}$$

with

$$< \mathbf{r}|A[\Lambda]|\mathbf{r} >_{ij}^{\alpha\alpha'} = -z^2\delta_{ij}\delta_{\alpha\alpha'} - c_0^2\delta_{\alpha\alpha'}\nabla_i\nabla_j - \nabla_i\Lambda_{\alpha\alpha'}(\mathbf{r},z)\nabla_j \tag{14}$$

We are now looking for a saddle-point which makes the exponents in (12) stationary. The corresponding saddle-point equations can be solved with a replica-diagonal and $\mathbf{r}$ independent effective field[26] $\Lambda_{\alpha\alpha'}(\mathbf{r},z) = \Lambda(z)\delta_{\alpha\alpha'}$. ¿From the stationarity condition one obtains the following self-consistent equation:

$$\Lambda(z) = -\frac{\gamma}{2}\sum_{|\mathbf{k}|<k_D}\frac{k^2}{-z^2+k^2(c_0^2+\Lambda(z))}\quad , \tag{15}$$

where k_D is the Debye wavenumber cutoff. This approximation is the self-consistent Born approximation (SCBA). It can also be derived by conventional perturbation theory.[27,28] In such a treatment the irrudicible graphs can be classified to comprise a so-called self-energy function $\Sigma(z)$, and, as it turns out, minus the function $\Lambda(z)$ plays the role of this function. We therefore define

$$\Sigma(z) = -\Lambda(z) = \frac{\gamma}{2} \sum_{|\mathbf{k}|<k_D} \frac{k^2}{-z^2 + k^2(c_0^2 - \Sigma(z))} \tag{16}$$

The local configurationally averaged Green's function is obtained as

$$G(z) = \sum_{|\mathbf{k}|<k_D} G(\mathbf{k}, z) = \sum_{|\mathbf{k}|<k_D} \frac{1}{-z^2 + k^2(c_0^2 - \Sigma(z))} \quad , \tag{17}$$

where $G(\mathbf{k}, z)$ is the Fourier transform of $\langle G_{ii}(|\mathbf{r} - \mathbf{r}'|, z)\rangle$. From $G(z)$ the DOS can be calculated as follows:

$$g(\omega) = \frac{2\omega}{\pi} \mathrm{Im}\{G(z)\} \tag{18}$$

It is interesting to notice that the SCBA becomes equivalent to the coherent-potential approximation (CPA)[9,27] in the continuum limit and in the limit of small disorder, i. e. $\gamma \ll 1$. The latter condition is, however, always fulfilled, because the system becomes unstable for $\gamma > 0.5$. It has been demonstrated in Ref.[9] that the results of the CPA compare very well with those of a numerical simulation of the same disordered system. We shall discuss the accuracy of the SCBA further in the end of the next section.

3. LOCAL HARMONIC OSCILLATORS, COUPLED TO ELASTIC WAVES

We consider N harmonic oscillators, which are located at positions $\mathbf{r}_i$ and have displacements $x_i(t)$. They are coupled to longitudinal waves that propagate with a sound velocity c_0.[29] The Lagrangian is

$$\begin{aligned} L &= \sum_{i=1}^{N} \frac{m}{2}(\dot{x}_i^2 - \omega_i^2 x_i^2) + \int \mathrm{d}^3\mathbf{r} \frac{m_0}{2} \left[\dot{\mathbf{u}}(\mathbf{r}, t)^2 - c_0^2 \left(\nabla \cdot \mathbf{u}(\mathbf{r}, t)\right)^2\right] \\ &\quad - \sum_i x_i \int \mathrm{d}^3\mathbf{r} v_i(\mathbf{r}) \left(\nabla \cdot \mathbf{u}(\mathbf{r}, t)\right) \end{aligned} \tag{19}$$

$v_i(\mathbf{r})$ is the potential energy of the host atoms in the presence of the inpurity:

$$v_i(\mathbf{r}) = v(\mathbf{r} - \mathbf{r}_i) \tag{20}$$

This could be, for example, a screened Coulomb potential:

$$v(\mathbf{r}-\mathbf{r}_i) = v_0 \frac{1}{|\mathbf{r}-\mathbf{r}_i|} e^{-\kappa|\mathbf{r}-\mathbf{r}_i|} \tag{21}$$

The equations of motion (Lagrange equations) for the two sets of coordinate are

$$\ddot{x}_i + \omega_i^2 x_i = \frac{1}{m}\int \mathrm{d}^2\mathbf{r} v_i(\mathbf{r})\left(\nabla\cdot\mathbf{u}(\mathbf{r},t)\right) \tag{22}$$

$$\ddot{\mathbf{u}}(\mathbf{r},t) - c_0^2\nabla\left(\nabla\cdot\mathbf{u}(\mathbf{r},t)\right) = \sum_i \frac{1}{m_0}\nabla v_i(\mathbf{r}) x_i(t) \tag{23}$$

Equation (22) can be readily solved for $x_i(z)$ in frequency space:

$$x_i(z) = \frac{1}{m}\int \mathrm{d}^2\mathbf{r} v_i(\mathbf{r})\left(\nabla\cdot\mathbf{u}(\mathbf{r},t)\right) G_{I,i}(z) \tag{24}$$

with the impurity Green's function

$$G_{I,i}(z) = \frac{1}{-z^2+\omega_i^2} \tag{25}$$

Inserting this into (23)leads to

$$-z^2\mathbf{u}(\mathbf{r},t) - c_0^2\nabla\left(\nabla\cdot\mathbf{u}(\mathbf{r},t)\right) = \sum_i \frac{1}{m_0}\nabla v_i(\mathbf{r})\frac{1}{m}\int \mathrm{d}^2\mathbf{r}' v_i(\mathbf{r}')\left(\nabla'\cdot\mathbf{u}(\mathbf{r}',t)\right) G_{I,i}(z) \tag{26}$$

We now introduce a spatial Fourier transform of $v_i(\mathbf{r})$:

$$v_i(\mathbf{r}) = v(\mathbf{r}-\mathbf{r}_i) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}_i)} v(\mathbf{k}) \tag{27}$$

with

$$v(\mathbf{k}) = \frac{1}{V}\int \mathrm{d}^3\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} v(|\mathbf{r}|) = \frac{4\pi v_0}{V}\frac{1}{k^2+\kappa^2} \tag{28}$$

Then the right-hand side of (26) takes the form

$$\frac{1}{m_0}\sum_i \nabla \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}_i)} v_k \frac{1}{m}\int \mathrm{d}^3\mathbf{r}' \sum_{\mathbf{k}'} e^{i\mathbf{k}'(\mathbf{r}'-\mathbf{r}_i)} v_k' \nabla'\cdot\mathbf{u}(\mathbf{r}',z) G_{I,i}(z) \tag{29}$$

Now, if the impurities are distributed randomly in space with concentration ρ, we can take an average over the positions of the impurities and the values of ω_i^2, so that we obtain

$$\overline{\sum_\ell e^{-i(\mathbf{k}+\mathbf{k}')\mathbf{r}_\ell} G_{I,\ell}(z)} = \rho\,\delta_{\mathbf{k},-\mathbf{k}'}\overline{G_I(z)} \tag{30}$$

Introducing now the spatial Fourier transform of the displacement fields and using the fact that we consider longitudinal excitations for which $\nabla(\nabla\cdot\mathrm{u}) = (\nabla\cdot\nabla)\mathrm{u}$ holds, we finally arrive at the following expression for the Green's function of the perturbed elastic waves:

$$G(\mathrm{k}, z) = \frac{1}{-z^2 + k^2\left[c_0^2 - \Sigma_I(z)\right]} \tag{31}$$

with the self energy being proportional to the averaged oscillator Green's function

$$\Sigma_I(z) = \rho\frac{v(0)^2}{m_0 m}\overline{G_I(z)} \equiv g\overline{G_I(z)} \tag{32}$$

where we have introduced a coupling parameter $g = \rho\frac{v(0)^2}{m_0 m}$ and assumed $\kappa \gg k_D$, which means that we can replace $v(\mathrm{k})$ by $v(0)$ in the range of integration.

We are now left with the task of calculating the average Green's function $\overline{G_I(z)}$, but this is trivial, because its imaginary part is proportional to a delta function so that

$$\overline{G_I''(\omega)} = \pi\int \mathrm{d}\omega_i^2 P(\omega_i^2)\delta(\omega^2 - \omega_i^2) = \pi P(\omega^2) \tag{33}$$

Instead of using the exact equation (33) one could assume a Gaussian distribution

$$P_G(\omega_i^2) = \frac{1}{\sqrt{2\pi\sigma}}e^{-\frac{1}{2\sigma}(\omega_i^2 - \omega_0^2)^2} \tag{34}$$

and perform the same steps that led to eq. (16) to derive a SCBA for the oscillators[31]

$$\Sigma_I(z) = \sigma\frac{1/2}{-z^2 + \omega_0^2 - \Sigma_I(z)} \tag{35}$$

which can be solved to

$$\Sigma_I(z) = \frac{\sigma}{2}G_I(z) = \frac{1}{2}[\tilde{z} - \sqrt{\tilde{z} - 2\sigma}] \tag{36}$$

with $\tilde{z} = \omega_0^2 - z^2$. Comparing this with (33) we have obtained in SCBA a Green's function that corresponds to a *half-elliptic* distribution with the same width.

$$P(\omega^2) = \frac{1}{\pi\sigma}\sqrt{2\sigma - (\omega^2 - \omega_0^2)^2} \tag{37}$$

In Fig. 1 we compare the Gaussian spectra with the half-elliptic ones for different width parameters σ. Obviously the main effect of the mean-field approximation is cutting off the tails of the distribution. From this result we

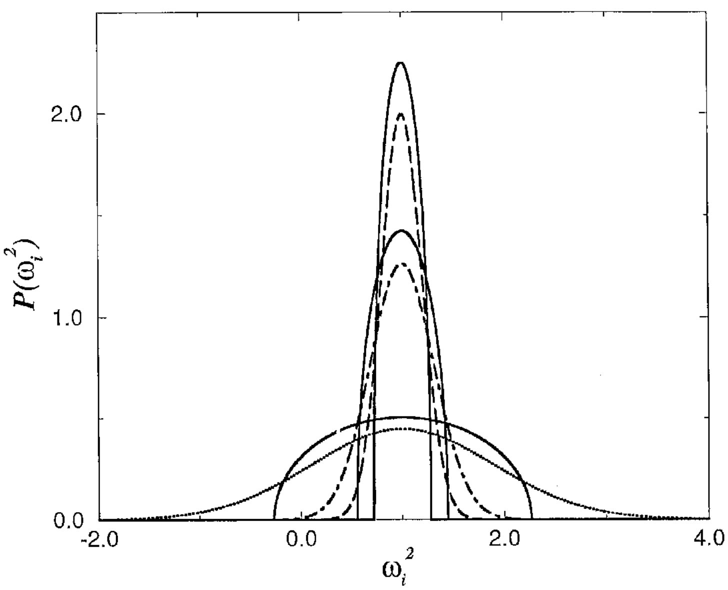

Fig. 1. Gaussian distribution for $\omega_0 = 0.9$, $\sigma = 0.04$ (dashes), 0.1 (dash-dots) and 0.8 (dots), compared with the corresponding half-elliptic distributions (full lines)

can draw some interesting conclusions concerning the accuracy of the SCBA and the use of a Gaussian distribution in the case of the *elastic disorder*:

For the elastic constants we have used a Gaussian distribution (4), although - even for small width γ - this always implies the presence of a small but finite amount of negative elastic constants $\tilde{K}$, which is unphysical. In SCBA, as it turns out, the spectrum is stable, provided $\gamma < \gamma_c = 0.5$. The same holds in the case of the oscillators (see Fig. 1): In the case of a Gaussian distribution there is a finite probability for the presence of negative ω_i^2 for any (even very small) value of σ. In SCBA - which corresponds to the half-elliptic distribution (37) - the tails of the Gaussian are cut off, and there is a sharp transition to instability for $\sigma_c = \frac{1}{2}\omega_0^4$. We conclude that an analogous thing happens in the case of elastic disorder: the tails of the Gaussian, which had to be used to be able to perform the functional integrals, are cut off by the SCBA.

On the other hand it is noteworthy in this context that an infinitely large random matrix, in which all off-diagonal elements are Gaussian distributed with the same variance has a *half-elliptic* spectrum[23,32,33] of the same width. The tails of the spectrum re-appear if the matrix is truncated to have finite size. If eq. (3) is discretized the equation of motion of the elastic constant model is governed by a *tri-diagonal* random dynamical matrix D with Gaussian distribution of the off-diagonal elements D_{ij}, but the diagonal elements are determined by the sum rule $\sum_j D_{ij} = 0$. The sum rule is due to momentum conservation and leads to Debye's $g(\omega) \propto \omega^2$ law for $\omega \to 0$. It has been demonstrated in ref.[9] that such a dynamical matrix has the same statistical properties, namely those of the Gaussian orthogonal ensemble (GOE)[33] as the infinitely large matrix. So we might conclude that the SCBA for the elastic disorder model, which gives the correct Debye behaviour and eliminates the negative ω^2 tail, might even be a better approximation than in the case of the oscillators.

Returning to the oscillators it is, of course, more sensible to use a half-elliptic (or other distribution with a sharp lower cutoff), than a Gaussian distribution. In our numerical calculation in the next section we shall do so and compare the results with the SCBA results of the elastic disorder model.

4. RESULTS AND DISCUSSION

In Fig. 2 we have plotted the reduced DOS[34] $g(\omega)/\omega^2$ against ω for the elastic disorder model for different values of the disorder parameter γ. Clearly there is a strong boson peak anomaly near 1/10 of the Debye frequency. Very similar results are obtained for the oscillator model with $\omega_0 = c_0 k_D = 1$ and $g = 1$ (Fig. 3). In Figs. 4 and 5 the influence of the variation of the parameters ω_0 and g are depicted.

In both models the boson peak becomes stronger and is shifted to lower frequencies if the disorder (given by the parameters γ and σ) is increased. In both cases there is an instability if the disorder is increased beyond the critical values $\gamma_c = 0.5$ and $\sigma_c = 0.5\omega_0^4$. This feature is shared with the earlier model calculations based on the random force-constant models and the CPA.[9,10,13] The boson peak occurs (as in the earlier investigations) as a precursor of the instability. As to be expected the boson peak appears also in the temperature dependence of the specific heat if represented as $C(T)/T^3$. $C(T)$ is calculated from the usual formula

$$C(T) = \int_0^{\omega_D} \mathrm{d}\omega g(\omega)(\omega/T)^2 \frac{e^{\omega/T}}{\left(e^{\omega/T}-1\right)^2} \tag{38}$$

In the following we shall demonstrate that the boson peak frequency ω_B

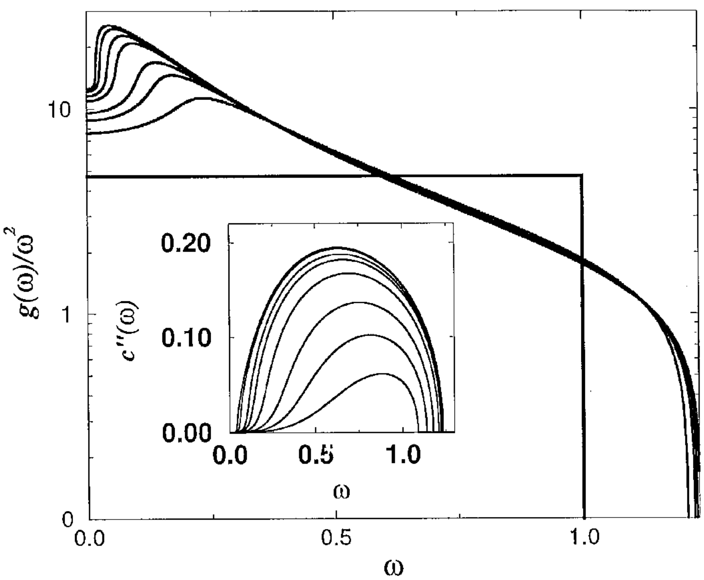

Fig. 2. Reduced DOS $g(\omega)/\omega^2$ for the elastic disorder model with (from top to bottom) $\gamma = 0.495, 0.49, 0.47, 0.45, 0.4, 0.3, 0.2, 0.1, 0.0$. In all pictures the frequencies are given in units of the Debye frequency $\omega_D = c_0 k_D \equiv k_B \Theta_D/\hbar$. Insert: the function $c''(\omega)$ for the same parameters

marks the "Ioffe-Regel frequency", where the mean free path becomes equal to the wavelength of the low-frequency excitations.[21,9] In order to do so we define an effective complex sound velocity[9]

$$c(z) = c'(\omega) - ic''(\omega) = \sqrt{c_0^2 - \Sigma(z)} \quad , \tag{39}$$

which is related to the scattering mean free path by

$$\frac{1}{\ell(\omega)} = \frac{2\omega c''(\omega)}{|c(z)|^2} \tag{40}$$

The wavelength is given by

$$\lambda(\omega) = 2\pi/\tilde{k}(\omega) = 2\pi c'(\omega)/\omega \tag{41}$$

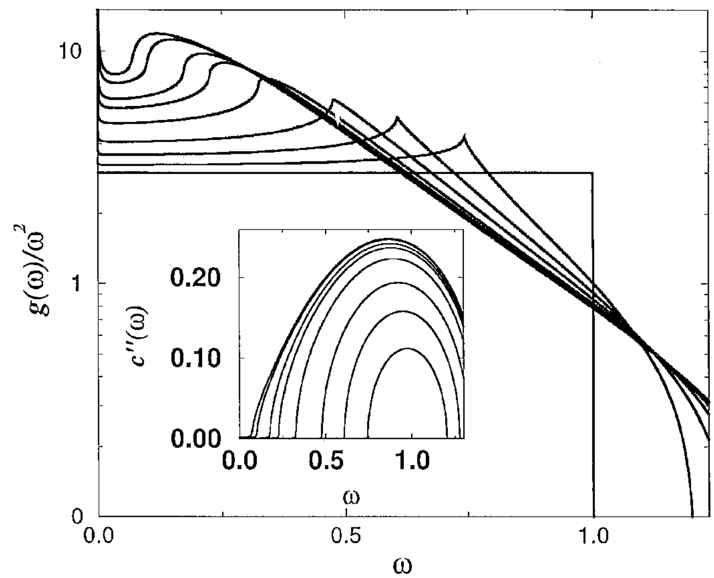

Fig. 3. Reduced DOS $g(\omega)/\omega^2$ for the oscillator model with $g = 1, \omega_0 = 1$ and (from top to bottom) $\sigma = 0.495, 0.49, 0.47, 0.45, 0.4, 0.3, 0.2, 0.1, 0.0$. Insert: the function $c''(\omega)$ for the same parameters

so that we obtain for the Ioffe-Regel ratio

$$\frac{\lambda(\omega)}{\ell(\omega)} = 4\pi \frac{c''(\omega)c'(\omega)}{|c(z)|^2} \approx 4\pi \frac{c''(\omega)}{c'(\omega)} \tag{42}$$

From the inserts of Figs 2 and 3 we see that the boson peak frequencies coincide with the frequencies at which $c''(\omega) \approx 0.1$, which corresponds to $\ell \approx \lambda$. We therefore can state that the boson peak appears just at the frequency where the waves start to be seriously be affected by the scattering and $\tilde{k}(0) = \omega/c'(0)$ ceases to be a "good" label to classify the modes (analogon to "good quantum number"). It has often been speculated that waves beyond the Ioffe-Regel limit are Anderson-localized.[35] However, it has been demonstrated in Refs.,[19,9] that the modes above the boson peak frequency are *not* localized but of diffusive nature. Just at the top of the band there is a mobility edge. In fact there is a fundamental difference between electron

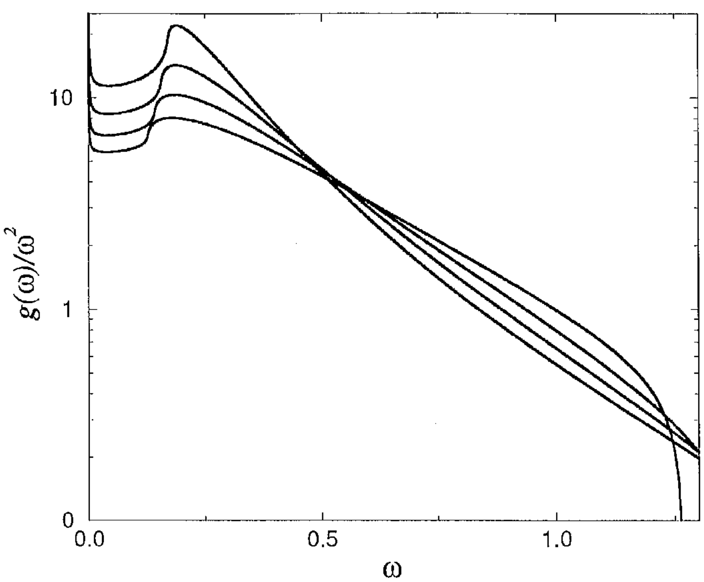

Fig. 4. Same as Fig. 3 with $g = 1, \sigma = 0.48$ and (from top to bottom) $\omega_0 = 1.2, 1.1, 1.0, 0.9$

localization and wave localization: In the case of electrons there is no physical limit for the disorder. So, if the mean free path becomes of the order of the de-Broglie wavelength, at both band edges localized states appear. The corresponding mobility edges move towards the center of the band as the disorder is increased until finally all states are localized. In the case of waves in a random medium the disorder cannot increased beyond a certain value given by γ_c and σ_c in our models. Therefore localized states will be confined to the vicinity of the Debye frequency.[30]

Let us now turn to a discussion of the "trans-boson" regime $\omega > \omega_B$. In the semilogarithmic representation of Figs. 2 - 5 we see that in this regime the reduced DOS of the systems with strong disorder can be approximately described as

$$g(\omega)/\omega^2 \propto e^{-\omega/\omega^*} \tag{43}$$

It has been shown recently[16] that such a behaviour is experimentally observed in a large number of disordered materials which exhibit a boson peak.

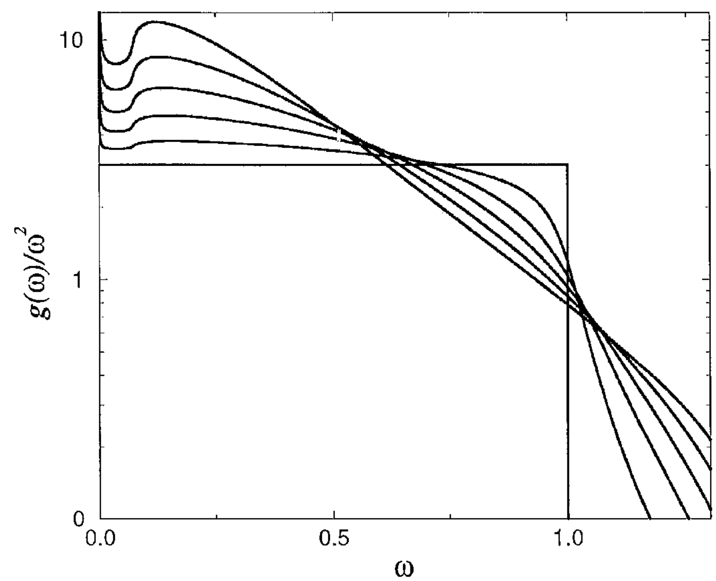

Fig. 5. Same as Fig. 3 with $\omega_0 = 1.0, \sigma = 0.495$ and (from top to bottom) $g = 1, 0.8, 0.6, 0.4, 0.2, 0.0$

We shall now give an explanation of this behaviour.

Eq. (17) for the local Green's function (valid for both models) can be rewritten using Parseval's theorem

$$G(z) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \mathrm{d}^3\mathbf{k} f(k, k_D) G(k, z) = \int_{-\infty}^{\infty} \mathrm{d}^3\mathbf{r} f(r, k_D) G(r, z) \tag{44}$$

with the cutoff function $f(k, k_D) = \theta(k_D - k)$, which has the Fourier transform

$$f(r, k_D) = \tilde{\rho} \frac{3}{(k_D r)^2} \left(\frac{sin(k_D r)}{k_D r} - cos(k_D r) \right) \tag{45}$$

where $\tilde{\rho} = k_D^3 / 6\pi^2$ is the number density. $G(r, z)$ takes the well-known form

$$G(r, z) = \frac{1}{4\pi c(z)^2 r} e^{i\omega r / c(z)} = \frac{1}{4\pi r \left[c_0^2 - \Sigma(z)\right]} e^{i\tilde{k}(\omega) r} e^{-r/2\ell(\omega)} \tag{46}$$

$f(r, k_D)$ is a function which equals 1 for $r k_D \ll 1$ and becomes very small beyond $r k_D > 1$. Therefore $r^2 f(r, k_D)$ has a peak below k_D^{-1} at, say, r_0.

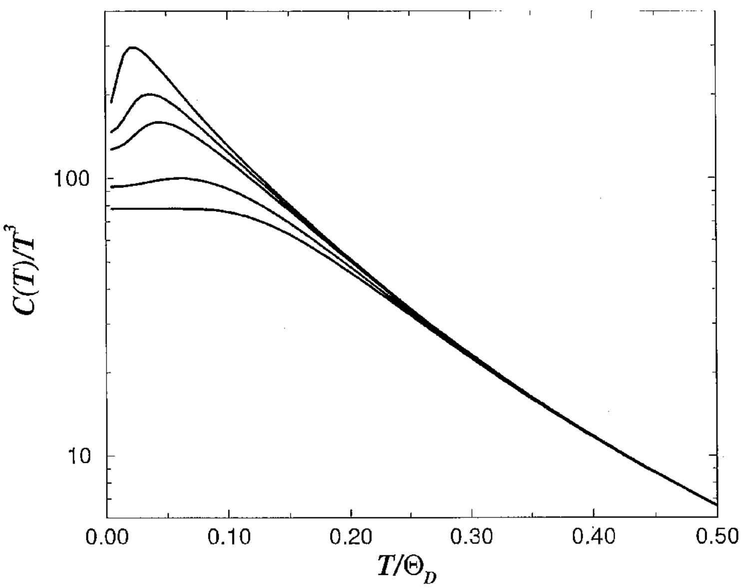

Fig. 6. Reduced specific heat capacity $C(T)/T^3$ for the elastic disorder model with (from top to bottom) $\gamma = 0.49, 0.45, 0.4, 0.2, 0.0$.

Because $\tilde{k}(\omega) < k_D$ holds, we can approximate $\sin(\tilde{k}r)$ by its argument. Replacing the r integral by the value of the Green's function at $r = r_0$, ignoring the frequency dependence of the denominator and using (18) we arrive at (43) with

$$\frac{1}{\omega^*} = \frac{r_0}{2\omega\ell(\omega)} = \frac{r_0 c''(\omega)}{|c(z)|^2} \tag{47}$$

In the regime, where $c''(\omega)$ is large and only weakly ω dependent we expect an approximate exponential decrease of the reduced DOS as shown in our SCBA calculations and in the experiental data. As demonstrated in Ref.[16] this exponential decay is also verified in the reduced DOS of a computer simulation of a quenched liquid. Furthermore, relation (47) has a remarkable relevance concerning the experimental method used in:[16] There it was noted that the DOS measured by nuclear elastic scattering from Fe^{57} inside large molecules, which are immersed in a disordered host, has an ω^* that is appreciably smaller than that obtained from neutron scattering data

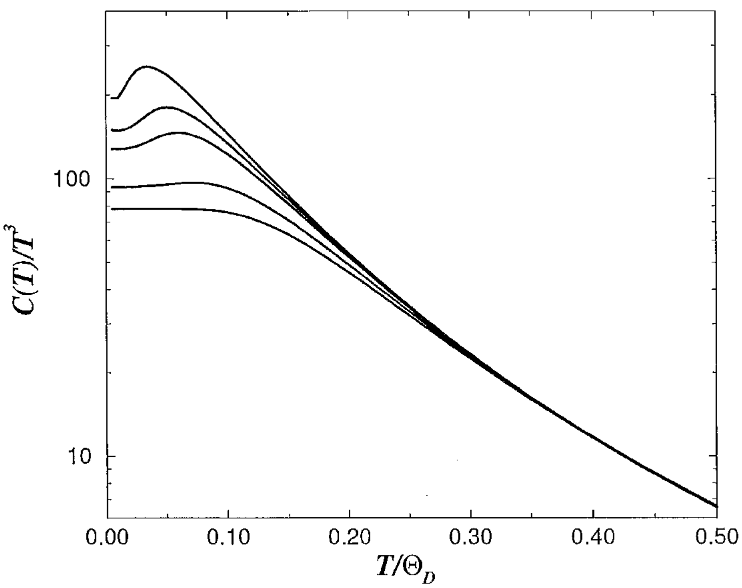

Fig. 7. Reduced specific heat capacity $C(T)/T^3$ for the oscillator model with $\omega_0 = 1, g = 1$ and (from top to bottom) $\sigma = 0.49, 0.45, 0.4, 0.2, 0.0$.

of the host. This observation can be attributed to a lesser sensitivity of the large probe to short-wavelength excitations leading to a k cuttoff smaller than k_D which, in turn, corresponds to a larger r_0.

Up to this point the discussion of the boson peak and the trans-boson exponential was explained by a $c''(\omega)$, which is similar for the two models, as verified in the inserts of Figs. 2 and 3. However, there is an important difference. From the SCBA equation (16) one easily derives the relation

$$\Sigma(z)[1 - \Sigma(z)] = \frac{\gamma}{2}[1 + z^2 G(z)] \quad , \tag{48}$$

from which we obtain the Rayleigh-Klemens relation[21,36] in the limit $\omega \to 0$ (using the $\omega = 0$ solution of (48) $2\Sigma(0) = 1 - \sqrt{1 - 2\gamma}$)

$$\Sigma''(\omega) = \frac{\gamma}{2\sqrt{1 - 2\gamma}} \pi \omega g(\omega) \propto \omega^3 \quad , \tag{49}$$

which implies Rayleigh's $\ell(\omega) \propto \omega^{-4}$ law. We are convinced that for any harmonic system with quenched disorder, in which translational invariance (which gives Debye's law) is guaranteed, there must be such a Rayleigh-Klemens asymptotics. This is so, because the scattering perturbation at low frequencies decreases as ω^2. Therefore, at low enough frequency, the SCBA (which reduces to the Born approximation in this limit) becomes exact.[37]

In the case of the oscillator model the frequency dependence of $\Sigma''(\omega)$ is identical to that of the distribution $P(\omega_i^2)$, just arbitrary. In the half-elliptic model (in the stable region) $\lim_{\omega\to 0}\Sigma''(\omega) = \lim_{\omega\to 0} P(\omega^2) = 0$. The spectrum just starts at a finite frequency. This failure of reproducing the Rayleigh law in the self energy is shared with earlier effective-medium theories[38] for the boson peak and can be traced to an incomplete incorporation of translation invariance into the theory. In the case of our oscillator model the defects are not allowed to move with the long-wavelength phonons, which then is the reason for the failure of reproducing the Rayleigh asymptotics. We believe that a recent theory dealing with low-density disordered solids, which does not show the Rayleigh asymptotics[13] faces a similar problematics. In experimental data, on the other hand, the low-frequency asymptotics is *not* governed by Rayleigh's law but by anharmonic effects[14,15] related to sound damping, which lead to $\ell(\omega) \propto \omega^2$. This will be demonstrated in detail in a forthcoming publication.[39]

Let us now discuss the physical relevance of the elastic constant model in comparison with the defect model. If we consider an amorphous material it is difficult to imagine the difference of "host" and "defect". The fluctuating elastic constant model is just what one expects as a first step for describing the influence of disorder on waves in a solid. The only fit parameter[40] in the theory is the disorder parameter γ, whereas (restricting ourselves to the half-elliptic distribution) there are three for the oscillator model. In the soft- potential defect model[7] there are even more fit parameters because the defects are described by anharmonic potentials. Of course in this theory a boson peak appears, because the quartic potentials effectively act as quasi-harmonic oscillators. We are convinced that defect models are more adequate for disordered crystals, in which the defects can be defined in a unique and physical way. The present exercise then allows for understanding why the boson peak and other disorder-induced features are so similar in disordered crystals and amorphous solids.

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