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Coherent potential approximation for diffusion and wave propagation in topologically disordered systems

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Using Gaussian integral transform techniques borrowed from functional-integral field theory and the replica trick we derive a version of the coherent potential approximation (CPA) suited for describing (i) the diffusive (hopping) motion of classical particles in a random environment, and (ii) the vibrational properties of materials with spatially fluctuating elastic coefficients in topologically disordered materials. The effective medium in the present version of the CPA is not a lattice but a homogeneous and isotropic medium, representing an amorphous material on a mesoscopic scale. The transition from a frequency-independent to a frequency-dependent diffusivity (conductivity) is shown to correspond to the boson peak in the vibrational model. The anomalous regimes above the crossover are governed by a complex, frequency-dependent self-energy. The boson peak is shown to be stronger for non-Gaussian disorder than for Gaussian disorder. We demonstrate that the low-frequency nonanalyticity of the off-lattice version of the CPA leads to the correct long-time tails of the velocity autocorrelation function in the hopping problem and to low-frequency Rayleigh scattering in the wave problem. Furthermore we show that the present version of the CPA is capable of treating the percolative aspects of hopping transport adequately.

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I. INTRODUCTION

The coherent potential approximation (CPA) is a very successful mean-field theory for calculating single-particle excitations in quenched-disordered[1–7] and strongly correlated[8–11] quantum systems. Quenched disorder in a solid can manifest itself as an impurity and alloy disorder in an otherwise crystalline material, and the CPA has nowadays become a powerful tool to calculate the electronic band structure of such materials.[12] The principle of the CPA is to introduce a crystalline effective medium in which the spatially fluctuating random potential is replaced by a constant but energy-dependent potential (coherent potential, self-energy). The self-energy is determined in such a way that the configurationally averaged Green's function is forced to be equal to the Green's function of the effective medium. Correspondingly, the T matrix due to scattering from the fluctuating potential minus the coherent potential vanishes.

A much more difficult task than the crystalline alloy problem is the calculation of the electronic excitations in a *topologically disordered solid* like a liquid or amorphous metal. This is so because one cannot use Bloch's theorem and the established band-structure methods for calculating the electronic structure of the effective medium. Based on the multiple-scattering theory of Lax[13] and Halperin[14] a CPA has been formulated by Györffy,[15] who already included correlations between the fluctuating potentials (see also the related paper by Hall and Faulkner).[16]

In order to include the short-range correlations of the amorphous solid in a more fundamental way, the tight-binding formalism for metals[17] has been used by a large number of authors to formulate effective-medium theories of liquid metals.[18–21] These approaches have been brought in mathematical correspondence to liquid-state integral-equation theories by Logan and Winn[22] and Winn and Logan.[23]

The Schrödinger equation for tight-binding electrons has a close resemblance to the equation of motion for diffusing particles as well as vibrations in a topologically disordered system. Correspondingly the single-site CPA on a lattice has been generalized to a two-site CPA in order to treat diffusion in a disordered crystal.[24–26]

Effective-medium theories for hopping transport in a topologically disordered system had been formulated along the lines of the electronic tight-binding theories.[27–29] However, the effective medium in these treatments is a Bethe lattice, i.e., a system without closed loops. In a disordered system it is just the closed paths, which must be included to calculate the correct nonanalyticity of the self-energy, which leads to long-time tails[30,31] and Rayleigh scattering.[32,33] Therefore Ganter and Schirmacher[34] combined the integral-equation scheme of Logan and Winn[22] with the repeated-indices renormalization technique of Feenberg[35] in order to formulate an effective-medium theory on the CPA level, in which the closed paths, and hence the nonanalyticities, were included. However, the resulting integral equations have very poor convergence properties, which, if applied to vibrations of vector character,[36] could only have been solved with severe simplifications. Later Ganter and Schirmacher[33] formulated a self-consistent hopping theory based on the so-called Euclidean random-matrix approach[37,38] which contains the appropriate nonanalyticity. The integral equations of this approach are easier to solve.

In the present work we derive a CPA for topologically disordered systems, in which no short-range correlations are considered, but in which the effective medium is not a crystal. Our effective medium is a homogenous and isotropic continuum. For the electronic problem a similar CPA has already been derived[39] along the lines of the formalism of Yonezawa and Morigaki,[4] and it has been shown there, how to introduce correlations.

In the present work we use a replica field-theoretical approach, in which the CPA appears as a saddle point of an interacting matrix field theory. The introduction of correlations will be postponed to future work.

Section II is devoted to the mathematically equivalent problems of diffusion and scalar waves with spatially fluctuating diffusivity/elastic modulus. For this model our version of the CPA is derived and solved. From the numerical solutions it is demonstrated that the existence of a dc-ac crossover in the diffusion problem corresponds to the presence of an excess of vibrational states (boson peak)[40–45] in the wave propagation problem. It is shown that the height of the boson peak is unrestricted for certain non-Gaussian distributions (inverse-power law distribution, log-normal distribution) but restricted for a box-shaped and a Gaussian distribution. For the non-Gaussian distributions a scaling relation between the height of the boson peak and its frequency position is shown to hold within the CPA. For weak disorder the CPA is shown to reduce to the self-consistent Born approximation (SCBA), which proved very successful to describe the anomalous vibrational properties of disordered solids.[40–45] In Sec. III the CPA for vector displacements in an elastic continuum with fluctuating shear modulus is presented (heterogeneous-elasticity theory).[40–45] The vector theory is shown to possess the same boson-peak features as the scalar theory.

II. DIFFUSION AND SCALAR VIBRATIONS IN A DISORDERED ENVIRONMENT

A. Models and mathematic correspondence

Let us start our discussion with considering hopping transport of electrons or ions in a disordered semiconductor, or—equivalently—among the impurities of a doped crystalline semiconductor.[46,47] Such a motion of particles between specific sites i,j in a disordered material can be described by a master equation for the probability $n_i(t)$ for being at site i at time t,

$$\frac{d}{dt}n_i(t) = -\sum_{j\neq i} W_{ij}(n_i(t) - n_j(t)), \tag{1}$$

where the transition (hopping) probabilities per unit time W_{ij} can depend on the distance $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and/or on an energy barrier E_{ij} between the sites i and j (representing a symmetrized version of diffusion in a landscape of states with disordered local energies with phonon-assisted transitions between them).[46,47] The distance dependence is supposed to fall off exponentially, so that we do not have a long-range model.

It has been shown recently[33] that by a coarse-graining procedure such a transport equation can be transformed to a diffusion equation on a *mesoscopic* scale,

$$\frac{\partial}{\partial t}n(\mathbf{r},t) = \nabla D(\mathbf{r})\nabla n(\mathbf{r},t), \tag{2}$$

with a spatially fluctuating diffusion coefficient $D(\mathbf{r})$, which is supposed to be a random variable in the three-dimensional space with a suitable distribution density $P[D(\mathbf{r})]$. Performing the Laplace transform $n(\mathbf{r},s) = \int_0^\infty dt e^{-st} n(\mathbf{r},t)$ with $s = i\omega + \epsilon$ we obtain from (2) the diffusion equation in frequency space (disregarding the $t = 0$ term),

$$sn(\mathbf{r},s) = \nabla D(\mathbf{r})\nabla n(\mathbf{r},s). \tag{3}$$

On a *macroscopic* scale the (quenched) disorder is known to lead to a diffusion equation with a space-independent but frequency-dependent complex diffusivity $D(s)$,

$$sn(\mathbf{r},s) = D(s)\nabla^2 n(\mathbf{r},s). \tag{4}$$

$D(s)$ is the Laplace transform of the velocity autocorrelation function $Z(t)$ of the moving particle. If the particle carries a charge q, $D(s)$ is related to the complex, frequency-dependent conductivity $\sigma(s)$ by the Nernst-Einstein relation,

$$\sigma(s) = n_\mu q^2 D(s), \tag{5}$$

where $n_\mu \equiv \partial n/\partial\mu$ is the derivative of the number of carriers with respect to the chemical potential. In degenerate quantum systems this quantity is equal to the density of electronic states at the Fermi level, in classical systems $n_\mu = n/k_B T$, where T is the temperature.

Let us now consider a topologically disordered mass-spring system in which the masses (which we suppose to be equal to unity) are connected by distance-dependent force constants, which we call K_{ij}. The corresponding equation of motion for the scalar displacements of the masses at point i is

$$\frac{d^2}{dt^2}u_i(t) = -\sum_{j\neq i} K_{ij}(u_i(t) - u_j(t)). \tag{6}$$

The same coarse-graining procedure, which leads from (1) to (2) produces the following stochastic wave equation:

$$\frac{\partial^2}{\partial t^2}u(\mathbf{r},t) = \nabla K(\mathbf{r})\nabla u(\mathbf{r},t), \tag{7}$$

or in frequency space,

$$s^2 u(\mathbf{r},s) \equiv \tilde{s}u(\mathbf{r},\tilde{s}) = \nabla K(\mathbf{r})\nabla u(\mathbf{r},\tilde{s}), \tag{8}$$

where now $K(\mathbf{r}) \equiv v(\mathbf{r})^2$ has the meaning of a space-dependent modulus, which is equal to the square of the wave velocity v. $K(\mathbf{r})$ is again a random variable in the three-dimensional space and can be identified with $D(\mathbf{r})$ in the diffusion problem.

On a macroscopic scale one deals with an equation of motion in frequency space for scalar wave amplitudes $u(\mathbf{r},z)$ with a frequency-dependent, complex sound velocity $v(\tilde{s})$,

$$\tilde{s}u(\mathbf{r},\tilde{s}) = K(\tilde{s})\nabla^2 u(\mathbf{r},\tilde{s}). \tag{9}$$

Here $\tilde{s} = s^2 = -\omega^2 + i\tilde{\epsilon}$ and $K(\tilde{s}) = v^2(\tilde{s})$ is a complex, frequency-dependent elastic modulus, which is equal to the square of a complex wave velocity. As in optics the imaginary part of $v(\tilde{s})$, $v''(\omega)$ is related to the disorder-induced mean-free path of the waves, $\ell(\omega)$, and to the sound-attenuation coefficient $\Gamma(\omega)$ by[33]

$$\frac{1}{\ell(\omega)} = \frac{2\omega v''(\omega)}{|v(\tilde{s})|^2} = \frac{1}{2|v(\tilde{s})|}\Gamma(\omega). \tag{10}$$

In a quenched-disordered system, i.e., a medium with either spatially fluctuating density or elastic modulus the sound attenuation exhibits Rayleigh scattering,[32,33]

$$\Gamma(\omega) \propto \omega^4 \quad \text{for} \quad \omega \to 0. \tag{11}$$

This means that both $v(\tilde{s})$ and $K(\tilde{s})$ have a contribution, which varies as $\tilde{s}^{3/2}$ for small frequencies. If we now mathematically identify the diffusion coefficient $D(s)$ with $K(\tilde{s})$ we conclude that $D(s)$ has a low-frequency nonanalytic $s^{3/2}$ contribution,

$$\Delta D(s) = D(s) - D(0) \propto s^{3/2}, \tag{12}$$

which becomes $\Delta D(s) \propto s^{d/2}$ in d dimensions. This nonanalytic asymptotics has been proven to hold for any quenched-disordered system governed by equations of motion of the form (1), (2), (6), and (7). As $D(s)$ is the Laplace transform of the velocity autocorrelation function $Z(t)$ one obtains the nonanalytic long-time asymptotics ("long-time tail") $Z(t) \propto -t^{(d+2)/2}$. This long-time-tail property, which has been known already for some time,[30,31,48] is obviously equivalent to Rayleigh scattering via the correspondence $D(s) \leftrightarrow K(\tilde{s})$.[33,49] The analogy, in fact, goes further: In a quenched-disordered system (which is the subject matter of the present work) it is known that a crossover happens between a frequency-independent diffusivity and a strong frequency dependence, which can be parametrized as $D(s) \propto s^x$ with $x \approx 0.8$.[50–52] This disorder-induced diffusivity transforms under the correspondence $D(s) \leftrightarrow K(\tilde{s})$ to disorder-induced anomalous frequency dependence of the elastic modulus, the onset of which corresponds to the boson peak.[53,54] This correspondence will be discussed in more detail below.

B. Derivation of the CPA

We now consider the mathematically equivalent problems Eqs. (3) and (8), identifying the quantities $D(\mathbf{r}) \leftrightarrow K(\mathbf{r})$, $D(s) \leftrightarrow K(\tilde{s})$, and $s \leftrightarrow \tilde{s}$. We define[55]

$$(s - \nabla D(\mathbf{r})\nabla)\delta(\mathbf{r} - \mathbf{r}') \equiv \langle \mathbf{r}'|\mathcal{A}[D(\mathbf{r})]|\mathbf{r}\rangle. \tag{13}$$

The Green's function corresponding to Eq. (2) is given by the inverse matrix element of $\mathcal{A}$:

$$\mathsf{G}(\mathbf{r},\mathbf{r}') = \langle \mathbf{r}'|\mathcal{A}^{-1}|\mathbf{r}\rangle. \tag{14}$$

Applying standard methods in replica field theory[56] we represent the Green's function as a functional integral over mutually complex conjugate fields $u(\mathbf{r})^\alpha$ and $\bar{u}(\mathbf{r})^\alpha$ present in $\alpha = 1, \ldots, n$ replicas of the system as follows:

$$\mathsf{G}(\mathbf{r},\mathbf{r}') = \prod_{\alpha=1}^{n} \int \mathcal{D}[\bar{u}^\alpha(\mathbf{r}), u^\alpha(\mathbf{r})]\bar{u}^1(\mathbf{r})u^1(\mathbf{r}')e^{-\sum_\alpha \langle u^\alpha|\mathcal{A}|u^\alpha\rangle} \tag{15}$$

$$= \frac{\delta}{\delta J^{(1)}(\mathbf{r},\mathbf{r}')}\mathcal{Z}[J(\mathbf{r},\mathbf{r}')], \tag{16}$$

with the generating functional,

$$\mathcal{Z}[J(\mathbf{r},\mathbf{r}')] = \prod_{\alpha=1}^{n} \int \mathcal{D}[\bar{u}^\alpha(\mathbf{r})]\mathcal{D}[u^\alpha(\mathbf{r})]\, e^{-\sum_\alpha \langle u^\alpha|\mathcal{A}|u^\alpha\rangle} \times e^{-\sum_\alpha \langle u^{(\alpha)}|J^{(\alpha)}|u^{(\alpha)}\rangle}, \tag{17}$$

and the source-field J^α. By an integration by part the matrix elements of the inverse Green operator $\mathcal{A}$ can be written as

$$\langle u^\alpha|\mathcal{A}[D]|u^\alpha\rangle = \int d^3\mathbf{r}(s|u^\alpha(\mathbf{r})|^2 + D(\mathbf{r})|\nabla u^\alpha(\mathbf{r})|^2). \tag{18}$$

We now apply the Fadeev-Popov procedure,[57] which consists of the replacement of the fluctuating diffusivity $D(\mathbf{r})$ by a complex auxiliary field $Q^{(\alpha)}(\mathbf{r},s)$ with the help of a delta functional, which, in turn, is represented by another auxiliary field $\Lambda^{(\alpha)}(\mathbf{r},s)$:

$$\begin{aligned}\mathcal{Z}[J] &= \int \mathcal{D}[u,\bar{u}] \int \mathcal{D}[Q]\, e^{-\langle u|\mathcal{A}[Q]-J|u\rangle}\delta[D-Q] \\ &= \int \mathcal{D}[u,\bar{u}]\,\mathcal{D}[Q,\Lambda]\, e^{-\langle\phi|\mathcal{A}[Q]-J|\phi\rangle}e^{\langle\Lambda|D-Q\rangle} \\ &= \int \mathcal{D}[Q,\Lambda]\, e^{-\mathrm{Tr}\{\ln[\mathcal{A}[Q]-J]\}}e^{\langle\Lambda|D-Q\rangle},\end{aligned} \tag{19}$$

where we have suppressed the replica indices for brevity. The third equality in Eq. (19) follows from integrating out the displacement fields $\bar{u}^\alpha$ and u^α. In order to proceed further we devise another coarse-graining procedure. We tile the total space into N_c cells of (approximate) volume $V_c = V/N_c$, where $V = L^3$ is the total volume.[58,81] This could just be done by means of a cubic grid. However, in order to avoid any relation to a crystalline lattice we think, instead, of a Voronoi tessellation around midpoints of a closed-packed hard-sphere structure. This gives $V_c = L_c^3 = (\pi/6)\eta_c d_c^3$, where $\eta_c \approx 0.56$ is the close-packed packing fraction, resulting in $L_c \approx 0.66 d_c$. Within a cell with label i we replace the diffusivity by their average in each cell and assume that a diffusion equation,

$$\frac{\partial}{\partial t}n(\mathbf{r},t) = \nabla D_i \nabla n(\mathbf{r},t), \tag{20}$$

holds within a cell with label i. We now assume that the random numbers D_i are independent of each other, i.e., the joint distribution density is assumed to factorize as $P(D_1 \cdots D_{N_c}) = \prod_i p(D_i)$.

Our assumption of independent fluctuations of the quantities D_i implies that the size of the cells L_c must be larger or at least equal to the correlation length ξ of the diffusivity fluctuations $\Delta D(\mathbf{r}) = D(\mathbf{r}) - \langle D\rangle$, which is defined by the spatial decay of the correlations of these fluctuations:

$$\xi^3 = \frac{1}{\langle \Delta D^2\rangle}\int d^3\mathbf{r}\langle \Delta D(\mathbf{r}+\mathbf{r}_0)\Delta D(\mathbf{r}_0)\rangle. \tag{21}$$

Correspondingly we confine the $\mathbf{k}$ summations in the subsequent analysis to remain below a cutoff $|\mathbf{k}| < k_\xi = \nu/\xi$, where ν is an adjustable number of the order of 1.

Within our model $D(\mathbf{r})$ is now a piecewise constant function in real space and the same should hold for the auxiliary fields Q and Λ, which are now labeled as $Q_i^{(\alpha)}$, $\Lambda_i^{(\alpha)}$. Using this the scalar product, which appears in the exponential in Eq. (19), can be written as

$$\langle \Lambda|D-Q\rangle = \frac{V_c}{V}\sum_\alpha\sum_i \Lambda_i^{(\alpha)}(\boldsymbol{r})\big(D_i^{(\alpha)} - Q_i^{(\alpha)}\big). \tag{22}$$

We now start to evaluate the configurational average. Due to the Fadeev-Popov transformation the only term to be averaged over is the term $e^{\langle\Lambda|D-Q\rangle}$.

Assuming that all the N_c coarse-graining cubes behave the same on average and using that the individual cubes are not

correlated, we can write

$$\langle e^{\langle \Lambda | D-Q \rangle} \rangle = \prod_{\alpha} \prod_{i} \left\langle e^{\frac{V_c}{V} \Lambda_i^{(\alpha)} (D_i^{(\alpha)} - Q_i^{(\alpha)})} \right\rangle_i = e^{\sum_\alpha \frac{V}{V_c} \ln \left(\langle \exp[-\frac{V_c}{V} \Lambda_i^{(\alpha)} (D_i^{(\alpha)} - Q_i^{(\alpha)})] \rangle_i \right)}. \quad (23)$$

Note that the two occurring volume ratios do not cancel each other due to the average inside the logarithm. Using (23) the generating functional (19) can be written as

$$\mathcal{Z}[\tilde{J}] = \int \mathcal{D}[Q,\Lambda]\, e^{-S_{\text{eff}}[Q,\Lambda,\tilde{J}]}, \quad (24)$$

where we have now replaced the source field $J^\alpha(\mathbf{r},\mathbf{r}')$ by the translational-invariant source field $\tilde{J}(\mathbf{r}-\mathbf{r}')$ which is not supposed to depend on the replica index α. The effective action takes the form,

$$S_{\text{eff}}[Q,\Lambda,\tilde{J}] = \text{Tr}\{\ln(\mathcal{A}[Q] - \tilde{J})\} - \sum_{\alpha=1}^{n} \frac{V}{V_c} \ln \left(\left\langle e^{-\frac{V_c}{V} \Lambda_i^{(\alpha)} (D_i^{(\alpha)} - Q_i^{(\alpha)})} \right\rangle_i \right). \quad (25)$$

Since the factor $\frac{V}{V_c}$ in the effective action (25) is much larger than unity a saddle-point approximation can be employed to evaluate the integral in (24). In general this factor will scale as

$$\frac{V}{V_C} = \left(\frac{L}{\xi} \right)^d \overset{d\to\infty}{\longrightarrow} \infty. \quad (26)$$

Accordingly the CPA becomes exact for $d \to \infty$.[7]

We now assume that the fields Q and Λ are replica independent.

$$S_{\text{eff}}[Q,\Lambda,0] = n\, S'_{\text{eff}}(\{Q_i\},\{\Lambda_i\}), \quad (27a)$$

$$S'_{\text{eff}}(\{Q_i\},\{\Lambda_i\}) = \text{tr}\{\ln[\,\widetilde{A}(Q)]\} - \sum_i \ln \left(\left\langle e^{-\frac{V_c}{V} \Lambda_i (D_i - Q_i)} \right\rangle_i \right), \quad (27b)$$

where "tr" now means a trace without the replica indices.

The saddle point is determined by the equations,

$$\left. \frac{\partial S'_{\text{eff}}}{\partial Q_i} \right|_{Q_i = Q_{i,S}} = 0, \quad \forall i, \quad (28a)$$

$$\left. \frac{\partial S'_{\text{eff}}}{\partial \Lambda_i} \right|_{\Lambda_i = \Lambda_{i,S}} = 0, \quad \forall i. \quad (28b)$$

The derivative with respect to Λ is easily performed and yields

$$0 = \frac{\left\langle -\frac{V_c}{V} \Lambda_{i,s} (D_i - Q_{i,s}) e^{-\frac{V_c}{V} \Lambda_i (D_i - Q_{i,s})} \right\rangle_i}{\left\langle e^{-\frac{V_c}{V} \Lambda_{i,s} (D_i - Q_{i,s})} \right\rangle_i}, \quad \Rightarrow \quad 0 = \left\langle \frac{D_i - Q_{i,s}}{\exp\left[\frac{V_c}{V} \Lambda_{i,s} (D_i - Q_{i,s}) \right]} \right\rangle_i. \quad (29)$$

Since $\frac{V_c}{V} \ll 1$ the exponential in the denominator can be expanded to first order,[59]

$$0 = \left\langle \frac{D_i - Q_{i,s}}{1 + \frac{V_c}{V} (D_i - Q_{i,s}) \Lambda_{i,s}} \right\rangle_i. \quad (30)$$

The second saddle-point equation gives

$$\left. \frac{\partial \,\text{tr}\{\ln[\widetilde{A}(Q)]\}}{\partial Q_i} \right|_{Q_i = Q_{i,s}} = \frac{\frac{V_c}{V} \Lambda_{i,s} \left\langle e^{-\frac{V_c}{V} \Lambda_i (D_i - Q_{i,s})} \right\rangle_i}{\left\langle e^{-\frac{V_c}{V} \Lambda_{i,s} (D_i - Q_{i,s})} \right\rangle_i} = \frac{V_c}{V} \Lambda_i. \quad (31)$$

The left-hand side can be evaluated under the assumption that the saddle-point field Q_S is constant in space,

$$Q_{i,s} \equiv Q, \quad \forall i.$$

This corresponds to the introduction of an effective homogeneous medium. In this medium (31) becomes

$$\frac{V_c}{V} \Lambda = \frac{V_c}{V} \frac{\partial}{\partial Q} \text{tr} \ln[A_{\text{eff}}] = \frac{V_c}{V} \sum_{\boldsymbol{k}} \frac{k^2}{s + Qk^2}. \quad (32)$$

In the second step the effective-medium operator,

$$A_{\text{eff}}(\boldsymbol{k},\tilde{\boldsymbol{k}}) = (s + Qk^2) \delta_{\boldsymbol{k}\tilde{\boldsymbol{k}}}, \quad (33)$$

was defined. From this representation one can see that in the CPA the following holds:

$$\langle G \rangle (\boldsymbol{k},\tilde{\boldsymbol{k}},s) = \frac{1}{s + Qk^2} \delta_{\boldsymbol{k}\tilde{\boldsymbol{k}}} = \left\langle \frac{1}{s + Dk^2} \right\rangle \delta_{\boldsymbol{k}\tilde{\boldsymbol{k}}}, \quad (34)$$

under the assumption that the averaged system exhibits translational invariance. This equation expresses the averaged Green's function in terms of the Green's function of a homogeneous medium, where the spatially fluctuating diffusivity is replaced by the self-energy Q, which, however, is now frequency dependent: The space dependence due to the disorder has been transformed to a disorder-induced frequency dependence.

From (32) it follows that if Q is homogeneous in space, the same holds for Λ. Defining a new field $\widetilde{\Lambda} = 3V_c/\widetilde{\nu} V \Lambda$ with $\widetilde{\nu} = \nu^3/2\pi^2$ and performing the summation in (32) with a cutoff $|\boldsymbol{k}| < k_\xi$ the CPA equations become

$$0 = \left\langle \frac{D_i - Q(s)}{1 + \frac{\widetilde{\nu}}{3} [D_i - Q(s)] \widetilde{\Lambda}(s)} \right\rangle_i, \quad (35a)$$

$$\widetilde{\Lambda}(s) = \frac{3}{k_\xi^3} \int_0^{k_\xi} dk k^2 \frac{k^2}{s + k^2 Q(s)} = \frac{1}{Q(s)} [1 - s G(s)], \quad (35b)$$

with the local Green's function,

$$G(s) = \frac{3}{k_\xi^3} \int_0^{k_\xi} dk k^2 \frac{1}{s + k^2 Q(s)}. \quad (35c)$$

We call $\widetilde{\Lambda}(s)$ the susceptibility function, because it is proportional to the local dynamic susceptibility of the diffusing particle.

The CPA equation (35a) can be cast into the following equivalent forms:

$$1 = \left\langle \frac{1}{1 + \frac{\widetilde{\nu}}{3} [D_i - Q(s)] \widetilde{\Lambda}(s)} \right\rangle_i, \quad (35d)$$

$$Q(s) = \left\langle \frac{D_i}{1 + \frac{\widetilde{\nu}}{3} [D_i - Q(s)] \widetilde{\Lambda}(s)} \right\rangle_i. \quad (35e)$$

It is worthwhile to note that the k integral in Eq. (35b) for the susceptibility function can be carried out analytically. The diffusion pole in the denominator of the integrand produces a $\widetilde{\Lambda}(s) = \widetilde{\Lambda}(0) + \text{const} \times s^{2/3}$ low-frequency asymptotics, which is inherited by the function $Q(s)$. So, independent of the type of disorder, we obtain a correct long-time behavior for $Z(t)$ and Rayleigh scattering for the wave problem. Because for the vibrational problem in the $s \to 0$ limit the disorder scattering is suppressed by the Rayleigh frequency dependence, the CPA expression for the imaginary part of $Q(z)$ can be shown to reduce to the Born approximation in agreement with the previous derivations.[32,33]

In the dc limit $s = 0$ we have $\widetilde{\Lambda}(0) = 1/Q(s)$, so we obtain from Eq. (35e),

$$Q(0) = \left\langle \frac{D_i}{1 - \frac{\widetilde{\nu}}{3} + \frac{\widetilde{\nu}}{3}\frac{D_i}{3Q(0)}} \right\rangle. \tag{36a}$$

[From now on we suppress the index i, which indicates the average over $p(D_i)$.] In the case $Q(0) \neq 0$ (which is not trivial; see the paragraph on percolation) one can divide by $3Q(0)/\widetilde{\nu}$ to obtain

$$\frac{\widetilde{\nu}}{3} = \left\langle \frac{1}{1 + \left(\frac{3}{\widetilde{\nu}} - 1\right)\frac{Q(0)}{D_i}} \right\rangle. \tag{36b}$$

C. Relation with previous effective-medium theories

1. Lattice CPA

The standard two-site coherent potential approximation for the hopping problem of Eq. (1) on a lattice is[24–26]

$$\left\langle \frac{W_{ij} - \Gamma(s)}{1 + (W_{ij} - \Gamma(s))\frac{2}{Z\Gamma(s)}(1 - sG_{ii}(s))} \right\rangle = 0. \tag{37}$$

Here $\Gamma(s)$ is the effective frequency-dependent hopping rate and $G_{ii}(s)$ is the local Green's function of the effective medium, which within this theory is a simple-cubic lattice with coordination number $Z = 2d = 6$. The lattice Green's function has the form,

$$G_{ii}(s) = \sum_{\mathbf{k}\in BZ} \frac{1}{s + \Gamma(s) f(\mathbf{k})}, \tag{38}$$

where the sum goes over the first Brillouin zone (BZ), and

$$f(\mathbf{k}) = 6 - 2[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)], \tag{39}$$

with a being the lattice constant. Defining the local susceptibility function,

$$\begin{aligned} \Lambda_{ii}(s) &= \frac{1}{\Gamma(s)}(1 - sG_{ii}(s)) \\ &= \sum_{\mathbf{k}\in BZ} \frac{f(\mathbf{k})}{s + \Gamma(s) f(\mathbf{k})}, \end{aligned} \tag{40}$$

the CPA equation (37) takes the form,

$$\left\langle \frac{W_{ij} - \Gamma(s)}{1 + (W_{ij} - \Gamma(s))\frac{1}{3}\Lambda_{ii}(s)} \right\rangle = 0. \tag{41}$$

Now we take the continuum limit by replacing the BZ $\mathbf{k}$ summation by $\sum_{\mathbf{k}} \to \frac{3}{k_\xi^3}\int_0^{k_\xi} dk$ and $f(\mathbf{k})$ by its low-wave-number limit k^2a^2. If we now define the local diffusivities by $D_i = W_{ij}a^2$, the effective-medium diffusivity by $Q(s) = \Gamma(s)a^2$, and the continuum susceptibility function by $\widetilde{\Lambda}(s) = \Lambda_{ii}(s)/a^2$ we arrive at the continuum-off-lattice CPA result (35a), provided we take $\widetilde{\nu} = 1$. In order to be consistent with the continuum limit of the lattice CPA one may take always this value. On the other hand, one can also use this value such that the CPA percolation threshold $p_c^{\text{CPA}} = \widetilde{\nu}/3$ (see below) agrees to the continuum percolation threshold p_c of a certain topology.[28,29]

2. Self-consistent Born approximation, SCBA

If one takes Gaussian disorder for the local diffusivity one can perform the disorder average over the generating functional (17) exactly, which leads to an interacting effective field theory with the variance of $D(\mathbf{r})$ as coupling constant. Taking apart this interaction by a Hubbard-Stratonovich approximation and then performing a saddle-point approximation [assuming a small relative variance of $D(\mathbf{r})$] one arrives at the *self-consistent Born approximation* for the scalar problem.[60–62] We can, however, recover the SCBA from the CPA in the following way. Defining D_0 to be the average of the fluctuating diffusivities and defining the quantities $Q(s) = D_0 - \Sigma(s)$, $D_i = D_0 - \Delta_i$, we obtain from (35a) the two (equivalent) CPA equations:

$$0 = \left\langle \frac{\Delta_i - \Sigma(s)}{1 - \frac{\widetilde{\nu}}{3}(\Delta_i - \Sigma(s))\widetilde{\Lambda}(s)} \right\rangle_i, \tag{42a}$$

$$\Sigma(s) = \left\langle \frac{\Delta_i}{1 - \frac{\widetilde{\nu}}{3}(\Delta_i - \Sigma(s))\widetilde{\Lambda}(s)} \right\rangle_i. \tag{42b}$$

We now expand the interior of the average in (42b) with respect to $\Delta_i - \Sigma(s)$ to lowest nonvanishing order (respecting $\langle \Delta_i \rangle = 0$) we obtain

$$\Sigma(s) = \langle D_i^2 \rangle \frac{\widetilde{\nu}}{3}\widetilde{\Lambda}(s), \tag{43}$$

which is the SCBA for the scalar problem. As indicated already above, the SCBA can also be obtained from the saddle-point equation (29) by putting the exponential not into the denominator but into the numerator and then expand with respect to the small number V_c/V to first order. Because then only the first two cumulants of the distribution of the D_i enter, this corresponds to assuming Gaussian disorder.

So we recover the SCBA from the CPA in the Gaussian and weak-disorder limit.

3. Network effective-medium approximation, EMA

The CPA-like effective-medium treatment of the impedances of a heterogeneous medium or network date back to Bruggeman[63] and Landauer.[64] For a disordered Z-fold coordinated network of fluctuating conductances g_i the expression for the effective-medium conductance g_m is[65]

$$0 = \left\langle \frac{g_m - g_i}{g_i + \left(\frac{Z}{2} - 1\right)g_m} \right\rangle. \tag{44}$$

It has been generalized for the ac problem,[52,66] setting $Z/2 = d$,

$$0 = \left\langle \frac{g_m(s) - g_i}{g_i + (d-1)g_m(s) + ds} \right\rangle, \tag{45}$$

which can be rearranged as

$$0 = \left\langle \frac{g - g_m(s)}{1 + [g - g_m(s)]\frac{1}{d}\frac{1}{g_m(s)+s}} \right\rangle, \tag{46}$$

which has—for $d = 3$—the same form as the CPA equation (35a) with

$$\widetilde{\Lambda}(s)_{\mathrm{EMA}} = \frac{1}{s + Q(s)}. \tag{47}$$

This EMA has the same analytical structure as EMA versions derived earlier in the literature.[27–29] While these *ac* effective-medium theories describe rather nicely measured hopping conductivity data they violate the nonanalyticity requirement (12). As stated above, in CPA the function $\widetilde{\Lambda}(s)$ has a contribution, which varies as $s^{3/2}$, whereas $\widetilde{\Lambda}(s)_{\mathrm{EMA}}$ does not, as can be clearly seen from Eq. (47).

D. CPA results for the *dc* diffusivity

1. Percolation

In order to treat the percolation problem, which can be considered as the continuum version of the Lorentz problem,[31,48,67,68] we assume a distribution of local diffusivities of the form,

$$P(D_i) = p\delta(D_i - D_0) + (1 - p)\delta(D_i), \tag{48}$$

where p is the volume fraction in which the diffusivity is nonzero. Inserting this into Eq. (36a) one obtains

$$Q(0)\frac{\widetilde{\nu}}{3} = Q(0)\frac{1}{1 + \left(\frac{3}{\widetilde{\nu}} - 1\right)\frac{Q(0)}{D_0}}, \tag{49}$$

which has, like Eq. (36a), always the trivial solution $Q(0) = 0$. For the case $Q(0) \neq 0$ we obtain from Eq. (49),

$$Q(0) = \tfrac{2}{3}D_0(p - p_c)/(1 - p_c), \tag{50}$$

with $p_c = \frac{\widetilde{\nu}}{3}$. For $p < p_c$ the trivial solution of (49), $Q(0) = 0$ takes over.

2. Activated diffusion

In this class of models the diffusion of a particle is considered to take place by jumps over barriers of height E_i with a certain distribution $P(\epsilon)$ ("random barrier model").[52] So we write

$$D_i = D_0 e^{-E_i/k_B T}, \tag{51}$$

and parametrize the dc diffusivity as $(\frac{3}{\widetilde{\nu}} - 1)Q(0) = D_0 e^{-E_a/k_B T}$. Then Eq. (36b) takes the form,

$$\frac{\widetilde{\nu}}{3} = \int dE\, P(E)\frac{1}{e^{(E-E_a)/k_B T} + 1}. \tag{52}$$

In the low-temperature limit the Fermi function becomes a step function and we obtain

$$\frac{\widetilde{\nu}}{3} = p_c = \int_0^{E_a} dE\, P(E), \tag{53}$$

which means that the parameter E_a becomes temperature independent. From this follows that in the random-barrier problem the dc diffusivity is *always* of Arrhenius form, as observed frequently in fast-ion conducting glasses.[69]

It is worthwhile to point out that (53) corresponds to the so-called percolation construction for obtaining the dc conductivity of a disordered hopping-conduction network.[47,52] It has been nicely demonstrated recently that the low-temperature physics of the random-barrier model is essentially percolation physics.[70]

3. Variable-range hopping

A rather widely investigated type of carrier diffusion in disordered materials is that of electrons performing phonon-assisted tunneling transitions between localized states ("hopping transport").[47] Understanding the mechanisms of electronic hopping transport has been shown recently to be of extreme importance for devising organic light-emitting diodes (OLEDs).[71] Here we show that by the CPA one recovers the classical results of Mott[72] and Efros, Shklovskiĭ[47] for variable-range hopping.

The local diffusivity depends on an activation barrier E and a characteristic hopping distance r with distributions $P(E)$ and $P(r)$,

$$D_i = D_0 e^{-\alpha r - \beta E}, \tag{54}$$

where $e^{-\alpha r}$ is the tunneling factor and $\beta = 1/k_B T$. Depending on the density of localized electronic states near the Fermi energy $P(E)$ is either considered to be constant (Mott hopping) or proportional to E^2 (Coulomb-gap, Efros-Shklovski hopping). The distribution of sites is

$$P(r) = \frac{1}{Z}4\pi\rho r^2\theta(R - r) = \frac{3}{R^3}r^2\theta(R - r), \tag{55}$$

where $Z = \frac{4}{3}4\pi\rho R^3$ is the number of adjacent sites within a given radius R. If we parametrize the dc diffusivity as $(\frac{1}{p_c} - 1)Q(0) = D_0 e^{-\xi}$, we obtain from Eq. (36b)

$$p_c = \int dE\, P(E) \int dr\, P(r)\frac{1}{e^{\alpha r + \beta E - \xi} + 1}. \tag{56}$$

In the low-temperature limit the Fermi function becomes again a step function, and, by means of integrations by part one obtains the famous results $\ln Q(0) \propto -(T_0/T)^{1/4}$ for $P(E) =$ const (Mott hopping); $\ln Q(0) \propto -(T_0/T)^{1/2}$ for $P(E) \propto E^2$ (Efros-Sklovskii hopping). Again, these results are equivalent to the percolation construction.[47]

E. CPA results for the ac diffusivity

We consider activated transport of the form (51) with a constant barrier distribution,

$$P(E) = \frac{1}{E^*}, \quad 0 \leqslant E \leqslant E^*, \tag{57}$$

which is equivalent to an inverse-Power distribution for D,

$$P(D) = \frac{1}{\ln \mu/\sigma}\frac{1}{D}, \quad \mu \leqslant D \leqslant \sigma, \tag{58}$$

with $\sigma = D_0$ and $\mu = D_0 e^{-\beta E^*}$.

In Fig. 1 we show ac conductivity data collected from the literature over a very wide range of frequencies by Wong and Angell[73] together with the CPA prediction for the constant-barrier model (57). The only input is the measured dc activation energy of $E_a = 75$ KJ/mole.[74] However, it

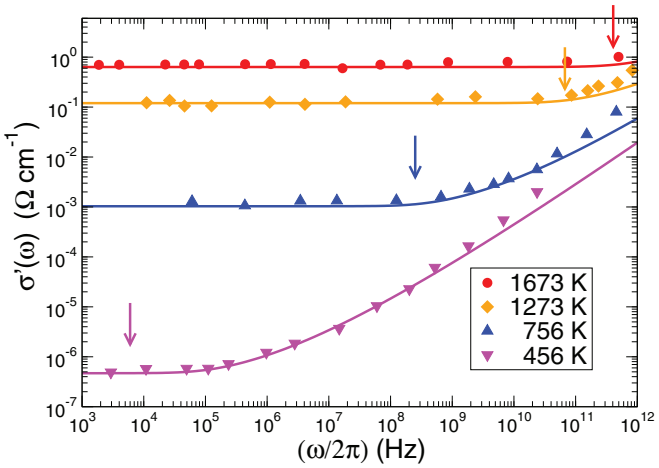

FIG. 1. (Color online) Comparison of ionic ac conductivity data of sodium trisilicate glass[73] with the CPA prediction for activated hopping with a constant-barrier distribution. We use units in which $D_0 = k_\xi = 1$. The arrows indicate the boson-peak positions $\omega_{\rm BP} \equiv \tilde{\omega}^2_{\rm BP}$ of Fig. 3.

should be made clear that the old EMA theories[27–29,75,76] are also able to produce such a fit. The difference to the CPA can be seen from the "loss function"[50,77] $[\sigma(\omega) - \sigma(0)]/\omega \propto [Q'(\omega) - 1]/\omega$, which is shown in Fig. 2. At low frequencies this function behaves as $\omega^{1/2}$ for $\omega \to 0$ due to the Rayleigh-type nonanalyticity. The old EMA theories do not exhibit this nonanalyticity. In the figure this behavior is demonstrated. There is experimental[77] and simulational[78] evidence for the presence of this low-frequency nonanalyticity of hopping transport.

F. Model calculations for the scalar phonon problem

We shall now exploit the mathematical correspondence $i\omega \leftrightarrow -\tilde{\omega}^2$, $Q(s) \equiv D(s) \leftrightarrow Q(\tilde{s}) \equiv K(\tilde{s})$ and, correspondingly, discuss the vibrational anomalies induced by the quenched disorder, as given in CPA. Similar discussions have already been published in the literature,[53] where it was pointed

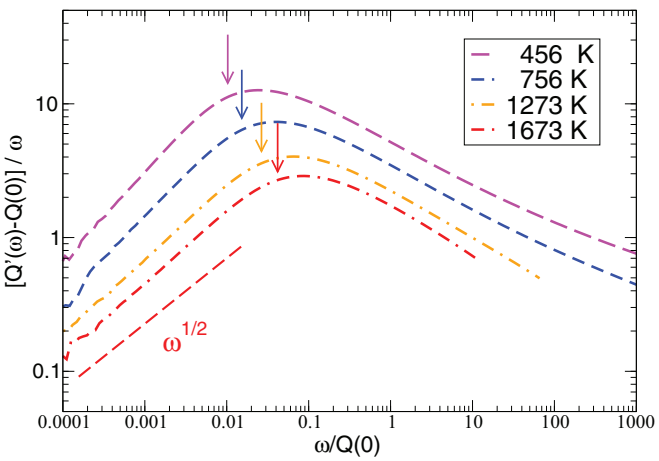

FIG. 2. (Color online) Loss function $[Q'(\omega) - Q(0)]/\omega \propto [\sigma(\omega) - \sigma(0)]/\omega$ calculated from the CPA curves in Fig. 1. Below the dc-ac crossover the Rayleigh-type nonanalyticity is visible.

TABLE I. Probability distributions used to model the disorder.

Name	P(K)
Uniform	$(\sigma - \mu)^{-1}$, $K \in [\mu,\sigma]$
Truncated Gaussian	$\sqrt{\frac{2}{\pi\sigma}} \frac{\exp[-(K-\mu)^2/(2\sigma)]}{1+\mathrm{Erf}(\mu/\sqrt{2\sigma})}$
Power law	$(K \ln[\frac{\sigma}{\mu}])^{-1}$, $K \in [\mu,\sigma]$
Log-normal	$\frac{1}{\sqrt{2\pi\sigma}} \frac{1}{K} e^{-\ln[\frac{K}{\mu}]^2/(2\sigma)}$

out that the boson peak (BP) in the vibrational problem corresponds to the dc-ac crossover in the diffusion problem.

As shown in the last subsection, the activated-diffusion model with a constant barrier distribution corresponds to an inverse-power-law distribution for the local diffusivities. For the corresponding local moduli K we rewrite this distribution:

$$P(K) = \frac{1}{\ln \mu/\sigma} \frac{1}{K}, \quad \mu \leqslant K \leqslant \sigma. \tag{59}$$

Other possible distributions, namely a uniform distribution, a Gaussian distribution, truncated at $K = 0$ and a log-normal distribution are detailed in Table I. The density of states (DOS) of the scalar phonons can be calculated as

$$g(\omega) = \frac{2\omega}{\pi} \mathrm{Im}\{G(\tilde{s})\}, \tag{60}$$

where $G(\tilde{s})$ is given by Eq. (35c), and we identify the correlation cutoff k_ξ with the Debye cutoff k_D.

As mentioned above, the CPA makes it possible to describe highly disordered systems, i.e., systems in which the variance of the spatial fluctuations of the quantity of interest exceeds the square of its average. In order to quantify the strength of the disorder, we define a disorder parameter as the ratio between the variance and the squared mean of the disorder distribution $\gamma = \langle K^2 \rangle / \langle K \rangle^2$. For the truncated Gaussian and the uniform distribution γ has an upper bound. For the uniform distribution a maximum disorder strength of $\gamma = \frac{1}{3}$ can be reached; for the truncated Gaussian this limit is $\gamma = \frac{\pi}{2} - 1$. Thus two of the four distributions can only model medium to weak disorder. On the other hand, the inverse-power and log-normal distributions have no upper bound of the disorder parameter. In particular, for the inverse-power distribution with $\mu = \sigma e^{-\beta E^*}$ the relation $\gamma = \beta E^*/2$ holds.

In Fig. 3 we show the so-called reduced DOS $g(\tilde{\omega})/g_D(\tilde{\omega})$, calculated for the inverse-power-law distribution. We use units, in which $k_\xi = k_D = 1$ and $K_0 = 1$. $g_D(\omega) = 3\omega^2/\omega_D^3$ is the Debye DOS, and $\omega_D = \sqrt{Q(0)}$ is the Debye frequency.

The disorder parameters $\gamma = \beta E^*/2$ have been chosen to agree to those in the conductivity calculations of Fig. 1. The boson peaks shown in Fig. 3 increase with increasing disorder, while its position decreases. The positions $\tilde{\omega}_{\rm BP}$ of the boson peaks are indicated in Figs. 1 and 2 via the correspondence $\omega_{\rm BP} \leftrightarrow \tilde{\omega}^2_{\rm BP}$. It is clearly seen that the boson peak marks the onset of the disorder-induced frequency dependence of the diffusivity (≡conductivity). Via the correspondence $D(\omega) \leftrightarrow K(\tilde{\omega}) = v(\tilde{\omega})^2$ this means that the boson peak marks the beginning of the frequency dependence of the sound velocity in the disordered vibration model. This is in agreement with earlier conclusions from effective-medium calculations using the EMA[53,54] and the SCBA.[40–45]

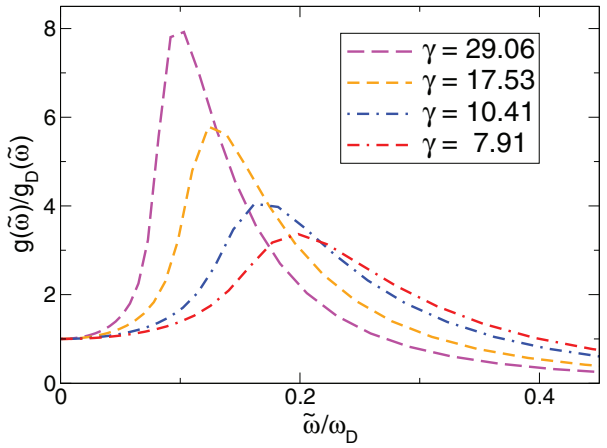

FIG. 3. (Color online) Reduced density of states $g(\tilde{\omega})/g_D(\tilde{\omega})$ for inverse-power-law disorder with the same disorder parameters as in Figs. 1 and 2. As the disorder increases so does the height of the boson peak; it is also shifted to lower frequencies.

In Fig. 4 the boson-peak height is plotted against its frequency position for all four distributions considered. We include also the prediction of the self-consistent Born approximation (SCBA). Figure 5 shows a closeup of the small-disorder region.

The down-shift and reinforcement of the boson peak with increasing disorder has been shown in the SCBA-based earlier treatments of vibrational anomalies[45] to result from the disorder-induced level repulsion, which is present in the anomalous frequency regime above the boson peak. This level repulsion, which is typical for random-matrix spectra, results from the absence of symmetries on the microscopic scale.

From our CPA calculations, displayed in Fig. 4 it follows that the height of the BP scales with its frequency position $\omega_{\rm BP}$ as $\frac{g(\omega_{\rm BP})}{g_D(\omega_{\rm BP})} \propto (\omega_{\rm BP})^c$ with $c = 1.25$. It is suggestive that this scaling should be related to the power-law frequency dependence of the diffusivity in the mathematically equivalent diffusion problem, but we did not find a way to prove this.

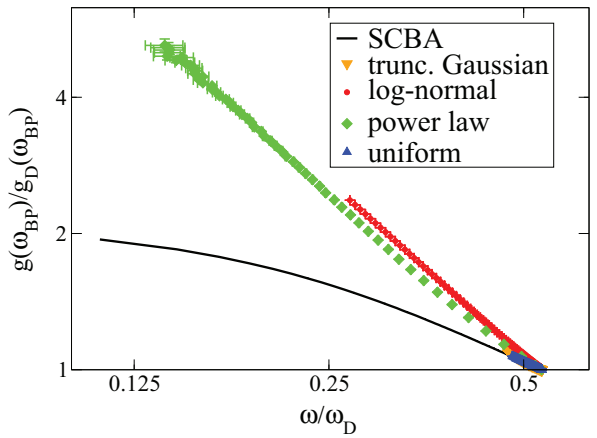

FIG. 4. (Color online) Relation between boson peak height and position for the CPA solutions of different distributions and disorder strength for $k_\xi = k_D$.

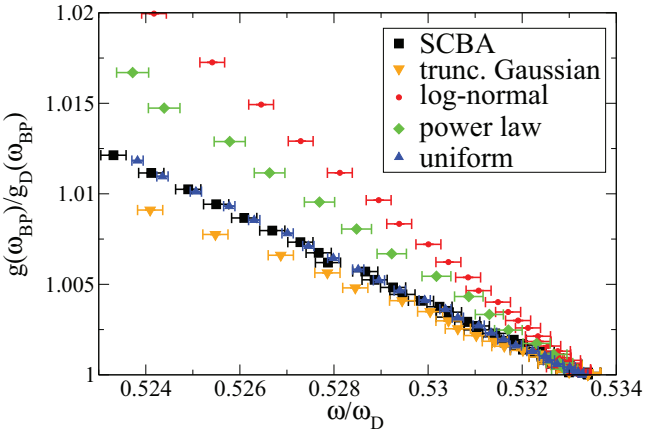

FIG. 5. (Color online) Closeup of the low disorder region of Fig. 4. Note that in the low-disorder limit $\omega_{\rm BP} \to 0.5333$, independently of of the chosen disorder distribution.

III. CPA FOR HETEROGENEOUS-ELASTICITY THEORY

A. Model

We start with the equations of motion of elasticity theory in frequency space, formulated in terms of the stress tensor $\sigma_{ij} = \rho\tilde{\sigma}_{ij}$ (ρ is the mass density):[79]

$$-\omega^2 u_i(\mathbf{r},\omega) - \sum_j \partial_j \tilde{\sigma}_{ij}(\mathbf{r},\omega) \equiv \sum_j A_{ij} u_j(\mathbf{r},\omega), \qquad (61)$$

where $u_i(\mathbf{r},\omega)$ are the Cartesian components of the displacement field. We consider an elastic medium in which the elastic shear modulus may fluctuate in space. If the system is assumed to be still isotropic, the stress tensor can be represented in two ways:

$$\tilde{\sigma}_{ij} = \frac{1}{\rho}\sigma_{ij} = \tilde{\lambda}\delta_{ij}\mathrm{tr}\{\epsilon\} + 2\tilde{G}(\mathbf{r})\epsilon_{ij} \qquad (62a)$$

$$= \frac{1}{\rho}\sigma_{ij} = \tilde{K}\delta_{ij}\mathrm{tr}\{\epsilon\} + 2\tilde{G}(\mathbf{r})\widehat{\epsilon}_{ij}. \qquad (62b)$$

Here $\lambda = \rho\tilde{\lambda} = K + \frac{2}{3}G$ is the longitudinal Lamé modulus, $K = \rho\tilde{K}$ is the bulk modulus, and $G = \rho\tilde{G}$ the shear modulus. ϵ_{ij} is the strain tensor ($\partial_j \equiv \partial/\partial x_j$):

$$\epsilon_{ij} = 1/2(\partial_i u_j + \partial_j u_i), \qquad (63)$$

and $\widehat{\epsilon}_{ij}$ the traceless strain tensor,

$$\widehat{\epsilon}_{ij} = \epsilon_{ij} - \tfrac{1}{3}\delta_{ij}\mathrm{tr}\{\epsilon\}, \qquad (64)$$

($\partial_j \equiv \partial/\partial x_j$). The spatial fluctuations of the shear modulus can be modeled in two ways: In what we call Model I[40,41] the longitudinal Lamé modulus λ is assumed to be constant [referring to the representation (62a)], in Model II[42,43] the K modulus [referring to the representation (62b)] is assumed to be constant. As can be shown easily, in model I the macroscopic longitudinal Lamé modulus is frequency independent; in model II the macroscopic bulk modulus is frequency independent.[40,42,43]

B. Derivation of the CPA for heterogeneous elasticity

For model I the matrix A_{ij} takes the explicit form,

$$A_{ij} = -\omega^2\delta_{ij} - \tilde{\lambda}\partial_i\partial_j - \left(\partial_j\tilde{G}(\mathbf{r})\partial_i + \delta_{ij}\sum_\ell \partial_\ell\tilde{G}(\mathbf{r})\partial_\ell\right), \tag{65}$$

for model II we have

$$A_{ij} = -\omega^2\delta_{ij} - \tilde{K}\partial_i\partial_j + \frac{2}{3}\partial_i G(\mathbf{r})\partial_j - \left(\partial_j\tilde{G}(\mathbf{r})\partial_i + \delta_{ij}\sum_\ell \partial_\ell\tilde{G}(\mathbf{r})\partial_\ell\right). \tag{66}$$

The Green matrix $G = A^{-1}$ is represented as

$$\mathsf{G}(\mathbf{r},\mathbf{r}')_{ij} = \prod_{\alpha=1}^{n}\int \mathcal{D}\left[\bar{u}^\alpha_\ell(\mathbf{r}),u^\alpha_m(\mathbf{r})\right]\bar{u}^1_i(\mathbf{r})u^1_j(\mathbf{r}')e^{-\sum_\alpha\langle u^\alpha_\ell|\mathcal{A}|u^\alpha_m\rangle} \tag{67}$$

$$= \frac{\delta}{\delta J^{(1)}_{ij}(\mathbf{r},\mathbf{r}')}\mathcal{Z}[J(\mathbf{r},\mathbf{r}')], \tag{68}$$

with the generating functional,

$$\mathcal{Z}[J(\mathbf{r},\mathbf{r}')] = \prod_{\alpha=1}^{n}\int \mathcal{D}\left[\bar{u}^\alpha_\ell(\mathbf{r})u^\alpha_m(\mathbf{r})\right]e^{-\sum_\alpha\langle u^\alpha_\ell|\mathcal{A}|u^\alpha_m\rangle}, \times e^{-\sum_\alpha\langle u^\alpha_\ell|J^\alpha_{\ell m}|u^\alpha_m\rangle}, \tag{69}$$

and the source-field matrix J^α. By an integration by part one arrives at the following representation of the action:

$$\sum_{ij}\langle u^\alpha_i|\mathcal{A}[G]|u^\alpha_j\rangle = \int d^3\mathbf{r}\left(\tilde{s}\sum_i|u^\alpha_i(\mathbf{r})|^2 + \frac{1}{2}\tilde{K}\,\mathrm{tr}\{\epsilon^\alpha(\mathbf{r})\}^2 + G(\mathbf{r})\sum_{ij}|\widehat{\epsilon}^\alpha_{ij}(\mathbf{r})|^2\right). \tag{70}$$

Applying again the Fadeev-Popov procedure and performing all the steps we have done before, we arrive at an effective action, which looks similar to that of the diffusion problem (25):

$$S_{\mathrm{eff}}[Q,\Lambda,\tilde{J}] = \mathrm{Tr}\{\ln(\mathcal{A}[Q]-\tilde{J})\} - \sum_{\alpha=1}^{n}\frac{V}{V_c}\ln\left(\left\langle e^{-\frac{V_c}{V}\Lambda^{(\alpha)}_i(D^{(\alpha)}_i-Q^{(\alpha)}_i)}\right\rangle_i\right). \tag{71}$$

But now the trace operation goes also over the Cartesian indices.

The homogeneous matrix $A_{\mathrm{eff}}[Q]$ is both diagonal in the Cartesian indices and with respect to the $\mathbf{k}$ vectors. The diagonal elements are $1/G_L(\mathbf{k},\tilde{s})$ and twice $1/G_T(\mathbf{k},\tilde{s})$, which are given by

$$1/G_L(\mathbf{k},\tilde{s}) = \tilde{s} + k^2[\tilde{\lambda}+2Q(\tilde{s})] \quad \text{Model I}, \tag{72a}$$

$$1/G_L(\mathbf{k},\tilde{s}) = \tilde{s} + k^2\left[\tilde{K}+\tfrac{4}{3}Q(\tilde{s})\right] \quad \text{Model II}, \tag{72b}$$

$$1/G_T(\mathbf{k},\tilde{s}) = \tilde{s} + k^2 Q(\tilde{s}). \tag{72c}$$

The saddle-point equations, followed by the expansion of the exponential in the denominator leads to the CPA equations,

$$0 = \left\langle\frac{G_i - Q(\tilde{s})}{1+\frac{\tilde{\nu}}{3}(G_i-Q(\tilde{s}))\Lambda(\tilde{s})}\right\rangle_i. \tag{73a}$$

The susceptibility functions for the models $\alpha = I, II$ take the form,

$$\Lambda_\alpha(\tilde{s}) = \frac{3}{k^3_\xi}\int_0^{k_\xi} dk k^4(q_\alpha G_L(k,\tilde{s}) + 2G_T(k,\tilde{s})), \tag{73b}$$

with $q_I = 2$ and $q_{II} = 4/3$. The density of states is calculated from the well-known formula,

$$g(\omega) = \mathrm{Im}\left\{\frac{2\omega}{3\pi}(G_L(\tilde{s}) + 2G_T(\tilde{s}))\right\}, \tag{74}$$

where we have introduced the local longitudinal and transverse functions (identifying again ξ with k_D),

$$G_{L,T}(\tilde{s}) = \frac{3}{k^3_D}\int_0^{k_D} dk G_{L,T}(k,\tilde{s}). \tag{75}$$

We can write the susceptibility function $\Lambda_\alpha(\tilde{s})$ as follows:

$$\Lambda_\alpha(\tilde{s}) = \frac{1-\tilde{s}G_T(\tilde{s})}{Q(\tilde{s})} + q_\alpha\frac{1-\tilde{s}G_L(\tilde{s})}{p_\alpha + q_\alpha Q(\tilde{s})} = \widetilde{\Lambda}(\tilde{s})\left(1+\frac{q_\alpha Q(\tilde{s})}{p_\alpha+q_\alpha Q(\tilde{s})}\frac{1-\tilde{s}G_L(\tilde{s})}{1-sG_T(\tilde{s}}\right), \tag{76}$$

with $p_I = \tilde{\lambda}$ and $p_{II} = \tilde{K}$. $\widetilde{\Lambda}(\tilde{s})$, which is the transverse local susceptibility, is the same mathematical function of Q as the susceptibility function of Eq. (35b) for the scalar phonon problem. Because the function inside the big brackets is only weakly frequency dependent and the density of states is dominated by the transverse Green's function all the results derived and presented for the scalar phonon problem hold also for the vector phonon problem.

In particular, for non-Gaussian distributions of the shear modulus the quantity $g(\omega)/g_D(\omega)$ can have boson peaks with arbitrary heights, and a scaling as depicted in Fig. 4 holds.[80] As an example we show in Fig. 6 the reduced density of states,

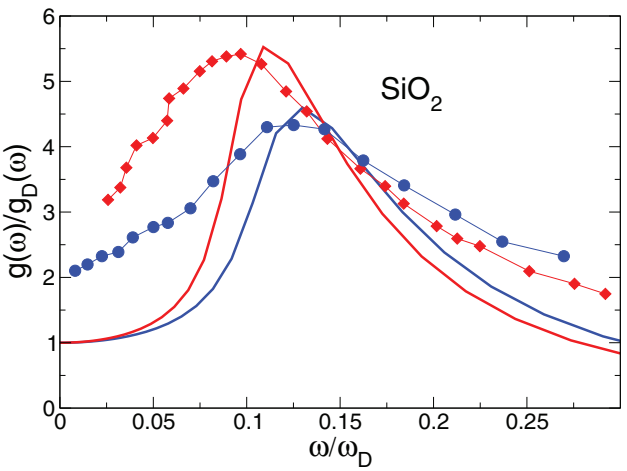

FIG. 6. (Color online) Boson peak data for SiO_2[81] compared with the reduced DOS for the inverse-power model with two different lower cutoffs μ.

extracted from inelastic x-ray measurements by Baldi *et al.*[81] together with the corresponding quantity calculated for the inverse-power distribution $P(G)$ given by Eq. (59).

The important difference between the scalar model and the vector theory (heterogeneous elasticity theory) is that it describes the physically relevant vector displacements, in which dilatational and shear degrees of freedom can be distinguished. Model II represents a theory, in which the disorder-induced anomalous frequency dependence is dominated by the dilatation-free shear degrees of freedom in agreement with recent computer simulations.[42,43,82,83]

IV. CONCLUSIONS

We have derived a version of the coherent-potential approximation for both diffusional and vibrational motion in a quenched-disordered environment, which is suitable for topologically disordered materials. The effective medium is not a crystalline lattice but a homogeneous and isotropic system with frequency-dependent diffusivity or elastic constants, respectively. The results can be directly applied to experimentally measured spectra. In the weak-disorder limit the CPA reduces to the self-consistent Born approximation, which is based on Gaussian disorder. In the strong-disorder limit, in which the local diffusivities or elastic quantities vary exponentially, the CPA describes correctly the percolative aspects of such systems. It has been demonstrated that the disorder-induced vibrational anomalies become stronger as the disorder is increased. In particular the height of the boson peak has been shown to increase indefinitely with the disorder.

In contrast to some earlier effective-medium theories for the heterogeneous diffusion and wave propagation problem the present theory includes the correct low-frequency nonanalyticity, which leads to a long-time tail of the velocity autocorrelation function of the diffusion problem and to Rayleigh scattering in the vibrational problem.

The present version of the CPA does not treat correlated spatial disorder. How to include correlations into the CPA has been shown by Zimmermann and Schindler.[39] It is straightforward to modify the present theory along the lines of Ref. 39. The inclusion of correlations will modify the shape of the calculated spectra but not the general conclusions for the influence of quenched disorder on these spectra.

ACKNOWLEDGMENT

S.K. and W.S. are grateful to Friederike Schmid for helpful discussions.

APPENDIX: ELECTRONS IN A RANDOM POTENTIAL

The method developed above for the diffusion and scalar phonon problem can, with slight modifications, be applied to the problem of an electron gas in a random potential. This model is governed by the Schrödinger equation:

$$\int d^3x\, \Psi^\dagger(\boldsymbol{x})\left(\frac{\hbar^2}{2m}\Delta - V(\boldsymbol{x}) - \widetilde{E}\right)\Psi(\boldsymbol{x})|\varphi\rangle = \mathbb{A}|\varphi\rangle = 0,$$
$$\widetilde{E} = \frac{E + i\varepsilon}{N}. \tag{A1}$$

The corresponding Green's function can then be expressed with a coherent-state path integral over the Grassmann fields θ and $\bar{\theta}$:

$$G(\boldsymbol{x},\boldsymbol{x}',\widetilde{E}) = \frac{1}{\zeta[0]}\frac{\delta\zeta[J]}{\delta J(\boldsymbol{x}',\boldsymbol{x})}\bigg|_{J=0}, \tag{A2}$$
$$\zeta[J] = \int \mathcal{D}[\theta,\bar{\theta}]\, e^{\langle\theta|A+J|\theta\rangle}. \tag{A3}$$

From here on all steps are analogous to the previous section. First the replica trick is performed and a coarse-grained potential,

$$V(\boldsymbol{x}) = \sum_i v_i\,\chi_i(\boldsymbol{x}), \tag{A4}$$

with no correlation between the coarse-graining boxes is introduced. $V(x)$ is subsequently replaced in A via the Fadeev-Popov procedure by an auxiliary field Q yielding

$$\langle\zeta^n[J]\rangle = \int \mathcal{D}[Q,\Lambda]\, e^{-nS_{\text{eff}}[Q,\Lambda,J]}, \tag{A5}$$

with the effective action,

$$S_{\text{eff}}[Q,\Lambda,J] = -\text{tr}\ln(A+J) - \sum_i \ln\langle e^{V_c/V\Lambda_i(v_i-Q_i)}\rangle_i. \tag{A6}$$

As described in the body of the paper, the CPA equations determine the saddle point of (A5). The saddle-point equations read

$$\Lambda' = -\frac{V_c}{V\widetilde{\nu}}\sum_{\boldsymbol{k}}\frac{1}{\widetilde{E} - \frac{\hbar^2}{2m}k^2 - Q}, \tag{A7a}$$
$$Q = \left\langle\frac{v}{1+\widetilde{\nu}(v-Q)\Lambda'}\right\rangle. \tag{A7b}$$

The k-space summation can now be evaluated and the CPA equations solved. From these results the calculation of the density of states can be done.

The effective-medium operator that is defined by Eq. (A7) is

$$A_{\text{eff}}(\boldsymbol{k},\boldsymbol{k}',z) = \left(z - \frac{\hbar^2k^2}{2m} - Q\right)\delta_{\boldsymbol{k}\boldsymbol{k}'}. \tag{A8}$$

This result has already been obtained in an independent discussion of the CPA for electrons in a random potential[39] and can be interpreted as the continuum version of the classical lattice theories, e.g.[4]

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