

# Mean-field theories for the description of waves in disordered materials

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## 1 Preliminaries: Wave equations without disorder

### 1.1 Scalar waves

#### A Electrons

A single electron in the presence of an external potential  $V(\mathbf{r})$  obeys Schrödinger's wave equation

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \mathcal{H} \psi(\mathbf{r}, t) \quad (1.1)$$

with the Hamilton operator

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 - v(\mathbf{r}) \quad (1.2)$$

Going into frequency space  $\hbar\omega = E$  we obtain the stationary Schrödinger equation

$$E\psi(\mathbf{r}, E) = \mathcal{H}\psi(\mathbf{r}, E) = \left( -\frac{\hbar^2}{2m}\nabla^2 - v(\mathbf{r}) \right)\psi(\mathbf{r}, E) \quad (1.3)$$

where  $k_F = \frac{m}{\hbar}v_F$  is the Fermi wavenumber and  $v_F$  the Fermi velocity.

## B Scalar classical waves

In liquids and air the pressure deviations  $u(\mathbf{r}, t) = p(\mathbf{r}, t) - p_0$  obey the equation of motion

$$\frac{\partial^2}{\partial t^2}u(\mathbf{r}, t) = v^2\nabla^2u(\mathbf{r}, t) \quad (1.4)$$

In the frequency domain (Fourier transform of  $\mathbf{u}(\mathbf{r}, t)$ ) we obtain

$$-\omega^2u(\mathbf{r}, \omega) = v^2\nabla^2u(\mathbf{r}, \omega) \quad (1.5)$$

Eq. (1.5) is also called Helmholtz equation

## C Diffusion equation

If particles in a liquid or solid are able to move randomly due to the thermal excitations by which they are pushed, any imbalance of the particle's concentration  $\rho(\mathbf{r}, t)$  will cause a current  $\mathbf{j}(\mathbf{r}, t)$  in the direction of the negative concentration gradient. This is Fick's law and is expressed mathematically

$$\mathbf{j}(\mathbf{r}, t) = -D\nabla\rho(\mathbf{r}, t) \quad (1.6)$$

On the other hand particle number conservation leads to the continuity equation

$$\frac{\partial}{\partial t}\rho(\mathbf{r}, t) = -\nabla \cdot \mathbf{j}(\mathbf{r}, t) \quad (1.7)$$

If we combine Eqs. (1.6) and (1.7) we obtain the diffusion equation

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) = D \nabla^2 \rho(\mathbf{r}, t) \quad (1.8)$$

which, in the frequency domain reads

$$-i\omega \rho(\mathbf{r}, t) = D \nabla^2 \rho(\mathbf{r}, t) \quad (1.9)$$

If we compare this with the scalar wave equation (1.5), we see, that the “only” difference between the two is that  $-\omega^2$  is replaced by  $-i\omega$ . This mathematical correspondence between wave motion and diffusive motion will be exploited throughout these lectures.

## 1.2 Vector waves

### A Elastic medium

In an isotropic and homogeneous elastic medium the displacement vectors of the medium obey the equation of motion

$$\rho \ddot{\mathbf{u}}(\mathbf{r}) = (\lambda + 2G) \nabla \nabla \cdot \mathbf{u}(\mathbf{r}, t) - G \nabla \times \nabla \times \mathbf{u}(\mathbf{r}, t) \quad (1.10)$$

where  $G$  is the shear modulus,  $\lambda = K - \frac{2}{3}G$  is the Lamé modulus and  $K$  is the bulk modulus.

We split  $\mathbf{u}(\mathbf{r}, t)$  into a longitudinal and transverse part

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{u}_L(\mathbf{r}, t) + \mathbf{u}_T(\mathbf{r}, t) \quad \nabla \times \mathbf{u}_L = 0 \quad \nabla \cdot \mathbf{u}_T = 0 \quad (1.11)$$

If we use the vector analysis identity

$$\nabla \times \nabla \times \mathbf{A} = -\nabla^2 \mathbf{A} + \nabla(\nabla \cdot \mathbf{A}) \quad (1.12)$$

we obtain the following decoupled wave equations

$$\ddot{\mathbf{u}}_{L,T}(\mathbf{r}, t) = v_{L,T}^2 \nabla^2 \mathbf{u}_{L,T}(\mathbf{r}, t) \quad (1.13)$$

and in frequency space

$$-\omega^2 \mathbf{u}_{L,T}(\mathbf{r}, \omega) = v_{L,T}^2 \nabla^2 \mathbf{u}_{L,T}(\mathbf{r}, \omega) \quad (1.14)$$

with the longitudinal ( $L$ ) and transverse ( $T$ ) sound velocities

$$v_L^2 = \frac{1}{\rho}(\lambda + 2G) \equiv \frac{1}{\rho}M = \frac{1}{\rho}\left(K + \frac{4}{3}G\right) \quad v_T^2 = \frac{1}{\rho}G \quad (1.15)$$

$\lambda$  = longitudinal Lamé modulus

$K$  = bulk modulus

$G$  = shear modulus

$M$  = longitudinal modulus

## B Electromagnetic waves

Maxwell's equations in a homogeneous, isotropic medium are

$$\nabla \cdot \mathbf{B} = 0 \quad \nabla \cdot \mathbf{E} = 0$$

$$\nabla \times \mathbf{B}(\mathbf{r}, t) = \frac{\epsilon}{c^2} \frac{\partial}{\partial t} \mathbf{E}(\mathbf{r}, t)$$

$$\nabla \times \mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t} \mathbf{B}(\mathbf{r}, t)$$

For deriving a wave equation for the electromagnetic fields one can either solve for the electrical field  $\mathbf{E}(\mathbf{r}, t)$  for the magnetic field  $\mathbf{B}(\mathbf{r}, t)$ . In the first case one has to decompose the double curl of  $\mathbf{E}$ , whereas in the second case the double curl of  $\mathbf{B}$ :

$$\begin{aligned} \frac{\epsilon}{c_0^2} \frac{\partial^2}{\partial t^2} \mathbf{E}(\mathbf{r}, t) &= -\nabla \times \nabla \times \mathbf{E}(\mathbf{r}, t) \\ &= \nabla^2 \mathbf{E}(\mathbf{r}, t) - \nabla(\nabla \cdot \mathbf{E}(\mathbf{r}, t)) \\ \frac{\epsilon}{c_0^2} \frac{\partial^2}{\partial t^2} \mathbf{B}(\mathbf{r}, t) &= -\nabla \times \nabla \times \mathbf{B}(\mathbf{r}, t) \\ &= \nabla^2 \mathbf{B}(\mathbf{r}, t) - \nabla(\nabla \cdot \mathbf{B}(\mathbf{r}, t)) \end{aligned} \quad (1.16)$$

where we have assumed  $\nabla \cdot \mathbf{B} = 0$  and  $\nabla \cdot \mathbf{E} = 0$ . In the frequency domain we get

$$-\omega^2 \mathbf{E}(\mathbf{r}, \omega) = \frac{c_0^2}{\epsilon} \nabla^2 \mathbf{E}(\mathbf{r}, \omega) \quad -\omega^2 \mathbf{B}(\mathbf{r}, \omega) = \frac{c_0^2}{\epsilon} \nabla^2 \mathbf{B}(\mathbf{r}, \omega) \quad (1.17)$$

## 1.3 Green's functions

### A One-electron Green's function

The one-electron Green's function obeys the following inhomogeneous Schrödinger equation with a  $\delta$  function inhomogeneity:

$$\left(i\hbar\frac{\partial}{\partial t} - \mathcal{H} \mp i\epsilon\right)G_{\pm}(\mathbf{r}, \mathbf{r}', t, t') = -\delta(\mathbf{r} - \mathbf{r}')\delta(t - t') \quad (1.18)$$

The  $\delta$  function is defined by  $\delta(x) = 0, x \neq 0$   $\int_{-\infty}^{\infty} dx\delta(x) = 1$ .

$G_+$  is called *advanced* Green's function,  $G_-$  *retarded* Green's function,

We now assume that  $\mathcal{H}$  is stationary, so that we obtain the Eigenvalue problem

$$\mathcal{H}|\psi_n\rangle = E_n|\psi_n\rangle \quad (1.19)$$

and we have

$$\psi_n(\mathbf{r}, t) = e^{-\frac{i}{\hbar}E_n t} \underbrace{\psi_n(\mathbf{r})}_{\langle \mathbf{r} | \psi_n \rangle} \quad (1.20)$$

One can show that (3.47) is solved by

$$G_{\mp}(\mathbf{r}, \mathbf{r}', t, t') = \pm \frac{i}{\hbar} \sum_n \psi_n(\mathbf{r})\psi_n^*(\mathbf{r}')e^{-(i/\hbar)[E_n \pm i\epsilon](t-t')}\theta(\mp(t-t')) \quad (1.21)$$

Here  $\theta(x) = 1$  for  $x \geq 0$  and  $\theta(x) = 0$  for  $x < 0$  (step function).

As the Green's function depends only on the time difference  $\tau = t - t'$  we can perform a Fourier transform with respect to  $\tau$ :

$$G_{\pm}(\mathbf{r}, \mathbf{r}', \omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G_{\pm}(\mathbf{r}, \mathbf{r}', \tau) = \sum_n \frac{\psi_n(\mathbf{r})\psi_n^*(\mathbf{r}')}{\underbrace{-E \pm i\epsilon + E_n}_{z_{\pm}}} \quad (1.22)$$

with  $E = \hbar\omega$ .

We define now the *resolvent operator* (or "Green operator") as

$$\mathcal{G}(z) = [z1 + \mathcal{H}]^{-1} \equiv \frac{1}{z + \mathcal{H}} \quad (1.23)$$

from which we obtain



$$G_{\pm}(\mathbf{r}, \mathbf{r}', \omega) = \langle \mathbf{r} | \frac{1}{z_{\pm} + \mathcal{H}} | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathcal{G}(z_{\pm}) | \mathbf{r}' \rangle \quad (1.24)$$

One can, of course also consider matrix elements of  $\mathcal{G}(z)$  in an arbitrary basis  $|\alpha\rangle$

$$G_{\alpha\beta}(z) = \langle \alpha | \mathcal{G}(z) | \beta \rangle . \quad (1.25)$$

In particular we shall make use of the plane wave basis normalized with the sample volume  $V$  and periodic boundary conditions

$$\langle \mathbf{r} | \mathbf{k} \rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\mathbf{r}}; \quad \langle \mathbf{k} | \mathbf{r} \rangle = \frac{1}{\sqrt{V}} e^{-i\mathbf{k}\mathbf{r}} . \quad (1.26)$$

A sum over  $\mathbf{k}$  vectors is given by

$$\sum_{\mathbf{k}} \dots = \frac{V}{(2\pi)^3} \int d^3\mathbf{k} \dots$$

If the potential is equal to zero (which corresponds to the classical wave equation (1.5),  $\mathcal{H} \equiv \mathcal{H}_0$  is diagonal in the  $\mathbf{k}$  representation and we have

$$G_0(\mathbf{k}, \mathbf{k})(z) \equiv G_0(\mathbf{k}, z) = \frac{1}{z + \frac{\hbar^2}{2m} k^2} . \quad (1.27)$$

## B Relation with Laplace transform

The Laplace transform of a time-dependent function  $f(t)$  is defined by

$$f(s) \equiv \mathcal{L}\{f(t)\} = \int_0^{\infty} dt e^{-st} f(t) \quad (1.28)$$

where  $s$  is a complex number with  $\mathcal{R}e\{s\} > 0$ .

We now take a closer look at the Fourier transform of the retarded Green's function, which is proportional to  $\theta(\tau)$ :

$$\begin{aligned} G_-(\mathbf{r}, \mathbf{r}', \omega) &= \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} G_-(\mathbf{r}, \mathbf{r}', \tau) \\ &= \frac{i}{\hbar} \int_0^{\infty} d\tau e^{i\omega\tau} \sum_n \langle \mathbf{r}' | \psi_n \rangle e^{-(i\tau/\hbar)E_n} \langle \psi_n | \mathbf{r} \rangle e^{-(\epsilon/\hbar)\tau} \end{aligned}$$

$$= \int_0^{\infty} d\tau e^{i\omega\tau} e^{-(\epsilon/\hbar)\tau} \underbrace{\frac{i}{\hbar} \langle \mathbf{r}' | e^{-(i\tau/\hbar)\mathcal{H}} | \mathbf{r} \rangle}_{\tilde{G}(\mathbf{r}, \mathbf{r}', \tau)} \quad (1.29)$$

which identifies the retarded Green's function as the Laplace transform of the “correlation function”  $\tilde{G}(\mathbf{r}, \mathbf{r}', \tau)$  with Laplace parameter  $s = \epsilon/\hbar - i\omega$ .

### C Relation to the density of states

Let us consider the difference of the trace of the resolvent taken with  $z$  just above and below the real axis:

$$\begin{aligned} \text{tr}\{\mathcal{G}(z_-) - \mathcal{G}(z_+)\} &= \sum_n \left[ \frac{1}{E - i\epsilon - E_n} - \frac{1}{E + i\epsilon - E_n} \right] \\ &= 2i \mathcal{I}m \left\{ \text{tr}\{\mathcal{G}(z_-)\} \right\} = -2i \mathcal{I}m \left\{ \text{tr}\{\mathcal{G}(z_+)\} \right\} \\ &= \sum_n \frac{2i\epsilon}{(E - E_n)^2 + \epsilon^2} \xrightarrow{\epsilon \rightarrow 0} 2\pi i \sum_n \delta(E - E_n) \end{aligned}$$

In the limit  $\epsilon \rightarrow 0$  we obtain

$$g(E) = \frac{1}{n} N(E) = \frac{1}{\pi N} \mathcal{I}m \left\{ \text{tr}\{\mathcal{G}(z_-)\} \right\} = -\frac{1}{\pi N} \mathcal{I}m \left\{ \text{tr}\{\mathcal{G}(z_+)\} \right\} \quad (1.30)$$

### D Laplace transform and Green's function for classical waves

We want to solve the classical scalar wave equation

$$\frac{\partial^2}{\partial t^2} u(\mathbf{r}, t) = v^2 \nabla^2 u(\mathbf{r}, t) \quad (1.31)$$

with the help of Laplace transform. We first perform a spatial Fourier transform

$$u(\mathbf{k}, t) = \int_V d\mathbf{r} e^{i\mathbf{k}\mathbf{r}} u(\mathbf{r}, t) \quad (1.32)$$

The wave equation for this quantity reads

$$\frac{\partial^2}{\partial t^2} u(\mathbf{k}, t) = -v^2 k^2 u(\mathbf{k}, t) \quad (1.33)$$

The rules for Laplace-transforming a time derivative of a function are

$$\mathcal{L}\{\dot{f}(t)\} = s f(s) - f(t=0) \quad (1.34)$$

from which follows

$$\mathcal{L}\{\ddot{f}(t)\} = s[sf(s) - f(t=0)] - \dot{f}(t=0) \quad (1.35)$$

If we consider only cases, in which  $\dot{f}(0) = 0$  we obtain from (1.33) and (1.35)

$$s^2 u(\mathbf{k}, s) - u(\mathbf{k}, t=0) = -v^2 k^2 u(\mathbf{k}, s) \quad (1.36)$$

If we compare this with the frequency wave equation (1.5) we identify  $s^2$  with  $-\omega^2$ . But stop:  $s$  must have a nonvanishing real part! so we write - in accordance with our Green's function treatment of the electrons

$$s = -i\omega + \epsilon \quad s^2 = -\omega^2 - i \underbrace{2\epsilon\omega}_{\tilde{\epsilon}} \quad (1.37)$$

we can now solve (1.36) to obtain

$$u(\mathbf{k}, s) = \frac{u(t=0)}{-\omega^2 - i\tilde{\epsilon} + v^2 k^2} \equiv u(t=0)G_0(k, z) \quad (1.38)$$

with

$$G_0(k, z) = \frac{1}{z + v^2 k^2} \quad z = -\omega^2 - i\tilde{\epsilon} \quad (1.39)$$

## E Laplace transform and Green's function for diffusion

In  $\mathbf{k}$  space the diffusion equation

$$\frac{\partial}{\partial t} \rho(\mathbf{k}, t) = D \nabla^2 \rho(\mathbf{k}, t) \quad (1.40)$$

becomes

$$\frac{\partial}{\partial t} \rho(\mathbf{k}, t) = -D k^2 \rho(\mathbf{k}, t) \quad (1.41)$$

Going to the Laplace transform we get

$$(s + D k^2) \rho(\mathbf{k}, s) = \rho(t=0) \quad (1.42)$$

with the solution

$$\rho(\mathbf{k}, s) = \frac{\rho(t=0)}{s + Dk^2} = \rho(t=0)G_0(\mathbf{k}, s) \quad (1.43)$$

From the comparison with (1.9) and the condition  $\mathcal{R}e\{s\} > 0$  we must have

$$G_0(k, s) = \frac{1}{s + v^2k^2} \quad s = -i\omega + \epsilon \quad (1.44)$$

So — going from waves to diffusion we have to take

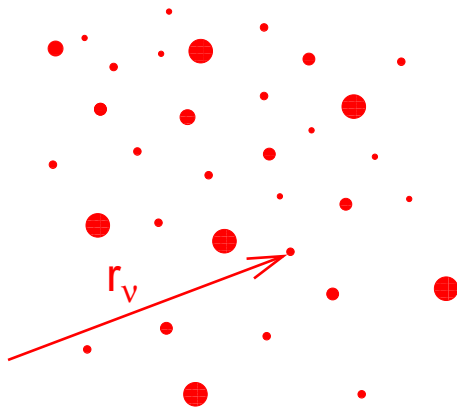
$$z = -\omega^2 - i\tilde{\epsilon} \quad \longrightarrow \quad s = -i\omega + \epsilon$$

## 2 Waves in the presence of disorder

### 2.1 Potential-type disorder

#### A Impurity disorder

- We assume that the perturbing potentials are centered at certain points  $\mathbf{r}_i$ , which are distributed randomly in space.



$$v(\mathbf{r}) = \sum_{\nu} v(\mathbf{r} - \mathbf{r}_{\nu}) \quad (2.1)$$

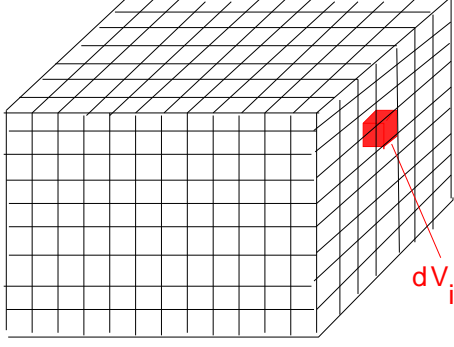
- In  $\mathbf{k}$  space we get

$$\langle \mathbf{k} + \mathbf{q} | v | \mathbf{k} \rangle \equiv v(\mathbf{q}) = v(\mathbf{q}) \sum_i e^{i\mathbf{q}\mathbf{r}_i} \quad (2.2)$$

- We may shift the energy scale in such a way that the impurity average  $\langle v \rangle = 0$ .

#### B Continuous Gaussian disorder

If we do not want to make a specific disorder model we just assume that the potential  $V(\mathbf{r})$  exhibits spatial fluctuations. We may again choose the energy scale such that  $\langle v \rangle = 0$ . We now assume  $v(\mathbf{r})$  to exhibit Gaussian fluctuations, which we describe as follows:



- We divide our sample of volume  $V$  into  $N$  volume elements  $dV_i$  of volume content  $\Delta V$ .

We assume that

- $v(\mathbf{r}) = \text{const} = v_i$  inside the volume element
- all random numbers  $v_i$  are independent

If we denote  $\sigma_V^2 = \langle v_i^2 \rangle$  to be the standard deviation (square-root of the variance), we have

$$\langle v_i v_j \rangle = \sigma_V^2 \delta_{ij} \quad (2.3)$$

The random numbers  $v_i$  obey the distribution

$$p(v_i) = p_0 e^{-\frac{1}{2}v_i^2/\sigma_V^2} \quad (2.4)$$

We may now write the Joint probability density

$$P(v_1 \dots v_i \dots v_N) = \prod_{i=1}^N p(v_i) = p_0^N e^{-\frac{1}{2\sigma_V^2} \sum_{i=1}^N v_i^2} \quad (2.5)$$

In the continuum limit  $\Delta V \rightarrow 0$ ,  $N \rightarrow \infty$ ,  $N\Delta V \rightarrow V$  we obtain

$$P[v(\mathbf{r})] = \tilde{P}_0 \exp \left\{ -\frac{1}{2\gamma} \int_V d\mathbf{r} v(\mathbf{r})^2 \right\} \quad (2.6)$$

Here

$$\gamma = \sigma^2 V_\xi \quad (2.7)$$

where  $V_\xi$  is the correlation volume, which is the smallest volume, for which the correlations between the fluctuations can be neglected, i.e.  $V_\xi \propto \xi^3$ , where  $\xi$  is the correlation length.

The continuum limit of Eq. (2.3) is then

$$\langle v(\mathbf{r})v(\mathbf{r}') \rangle = \gamma \delta(\mathbf{r} - \mathbf{r}') \quad (2.8)$$

In Eq. (2.3) we introduced the  $\delta$  function with

$$\delta(\mathbf{r}) = 0, |\mathbf{r}| \neq 0 \quad \int d\mathbf{r} \delta(\mathbf{r}) = 1 \quad (2.9)$$

## 2.2 Modulus-type disorder

We now consider the Helmholtz equation (1.5) with a spatially fluctuating elastic modulus, which we call  $M$  as in the equation for the longitudinal waves.

$$-\omega^2 u(\omega, \mathbf{r}) = \nabla \tilde{M}(\mathbf{r}) \nabla u(\omega, \mathbf{r}) \quad (2.10)$$

We further separate out the average of the ‘‘longitudinal’’ modulus (in this model there is no transverse one)  $\tilde{M} = v^2 = M/\rho$ , where  $v$  is the sound velocity and  $\rho$  the mass density  $\tilde{M}_0 = \langle \tilde{M} \rangle$ :

$$\tilde{M}(\mathbf{r}) = \tilde{M}_0 + \Delta(\mathbf{r}) \quad (2.11)$$

We now assume the deviations  $\Delta(\mathbf{r})$  to exhibit uncorrelated Gaussian fluctuations:

$$\langle \Delta(\mathbf{r}) \Delta(\mathbf{r}') \rangle = \gamma \delta(\mathbf{r} - \mathbf{r}') \quad (2.12)$$

with  $\gamma = \sigma_{\Delta}^2 V_{\xi}$ ,

$$P[\Delta(\mathbf{r})] = \tilde{P}_0 \exp \left\{ -\frac{1}{2\gamma} \int_V d\mathbf{r} \Delta(\mathbf{r})^2 \right\} \quad (2.13)$$

## 2.3 Perturbation expansion and Born approximation

### A Potential-type disorder

We now consider electrons with a Hamiltonian of the form

$$\mathcal{H} = \mathcal{H}_0 - v \quad (2.14)$$

From the operator identity  $\frac{1}{A+B} = \frac{1}{A} \left(1 - \frac{B}{A+B}\right)$  we obtain

$$\mathcal{G}(z) = \frac{1}{z + \mathcal{H}_0} \left(1 + v \frac{1}{z + \mathcal{H}}\right) = \mathcal{G}_0(z) \left(1 + v \mathcal{G}(z)\right), \quad (2.15)$$

which one can iterate to obtain

$$\begin{aligned}
\mathcal{G} &= \mathcal{G}_0 + \mathcal{G}_0 v \mathcal{G}_0 + \mathcal{G}_0 v \mathcal{G}_0 \mathcal{G}_0 v \mathcal{G}_0 + \dots \\
&= \mathcal{G}_0 + \mathcal{G}_0 \frac{v}{1 - v \mathcal{G}_0} \mathcal{G}_0 \\
&\equiv \mathcal{G}_0 + \mathcal{G}_0 \mathcal{T} \mathcal{G}_0,
\end{aligned}$$

where we have defined the *scattering matrix* or *T-matrix*  $\mathcal{T}$ .

- In the following we denote a configurational average over the quenched disorder by  $\langle \dots \rangle$ .

In order to be able to calculate the (averaged) density of states of the disordered system we become interested in the *configurationally averaged resolvent*

$$\mathbf{G}(z) = \langle \mathcal{G}(z) \rangle = \left\langle \frac{1}{z + \mathcal{H}_0 - v} \right\rangle \equiv \frac{1}{z + \mathcal{H}_0 - \Sigma(z)} \quad (2.16)$$

Here we have introduced an unknown operator  $\Sigma(z)$  which looks like an effective potential of a fictitious system which is not disordered but, instead, depends on a complex parameter  $z$ . This (yet unknown) operator is called self-energy operator. We now insert the perturbation expansion (2.16) into (2.16) and solve for  $\Sigma(z)$ :

$$\begin{aligned}
\Sigma(z) &= z + \mathcal{H}_0 - \frac{1}{\langle \mathcal{G}(z) \rangle} \\
&= \frac{1}{\mathcal{G}_0} - \frac{1}{\mathcal{G}_0 + \mathcal{G}_0 \underbrace{\langle v \rangle}_0 \mathcal{G}_0 + \mathcal{G}_0 \langle v \mathcal{G}_0 \mathcal{G}_0 v \rangle \mathcal{G}_0 + \dots} \\
&= \frac{1}{\mathcal{G}_0} \left( 1 - \frac{1}{1 + \langle v \mathcal{G}_0 v \rangle \mathcal{G}_0 + \dots} \right)
\end{aligned}$$

To second order in  $v$  we get

$$\Sigma(z) = \frac{1}{\mathcal{G}_0(z)} \left\langle v \mathcal{G}_0(z) v \right\rangle \mathcal{G}_0(z). \quad (2.17)$$

We now use the  $|\mathbf{k}\rangle$  basis. The density of states is given by

$$N(E) = \left\langle \frac{1}{\pi V} \sum_{\mathbf{k}} \underbrace{\langle \mathbf{k} | \mathbf{G}(z_+) | \mathbf{k} \rangle}_{G(k,z)} \right\rangle \quad (2.18)$$

---

A note on the  $\mathbf{k}$  sum:

- On a disordered lattice the  $\mathbf{k}$  sum runs over the first Brillouin zone.
- In an amorphous system the  $\mathbf{k}$  we must introduce an upper cutoff, if the  $\mathbf{k}$  integral does not converge for high  $|\mathbf{k}|$ :

$$\sum_{\mathbf{k}} f(\mathbf{k}) = \frac{V}{(2\pi)^3} \int_{|\mathbf{k}| < k_c} d\mathbf{k} \quad (2.19)$$

$k_c$  can e.g. be the the inverse correlation length of the disorder fluctuations.

---

Note that the averaged Green's function depends only on the difference  $\mathbf{r} - \mathbf{r}'$

$$\langle G(\mathbf{r}, \mathbf{r}', z) \rangle = G(\mathbf{r} - \mathbf{r}', z) \quad (2.20)$$

From this it follows that both  $\mathbf{G}(z)$  as well as  $\Sigma(z)$  are diagonal in the  $|\mathbf{k}\rangle$  representation.

We now can write down the diagonal element of the self-energy operator, which is called the self-energy function to second order in  $v$ :

$$\begin{aligned} \Sigma(\mathbf{k}, z) &= \langle \mathbf{k} | \Sigma(z) | \mathbf{k} \rangle = \sum_{\mathbf{q}} \frac{1}{G_0(k, z)} \\ &\quad \times \left\langle \langle \mathbf{k} | V | \mathbf{k} + \mathbf{q} \rangle G_0(|\mathbf{k} + \mathbf{q}|, z) \langle \mathbf{k} + \mathbf{q} | V | \mathbf{k} \rangle \right\rangle G_0(k, z) \\ &= \frac{1}{V} \sum_{\mathbf{q}} \frac{1}{V} \underbrace{\left\langle \sum_{\ell m} e^{i\mathbf{q}(\mathbf{r}_\ell - \mathbf{r}_m)} \right\rangle}_{K(q) = S(q) |v(q)|^2} |v(q)|^2 G_0(|\mathbf{k} + \mathbf{q}|, z) \\ &= \frac{1}{V} \sum_{\tilde{\mathbf{q}}} K(\tilde{\mathbf{q}} - \mathbf{k}) G_0(\tilde{\mathbf{q}}) \quad (2.21) \\ &= \Sigma'(\mathbf{k}, E) + i\Sigma''(\mathbf{k}, E) \end{aligned}$$

- $K(q)$  is the correlation function of the impurity-induced potential fluctuations.  $S(q)$  is called the structure factor of the impurities.
- For the Gaussian uncorrelated fluctuations we have to set

$$K(q) = \langle \Delta^2 \rangle V_\xi \theta(q_c - q) \quad (2.22)$$



where  $V_\xi$  is the smallest coarse-graining volume for which the disorder fluctuations are uncorrelated (correlation volume). It is consistent to choose  $q_c$  of the order of  $V_\xi^{-1/3}$ .

Inserting (2.22) into (2.21) we get the uncorrelated version of the Born approximation

$$\Sigma(z) = \Sigma(k=0, z) = \langle \Delta^2 \rangle \frac{V_\xi}{2\pi^2} \int_0^{q_c} dq q^2 G_0(q, z) \quad (2.23)$$

Let us now discuss what consequences the disorder has for the electronic structure.

The Green's function (the imaginary part of which, summed over  $\mathbf{k}$ , gives the density of states) has the form

$$G(\mathbf{k}, z) = \frac{1}{z + E_{\mathbf{k}}^{(0)} - \Sigma(\mathbf{k}, z)} \quad (2.24)$$

The real part of  $\Sigma(\mathbf{k}, z)$  produces a *shift* (“renormalization”) of the band structure:

$$E_{\mathbf{k}} \equiv E_{\mathbf{k}}^{(0)} + \Sigma'(k, E) \quad E_{\mathbf{k}}^{(0)} = \frac{\hbar^2}{2m} k^2 \quad (2.25)$$

for free electrons

The density of states now takes the form

$$N(E) = \frac{1}{\pi V} \sum_{\mathbf{k}} \frac{\Sigma''(k, E)}{[E_{\mathbf{k}}]^2 + [\Sigma''(k, E)]^2} \quad (2.26)$$

The imaginary part of  $\Sigma(\mathbf{k}, z)$  introduces a new element into the density of states of our disordered system: The function  $E_{\mathbf{k}}$  is no more sharply defined but is “washed out” by the disorder-induced imaginary part of  $\Sigma(k, E)$ . This is so, because neither a lattice  $\mathbf{k}$  vector nor the free-electron  $\mathbf{k}$  vector can serve as a “good quantum number” for labeling the electronic states. However, the latter serves as “approximate quantum number” but one has to deal with the fact that in this “approximate” basis the  $E_{\mathbf{k}}$  resonances are washed out by disorder.

## B Self-consistent Born approximation

Let us look again at the lowest-order Born approximation for the self energy

$$\begin{aligned}
 G(\mathbf{k}, z) &= \frac{1}{z + E_{\mathbf{k}}^{(0)} - \Sigma(\mathbf{k}, z)} \\
 \Sigma(\mathbf{k}, z) &= \frac{1}{(2\pi)^3} \int d^3\mathbf{q} S(q) |v(q)|^2 \underbrace{\frac{1}{z + E_{\mathbf{k}+\mathbf{q}}^{(0)}}}_{G_0(\mathbf{k}+\mathbf{q}, z)}
 \end{aligned} \tag{2.27}$$

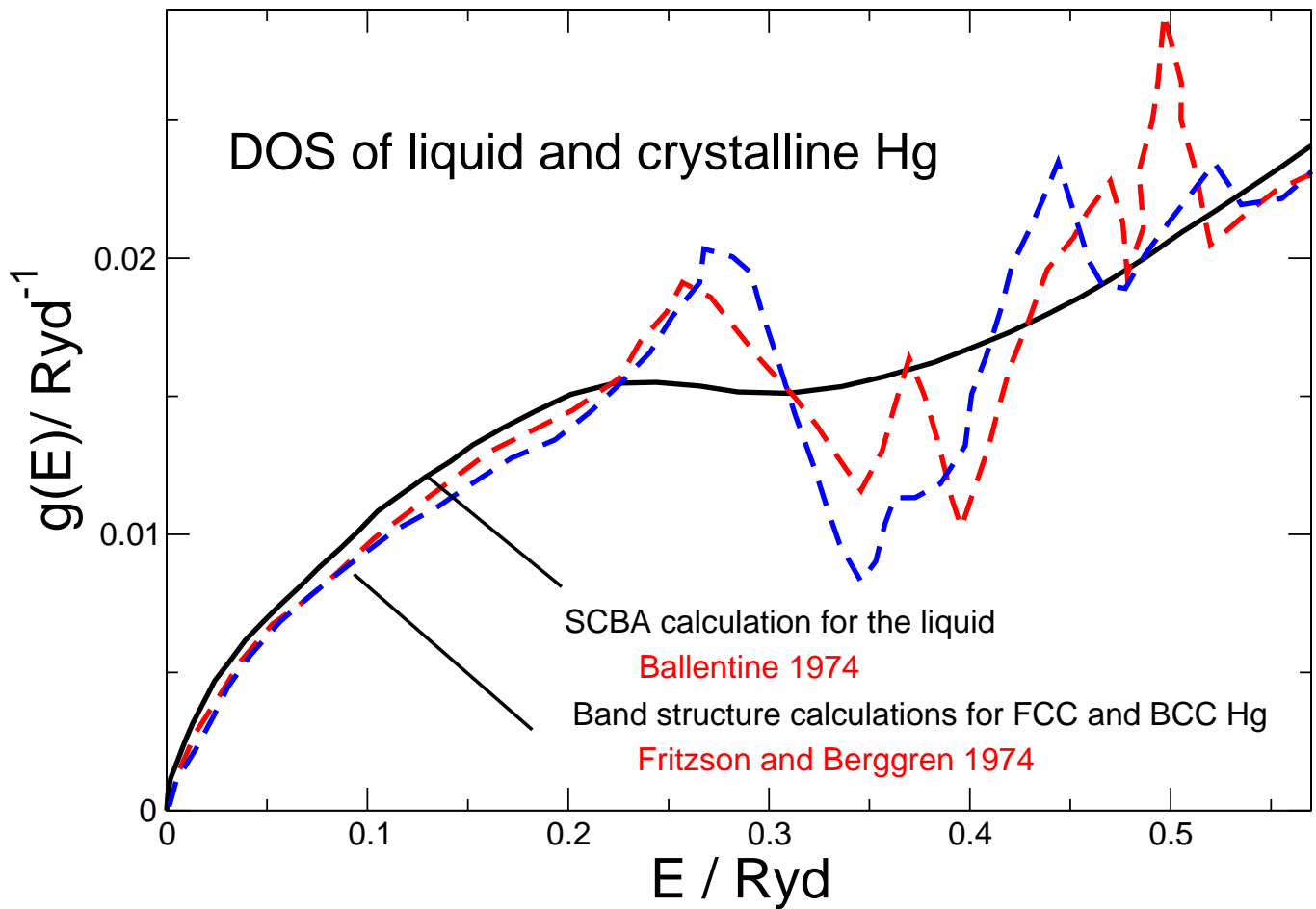
It is obviously not satisfactory to deal with two different Green's functions: the disorder-affected one  $G(\mathbf{k}, z)$  and the free one  $G_0(\mathbf{k}, z)$ . Therefore one made an ad-hoc replacement

$$G_0(\mathbf{k} + \mathbf{q}, z) \longrightarrow G(\mathbf{k} + \mathbf{q}, z)$$

which results in the Self-consistent Born approximation, SCBA:

$$\Sigma(\mathbf{k}, z) = \frac{1}{(2\pi)^3} \int d^3\mathbf{q} S(q) |v(q)|^2 \underbrace{\frac{1}{z + E_{\mathbf{k}+\mathbf{q}}^{(0)} - \Sigma(\mathbf{k} + \mathbf{q}, z)}}_{G(\mathbf{k}+\mathbf{q}, z)} \tag{2.28}$$

In the figure we have plotted the density of states of liquid mercury as calculated in SCBA by Ballentine 1974 using the measured liquid structure factor  $S(q)$ , the free electron band structure  $E_{\mathbf{k}}^{(0)} = \frac{1}{2m} \hbar^2 k^2$  and a suitable pseudopotential  $v(q)$ . We compare this with the FCC and BCC crystalline density of states obtained by band structure calculations of Fritzson and Berggren 1974. We see, as discussed above that the disorder smears out all ragged features present in the crystalline DOS.



Inserting the uncorrelated expression (2.22) for the correlation function we get the uncorrelated version of the SCBA:

$$\Sigma(z) = \Sigma(k=0, z) = \langle \Delta^2 \rangle \frac{V_\xi}{2\pi^2} \int_0^{q_c} dq q^2 \frac{1}{z + \frac{\hbar^2 k^2}{2m} - \Sigma(z)} \quad (2.29)$$

- In the next section we shall derive the uncorrelated version of the SCBA with the help of non-perturbative field-theoretical methods, namely using Gaussian functional integrals and a saddle-point approximation.

### C Modulus-type disorder: Rayleigh scattering

We study the scalar wave equation with modulus-type disorder, which is equivalent to a diffusion equation with modulus-type disorder via the correspondence  $z = -\omega^2 - i\tilde{\epsilon} \longleftrightarrow s = -i\omega + \epsilon$

$$-\omega^2 u(\omega, \mathbf{r}) = \nabla \tilde{M}(\mathbf{r}) \nabla u(\omega, \mathbf{r}) \quad \tilde{M}(\mathbf{r}) = \tilde{M}_0 + \Delta(\mathbf{r}) \quad (2.30)$$

The full Green's function obeys the equation of motion

$$(z - \tilde{M}_0 \nabla^2)G(\mathbf{r}, \mathbf{r}', z) - \nabla \Delta(\mathbf{r}) \nabla G(\mathbf{r}, \mathbf{r}', z) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.31)$$

The “unperturbed” Green's function obeys

$$(z - \tilde{M}_0 \nabla^2)G_0(\mathbf{r}, \mathbf{r}', z) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.32)$$

which is solved in  $\mathbf{k}$  space to give

$$G_0 = \frac{1}{z + k^2 \tilde{M}_0} \quad (2.33)$$

Now we follow exactly the same procedure as done in the previous paragraph for the electrons.

We, again, represent the averaged Green's function, which contains fluctuations, by means of a self-energy function  $\Sigma(\mathbf{k}, z)$  as follows

$$\mathbf{G}(\mathbf{k}, z) \equiv \langle G(z, \mathbf{k}\mathbf{k}') \rangle \delta(\mathbf{k} + \mathbf{k}') = \frac{1}{z + \tilde{M}_0 k^2 - \Sigma(\mathbf{k}, z)} \quad (2.34)$$

Performing the perturbation expansion *mutatis mutandis* (see appendix to this section) we get for the self energy in Born approximation

$$\Sigma(\mathbf{k}, z) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k}_1 K(\mathbf{k} - \mathbf{k}_1) (\mathbf{k} \cdot \mathbf{k}_1)^2 G_0(k_1, z) \quad (2.35)$$

where  $K(\mathbf{k} - \mathbf{k}')$  is the correlation function of the fluctuations

$$K(\mathbf{r}, \mathbf{r}') = \langle \Delta(\mathbf{r}) \Delta(\mathbf{r}') \rangle = K(\mathbf{r} - \mathbf{r}') \quad (2.36)$$

We now assume Gaussian uncorrelated disorder:

$$K(\mathbf{r}, \mathbf{r}') = \Delta^2 \delta(\mathbf{r} - \mathbf{r}') \quad \Leftrightarrow \quad K(\mathbf{k}) = \underbrace{\langle \Delta^2 \rangle V_\xi}_\gamma \theta(q_c - q) \quad (2.37)$$

Now the only angle dependence in the integral in Eq. (2.35) is in the squared scalar product  $(\mathbf{k} \cdot \mathbf{k}_1)$ , which therefore can be replaced by its angle average  $\frac{1}{3}k^2 k_1^2$ , and we get the uncorrelated version of the Born approximation:

$$\begin{aligned}\Sigma(\mathbf{k}, z) &= k^2 \Sigma(z) && \text{with} \\ \Sigma(z) &= \frac{\gamma}{6\pi^2} \int_0^{q_c} dk_1 k_1^4 G_0(k_1, z)\end{aligned}\quad (2.38)$$

We now remind ourselves of the form of the averaged Green's function, Eq. (2.34)

$$G(\mathbf{k}, z) = \frac{1}{z + \tilde{M}_0 k^2 - \Sigma(\mathbf{k}, z)} = \frac{1}{-\omega^2 - i\tilde{\epsilon} + \underbrace{k^2[\tilde{M}_0 - \Sigma(z)]}_{v^2(z)}} \quad (2.39)$$

where we have and defined a frequency dependent complex speed of light or sound by

$$v^2(z) = \tilde{M}_0 - \Sigma(z) \quad (2.40)$$

with

$$\begin{aligned}\Sigma(z) &= \frac{1}{k^2} \Sigma(\mathbf{k}, z) \Big|_{\mathbf{k}=0} = \frac{\gamma}{6\pi^2} \underbrace{\int_0^\infty dk_1 \frac{k_1^4}{z + \tilde{M}_0 k_1^2}}_{\propto z^{3/2}} \\ &= \Sigma'(\omega) + i\Sigma''(\omega)\end{aligned}\quad (2.41)$$

We now neglect in (2.39)  $i\tilde{\epsilon}$  against the imaginary part  $\mathcal{Im}\{\Sigma(z)\} = \Sigma''(\omega)$  and define a frequency dependent complex wave number as by

$$\begin{aligned}\kappa(\omega) &= \frac{\omega}{v(z)} = \frac{\omega}{\underbrace{\sqrt{\tilde{M}_0 - \Sigma'(0) - i\Sigma''(\omega)}}_{v^2}} \\ &= \frac{\omega}{v} \frac{1}{\sqrt{1 - i\Sigma''(\omega)/v^2}} \approx \frac{\omega}{v} \left(1 + i\frac{1}{2} \frac{\Sigma''(\omega)}{v^2}\right) \equiv \bar{k} + i\frac{1}{2\ell(\omega)}\end{aligned}\quad (2.42)$$

Here  $v$  is the speed of light in the medium, modified by the disorder and  $\ell(\omega)$  is the mean-free path.

Now the averaged Green's function can be written as

$$\mathbf{G}(\mathbf{k}, \omega) = \frac{1}{v(\omega)^2} \frac{1}{k^2 - \kappa(\omega)^2} \approx \frac{1}{v^2} \frac{1}{k^2 - \kappa(\omega)^2} \quad (2.43)$$

which has a Fourier transform

$$\mathbf{G}(\mathbf{r}, \omega) = \frac{1}{4\pi v^2 r} e^{i\kappa(\omega)r} = \frac{1}{4\pi v^2 r} e^{i\bar{\kappa}r} e^{-r/2\ell(\omega)} \quad (2.44)$$

For the scattered intensity we obtain

$$\left| \mathbf{G}(\mathbf{r}, \omega) \right|^2 \propto e^{-r/\ell(\omega)} \quad (2.45)$$

with a mean-free path

$$\frac{1}{\ell(\omega)} \propto \omega \Sigma''(\omega) \propto \omega [\omega^2]^{3/2} = \omega^4, \quad (2.46)$$

This is the well-known Rayleigh scattering, which holds for any waves in the presence of static disorder and which leads to the blue color of the sky and the red color of the sunset:



Neuschwanstein Castle, Germany



Lake of Konstanz, Germany

## D Appendix: Details of the perturbation expansion for Rayleigh scattering

We study the stochastic Helmholtz equation

$$-\omega^2 u(\omega, \mathbf{r}) = \nabla \tilde{M}(\mathbf{r}) \nabla u(\omega, \mathbf{r}) \quad \tilde{M}(\mathbf{r}) = \tilde{M}_0 + \Delta(\mathbf{r}) \quad (2.47)$$

The Green's function obeys the equation of motion

$$(z - \tilde{M}_0 \nabla^2) G(\mathbf{r}, \mathbf{r}', z) - \nabla \Delta(\mathbf{r}) \nabla G(\mathbf{r}, \mathbf{r}', z) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.48)$$

Fourier-transformed we obtain

$$z G(\mathbf{k}\mathbf{k}', z) - \delta(\mathbf{k} + \mathbf{k}') + \tilde{M}_0 k^2 G(\mathbf{k}\mathbf{k}', z) = -\frac{1}{(2\pi)^3} \int d^3 \mathbf{k}_1 \mathbf{k} \mathbf{k}_1 \Delta(\mathbf{k} - \mathbf{k}_1) G(\mathbf{k}_1 \mathbf{k}', z) \quad (2.49)$$

We now define

$$G_0(\mathbf{k}\mathbf{k}', z) = \frac{1}{z + \tilde{M}_0 k^2} \delta(\mathbf{k} + \mathbf{k}') \equiv G_0(k, z) \delta(\mathbf{k} + \mathbf{k}') \quad (2.50)$$

to be the Green's function without fluctuations. We note that  $G_0(k, z)$  depends only on the modulus  $k = |\mathbf{k}|$  of  $\mathbf{k}$ .

From Eq. (2.48) we now obtain

$$\frac{G(\mathbf{k}\mathbf{k}'z)}{G_0(\mathbf{k}, z)} = 1 - \frac{1}{(2\pi)^3} \int d^3\mathbf{k}_1 \mathbf{k} \cdot \mathbf{k}_1 \Delta(\mathbf{k} - \mathbf{k}_1) G(\mathbf{k}_1\mathbf{k}', z) \quad (2.51)$$

We represent the averaged Green's function, which contains fluctuations, by means of a self-energy function  $\Sigma(\mathbf{k}, z)$  as follows

$$\mathbf{G}(\mathbf{k}, z) \equiv \langle G(z, \mathbf{k}\mathbf{k}') \rangle \delta(\mathbf{k} + \mathbf{k}') = \frac{1}{z + \tilde{M}_0 k^2 - \Sigma(\mathbf{k}, z)} = \frac{1}{\frac{1}{G_0(\mathbf{k}, z)} - \Sigma(\mathbf{k}, z)} \quad (2.52)$$

From this we obtain

$$\Sigma(\mathbf{k}, z) = \frac{1}{G_0(\mathbf{k}, z)} - \frac{1}{\langle G(\mathbf{k}\mathbf{k}', z) \rangle} = \frac{1}{G_0(\mathbf{k}, z)} \left( 1 - \frac{G_0(\mathbf{k}, z)}{\langle G(\mathbf{k}\mathbf{k}', z) \rangle} \right) \quad (2.53)$$

Inserting (2.51) and expanding the denominator with respect to the fluctuations  $\Delta$  we get

$$\Sigma(\mathbf{k}, z) = \frac{1}{G_0(\mathbf{k}, z)} \left\langle \frac{1}{(2\pi)^3} \int d^3\mathbf{k}_1 \mathbf{k} \cdot \mathbf{k}_1 \Delta(\mathbf{k} - \mathbf{k}_1) G(\mathbf{k}_1\mathbf{k}'z) \right\rangle \quad (2.54)$$

Inserting (2.51) again, recognizing that the average over a fluctuation is 0 and restricting ourselves to lowest (second) order in the fluctuations we obtain

$$\begin{aligned} \Sigma(\mathbf{k}, z) = & \left\langle \frac{1}{(2\pi)^3} \int d^3\mathbf{k}_1 \mathbf{k} \cdot \mathbf{k}_1 \Delta(\mathbf{k} - \mathbf{k}_1) G_0(\mathbf{k}_1) \right. \\ & \left. \times \frac{1}{(2\pi)^3} \int d^3\mathbf{k}_2 \mathbf{k}_1 \cdot \mathbf{k}_2 \Delta(\mathbf{k}_1 - \mathbf{k}_2) G_0(\mathbf{k}_2) \right\rangle \end{aligned}$$

The correlation function of the fluctuations is

$$K(\mathbf{r}_1, \mathbf{r}_2) = \langle \Delta(\mathbf{r}_1) \Delta(\mathbf{r}_2) \rangle = K(\mathbf{r}_1 - \mathbf{r}_2) \quad (2.55)$$

Its Fourier transform obeys

$$K(\mathbf{k}_1, \mathbf{k}_2) = \langle \Delta(\mathbf{k}_1) \Delta(\mathbf{k}_2) \rangle = K(\mathbf{k}_1) (2\pi)^3 \delta(\mathbf{k}_1 + \mathbf{k}_2) \quad (2.56)$$

from which we obtain the identification

$$\mathbf{k} - \mathbf{k}_1 = \mathbf{k}_2 - \mathbf{k}_1 \quad \Rightarrow \quad \mathbf{k}_2 = \mathbf{k} \quad (2.57)$$



From this we get the Born approximation for modulus-type disorder

$$\Sigma(\mathbf{k}, z) = \frac{1}{(2\pi)^3} \int d^3\mathbf{k}_1 K(\mathbf{k} - \mathbf{k}_1) (\mathbf{k} \cdot \mathbf{k}_1)^2 G_0(k_1, z) \quad (2.58)$$