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# Sound in granular matter: a case of wave propagation in random media.

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# **Sound in granular matter:**

**A case of wave propagation in random media**

## **Part I.**

Lecture notes to a course given by

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## NOTE

The available experimental results on acoustic probing of compactified granular matter provide a unique insight into the interior of granular samples – difficult to access otherwise. Attempts at reviewing and comparing these results from a unified point of view meets with a difficulty, as the theoretical picture of sound propagation in a granular media is not complete. The simplest general characteristic of granular matter is its *randomness*. Sound in granular matter is thus an instance of wave propagation in random media. This more general topic is by now well developed and we may draw from both the accumulated physical understanding and the formalisms at hand. It is the purpose of these lectures first to explore this connection in some detail and then to employ it for a discussion of the case of granular matter. This should provide a basis for a more detailed analysis of the existing and conceivable acoustic experiments as a tool for investigating granular matter.

It should be noted that the theory of waves in random media is heavily loaded with technicalities and with a related jargon often borrowed from quantum field theory, which does not facilitate the access to the underlying physical notions. In these lectures, an attempt at discussing these matters in an informative and technically elementary way. This is connected with the idea that these lectures should primarily address students and interested non-specialists. In fact, there are barely more than a handful of specialists in sound&granular matter. This field is at a crossroad between many disciplines and approaches, and the lectures aim at paving the way for communication between experimentalists and theorists involved.

The text presented here corresponds to the actual subject matter presented in the course, although it gives more details than was possible to cover in the short time available for the lectures. The first part (presently distributed) covers about the first half of the topics considered in the course. The second part will present an elementary introduction to localisation of classical waves and a two-part discussion of sound in granular matter. The first part will consider the general questions of confined granular samples. The notes will be concluded by a discussion of several recent experimental studies of sound propagation in granular matter.

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# Chapter 1

## Lecture one: Classical waves in random media

### 1.1 Historical remarks

We will approach the behavior of acoustic excitations in granular matter in steps. There are still many unknowns in this problem, and our method will be to make use of the knowledge which has been accumulated about various waves propagating (or being captured) in other random media. In some sense, a vast historical circle has closed in about one hundred years. In 1871, lord Rayleigh published his paper entitled "On the Light from the Sky" (see an easier accessible Treatise on Sound [1]) containing many essentials of the scattering theory for classical waves. As early as in 1905–06, the Radiative Transfer theory was introduced in order to handle the problem of light in stellar atmospheres, in which the notion of a diffusive light propagation was born [2]. In 1913, Ewald formulated the multiple scattering approach to electromagnetic propagation in periodic structures. While this evolution continued, another area of wave phenomena developed explosively with the creation of Quantum Physics in 1925–26. There, the scattering processes played an essential role, and their theory was brought to perfection [3]. But we will be concerned more with a seemingly remote area of an electric transport in solids. Already in the thirties, F. Bloch showed that periodic structures must be transparent for electron waves, resolving thereby the lasting enigma of the classical electron theory of Lorentz and Drude. Soon thereafter, Nordheim explained the so-called residual (non-thermal) part of the resistance of metal alloys by electron scattering on the alloy disorder. Electron waves in a crystal moved in an electric field according to the Boltzmann equation, which described the electrons as though they effectively were classical (quasi)particles, performing a diffusive motion [4]. While already this analogy between the electrons and the classical waves was striking, the really important lessons from the area of electron transport were only to come. In 1958, P. W. Anderson published the celebrated paper [5], in which he showed that a sufficiently strong disorder may prevent electrons from diffusing, or, more precisely, that it will cause an electron wave packet not to spread indefinitely. This notion of strong (Anderson) localisation played a substantial role in the subsequent development of the physics of disordered systems, in particular of amorphous semiconductors, and was subject of an immense theoretical effort for more than two decades, until the evolution was synthesized into two approaches, the scaling theory of localisation [6] and the self-consistent theory of localisation [7]. The basic paper by Abrahams et. al. addressed the critical behavior of conductance near the Anderson transition. It spurred, at the same time, an intense work on a new quantum effect, the so-called weak localisation, physically identical with the coherent back-scattering effect. The self-consistent theory linked localisation with a more conventional approach to electron transport. It also incorporated the outcome of a parallel development, conceptually less striking, but very successful in practice, namely a self-consistent reformulation of the multiple scattering theory [8], usually identified with the Coherent potential approximation as its most widespread representative [9], [10]. All this had a direct impact on work in the area of low dimensional electron systems. The parallels with mesoscopic systems [11] keep their inspirational value for physics of classical waves even today. We will not explore this interesting field, however.

The important point emerging from this sketchy picture is that while localisation for historical reasons appeared first in the disguise of a quantum effect, it is related only with, and fully explicable in

terms of, the wave properties of electrons. Hence, the same picture should be valid for classical waves propagating through a random medium. No need to stress that this was realized soon, and the first experimental papers on weak localisation of light [13], [12] appeared as early as in 1985. An authoritative account of the ensuing research on classical waves, light, sound, and other is summarized in the book [14]. This, together with a more recent and pedagogical overview [15] may be considered two basic modern references for the area of classical waves in random media. They also give a fairly complete bibliography to original and review articles of interest.

## 1.2 Electron and sound waves compared

When thinking about the chances to observe some localisation effect as characterized above, the electrons, say, in a mesoscopic structure seem to have all disadvantages. Even at very low temperatures, the phase breaking inelastic processes due to phonons have their characteristic length in the micron range. Because a typical experiment involves a measurement of transport properties, we have to deal with the whole electron distribution and the electron-electron interactions modify substantially the picture of localized independent electrons. And yet the experiments on both weak and strong localisation are abundant. Meanwhile, for classical waves a fully convincing evidence for Anderson localisation is still wanting. The situation is much more favorable with studies of the classical analogues of weak localisation and of "universal fluctuations" of global transport quantities. Some important reasons for such distinction can be traced down to rather elementary differences between electrons and classical waves.

Let us consider the 3D case. We want to contrast a wave of one spin-less electron described by a scalar field ("wave function")  $\psi(\mathbf{r}, t)$  with a sound wave in an ideal fluid, which can also be described by a scalar field of local dilation  $\theta(\mathbf{r}, t) = \text{div } \mathbf{u}$  with  $\mathbf{u}$  the displacement field.

ELECTRONS	SOUND WAVE
<p>complex-valued field <math>\psi(\mathbf{r}, t)</math>  observable ... density <math> \psi ^2</math>  <i>intensity</i> sensitive measurement</p> $i\hbar\partial_t \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}, t) + V(\mathbf{r}) \cdot \psi(\mathbf{r}, t) \quad (1.1)$ <p style="text-align: center;">SCHRÖDINGER EQUATION</p> <p>◇ first order in time  ◇ randomness in the potential <math>V</math></p> <p>harmonic solutions <math>\psi(\mathbf{r}, t) = \Psi(\mathbf{r}) \cdot e^{-i\omega t}</math> obey  Time-independent Schrödinger equation</p> $\hbar\omega\Psi(\mathbf{r}) + \frac{\hbar^2}{2m}\Delta\Psi(\mathbf{r}) - V(\mathbf{r}) \cdot \Psi(\mathbf{r}) = 0 \quad (1.3)$	<p>real field <math>\theta(\mathbf{r}, t)</math>  observable ... dilation <math>\theta</math>  <i>amplitude</i> sensitive measurement</p> $\frac{1}{c(\mathbf{r})^2}\partial_{tt} \theta(\mathbf{r}, t) = \Delta\theta(\mathbf{r}, t) \quad (1.2)$ <p style="text-align: center;">WAVE EQUATION</p> <p>◇ second order in time  ◇ randomness in the velocity <math>c</math>, i.e. in the static fluid density</p> <p>harmonic solutions <math>\theta(\mathbf{r}, t) = \Theta(\mathbf{r}) \cdot e^{-i\omega t}</math> obey  Helmholtz equation</p> $\frac{1}{c(\mathbf{r})^2}\omega^2\Theta(\mathbf{r}) + \Delta\Theta(\mathbf{r}) = 0 \quad (1.4)$

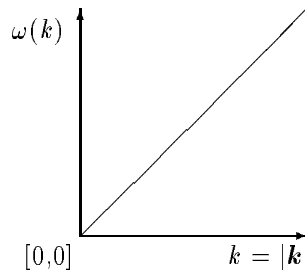
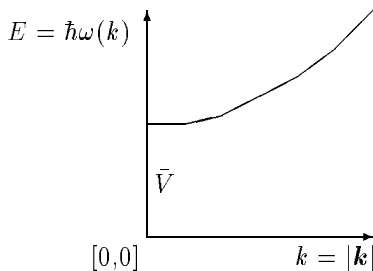
This table summarizes the formal analogies and differences between both physical situations. For homogeneous media, i.e. the random quantities reduced to their median values

$$V(\mathbf{r}) = \bar{V}, \quad c(\mathbf{r}) = \bar{c} \quad (1.5)$$

both wave equations have solutions of the plane wave form  $\exp(-i(\omega t - \mathbf{k}\mathbf{r}))$ , but with very different dispersion laws:

$$E(k) = \hbar\omega(k) = \bar{V} + \hbar^2(2m)^{-1} k^2 \quad (1.6)$$

$$\omega(k) = \bar{c} \cdot k \quad (1.7)$$



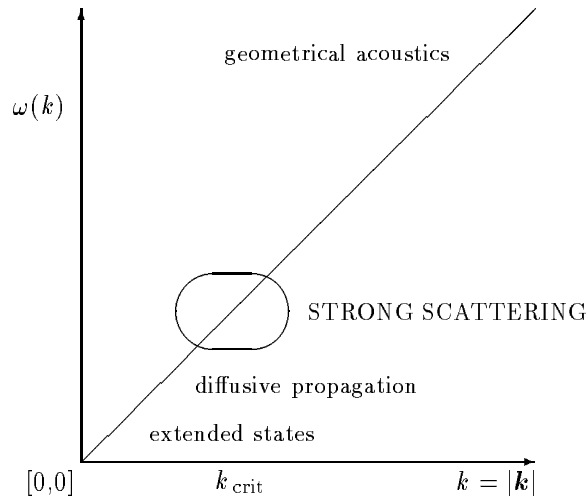
Sound is dispersionless, i.e., the dispersion law is linear. By contrast, the electrons have pronounced dispersion, and the phase velocity  $\omega(k)/k$  differs from the group velocity  $d\omega/dk$  by a factor of 2. Even more importantly, the absolute position of the electron dispersion law is of little importance, as it corresponds to an arbitrary choice of the origin of energies. The dispersion law for the sound waves starts, however, strictly at zero for fundamental reasons. In the case of sound, this is connected with the fact that to displace homogeneously the medium as a whole, no expense of the elastic energy is needed. Similar argument holds also for other classical waves. In fact, it has not much to do with the classicality of the waves in question: rather, they correspond to massless fields.

The disorder is reflected in fluctuations of  $V(\mathbf{r})$  around  $\bar{V}$ . The solutions of the time-independent Schrödinger equation are not plane waves any more, but for a weak random potential

$$V(\tilde{\mathbf{r}}) \equiv V(\mathbf{r}) - \bar{V} \quad (1.8)$$

a perturbation theoretical argument might suggest that the distorted states will still resemble the plane waves, in particular, that they will remain *extended* over the whole spatial extent of a large sample. This is not a correct assumption in general. Even for quite weak random potentials, there will always exist relatively extended negative fluctuations of  $V(\mathbf{r})$ , which may capture electrons in *fluctuation bound states*, which correspond to energies  $E = \hbar\omega < \bar{V}$ , that is below the edge of the band of unperturbed energies. The real question is about the behavior of the states with energies within the band. This, in fact, depends strongly on the dimension of the problem. In 1D and in 2D, *all* states become localized due to the action of the random potential. In 3D, the case originally investigated by Anderson, there is a richer variety of possibilities. Depending on the strength of the random potential, the states in the distorted band form two distinct classes: those below a characteristic energy  $E_c$  called the *mobility edge* are localized, non-propagating, those above remain extended, of course with a varying degree of distortion.

The fact that there is a spectral region below and above the band edge, where the disorder effects concentrate, made them so clearly manifest in many electron phenomena. The situation is very different for classical waves. First, no wave states can exist below the  $\omega^2$  threshold. Random or otherwise, no inhomogeneity can change the translation invariance argument about the long wavelength sound wave excitations. Second, the random perturbation appears at a different place in the Helmholtz equation, namely as a multiplier of  $\omega^2$ . For that reason, the effect of the randomness in the long wavelength limit, where  $\omega \rightarrow 0$ , is increasingly small, so that the very long sound waves are not only extended, but in fact nearly undistorted. The opposite limit of very short wavelengths, corresponding to  $\omega \rightarrow \infty$ , also leads to vanishingly small scattering, at least for smooth random fields: the wave achieves the regime of "geometrical acoustics" and propagates along the eikonal trajectories in the random landscape without being scattered. We are thus left with an intermediate region of frequencies/wavevectors, where more pronounced scattering effects may be expected, as sketched in the picture:



There are then several questions: which are the physical reasons for a strong scattering, where is the critical region characterized by  $k_{\text{crit}}$ , and, finally, what will the resulting effect be, just enhanced backscattering, or could perhaps strong localisation be achieved? Various mechanisms have been suggested, which might lead to a really intense scattering, like resonant scattering on inclusions (droplets, bubbles, ...), the so-called Mie resonances. A more efficient mechanism, paralleling the electron case, has been suggested on the basis of discrete microscopic model, which we will now briefly address.

### 1.3 Discrete models of random wave propagation

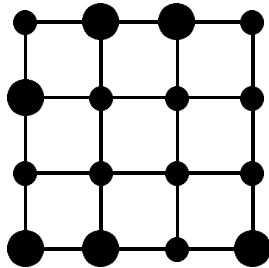
There have been proposed and theoretically analyzed many, many models, but we will comment on just two limiting, archetypal cases:

◊ *substitutional disorder* defined on regular, "crystal" lattice

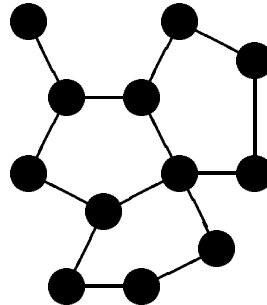
◊ *topological disorder* describing a random network

whose intuitive conception is sketched in the figure.

SUBSTITUTIONAL DISORDER



TOPOLOGICAL DISORDER



The idea of the discrete models is to represent the structure by a discrete set (matrix) of parameters characterising the nodes and links and then to solve a set of coupled ordinary differential equations for the excitations (waves), rather than to work with partial differential wave equations characteristic of continuous media.

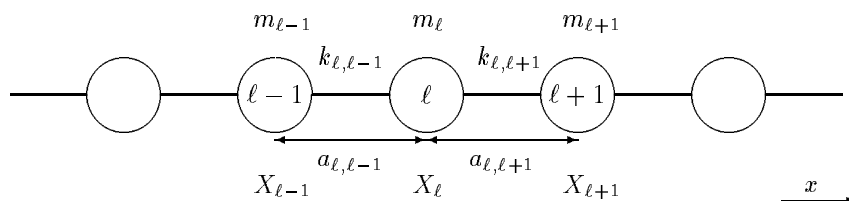
In the microscopic theory, the scheme applies both to electrons and to lattice vibrations, the nodes being atoms, and the links in turn being bonds, in both cases. In the parameter matrix, we have to distinguish the diagonal (single node) part, and the off-diagonal (site to site) part. For electrons, they



can be identified with atomic energy levels and with orbital overlaps, respectively, and the so-called LCAO (linear combinations of atomic orbitals), or TB (tight binding), scheme results. Anderson used a TB crystal with a purely diagonal disorder as his model in [5]. Lattice vibrations are directly related to our query about the elastic waves; in this case, the diagonal disorder concerns the atomic masses, while the off-diagonal disorder corresponds to variations in the strengths of the springs representing the mutual elastic couplings between the atoms; in other words, the system to be studied is a random array of balls and springs. As will be shown later, models of this type are particularly suited for granular media.

Substitutional disorder is better suited for a theoretical treatment: because it is assumed that the long range order of the underlying geometrical lattice is preserved, the *average* effect of the disorder can be represented by an effective fully periodic crystal. In the electron case, this means replacing the actual random potential by a properly selected periodic medium, the so-called Coherent Potential; the corresponding simplified but practicable construction is known under the name of CPA (Coherent potential approximation) [9], [10]. This captures, of course, only the overall features of the disorder, but it is relatively easy to build, on this basis, a more detailed understanding of, say, localisation effects. Topologically disordered systems are much harder for a systematic formal treatment [16],[17], and presently most of the related theoretical work is in fact based on numerical simulations followed by attempts to derive some general lessons from the output of the numerical experiments.

We cannot study the discrete models of lattice vibrations in detail, but we merely mention some results based on the simplest case of a 1D atomic chain of balls and springs between nearest neighbors. A segment of such chain may look as follows:



The reference "crystal" will have all quantities, masses  $m$ , spring stiffnesses  $k$ , and interatomic separations  $a$ , site  $\equiv$  node independent. The vibrations of such an ideal chain are easily found [4], and the dispersion law becomes

$$\omega(k) = c \cdot \sin(\frac{1}{2}ak)/\frac{1}{2}a, \quad 0 \leq k \leq \pi/a \equiv \frac{1}{2}B \quad (1.9)$$

where

$$c^2 = \frac{ka^2}{m} \quad (1.10)$$

As indicated, the dispersion law of the chain forms a finite band with a limiting wave vector  $k_{\text{crit}} = \frac{1}{2}B$ , and a limiting frequency,  $\omega_{\text{crit}} = 2c/a$ . Here,  $B$  denotes the shortest of the *Bragg vectors* of the lattice. In our case, a *stop band*, in which sound does not propagate, appears for  $k$  beyond the limit. In general, a finite stopband forms around each of the "Bragg reflections", called a "gap" in the microscopic theory. For  $\omega \rightarrow 0$ , this dispersion law becomes simply  $\omega = ck$ , and this represents the *continuum limit* of the discrete model dynamics, while  $c$  is identified with the sound velocity in the chain. Finally, we may rewrite the expression for  $c$  in terms of macroscopic quantities:

$$c^2 = \frac{ka^2}{m} = \frac{ka}{m/a} \equiv \frac{\kappa}{\rho} \quad (1.11)$$

where  $\rho$  is the linear mass density and  $\kappa$  is identified with a corresponding elastic modulus.

In this identification, nothing really referred to any "atomic" nature of the elements of the chain, and a similar procedure would be appropriate for a macroscopic system, like, e.g., a 1D chain of balls representing the simplest thinkable granular system. In such a system, given the order of magnitude of sound velocities, the macroscopic periodicity of the system can easily be adjusted so that the stop band occurred in the range of accessible acoustic frequencies. Now the vicinity of such a "gap" would be susceptible to strong effects of the disorder, precisely like has been described for the electronic case. It would only take to create a nearly periodic system, in which the disorder would be superimposed over an underlying "crystal", to obtain a situation favorable for the occurrence of pronounced localization (see S. John: *in* [14] for the analogous case of light). Presently, both "photonic crystals" and "sonic crystals" are in real existence, and this line of investigation is open.

## 1.4 Wave equations in electrodynamics and elastodynamics

We return now to the classical continuous random media again. So far, we wrote down the wave equation for sound in a rash way. Now, we will obtain some of the differential equations for inhomogeneous media in a more careful systematic way. Naturally, it would be just as important to also give the appropriate form of the boundary conditions, but this we will improvise only to the inevitable extent in this brief overview.

### 1.4.1 Maxwell equations

Let us consider (general reference: [18]) a non-magnetic insulating isotropic continuous medium and let its dielectric function be local in space and time. By the last assumption, we exclude optical dispersion. All of the assumptions are mere simplifications, except for space locality, which is crucial for our treatment, in which the medium is represented by a single function of position,  $\varepsilon_r(\mathbf{r})$ .

The Maxwell equations supplemented by the material relations read

$$\begin{aligned} \text{rot } \mathbf{H}(\mathbf{r}, t) &= \dot{\mathbf{D}}(\mathbf{r}, t), & \text{div } \mathbf{D}(\mathbf{r}, t) &= 0, & \mathbf{D}(\mathbf{r}, t) &= \varepsilon_0 \varepsilon_r(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) \\ \text{rot } \mathbf{E}(\mathbf{r}, t) &= -\dot{\mathbf{B}}(\mathbf{r}, t), & \text{div } \mathbf{B}(\mathbf{r}, t) &= 0, & \mathbf{B}(\mathbf{r}, t) &= \mu_0 \mathbf{H}(\mathbf{r}, t) \end{aligned} \quad (1.12)$$

It is now straightforward to eliminate all other vectors in favor of  $\mathbf{E}$  and to obtain

$$\begin{aligned} -\text{rotrot } \mathbf{E}(\mathbf{r}, t) &= \varepsilon_0 \mu_0 \varepsilon_r(\mathbf{r}) \ddot{\mathbf{E}}(\mathbf{r}, t) \\ \Delta \mathbf{E}(\mathbf{r}, t) - \text{graddiv } \mathbf{E}(\mathbf{r}, t) &= c^{-2} \varepsilon_r(\mathbf{r}) \ddot{\mathbf{E}}(\mathbf{r}, t) \end{aligned} \quad (1.13)$$

In the second line we introduce the vacuum speed of light,  $c = (\varepsilon_0 \mu_0)^{-\frac{1}{2}}$ . The equation resembles quite closely in form the wave equation we used in Sec 1.2, but there is an additional term on the l.h.s., which is very important and cannot be ignored. First of all, neglecting it would lead to violation of the divergence condition for  $\mathbf{D}$ , and by this also to non-conservation of charge and of the field energy. Second, it follows from the divergence condition, that

$$\text{div } \mathbf{E} = -\text{grad } \log \varepsilon_r \cdot \text{grad } \mathbf{E} \quad (1.14)$$

so that the additional term is of the same order in the random field as the r.h.s. itself. Only in the homogeneous case, it does vanish. Finally, this term is physically important, because  $\text{div } \mathbf{E}$  gives the polarisation charge induced by the field of the wave on inhomogeneities of the medium. Thus, it leads to coupling of all polarisations of the wave traversing through the inhomogeneities. Other forms of the wave equation may be useful, or the Maxwell equations may be rearranged into a convenient system of first order equations [19].

### 1.4.2 Elastodynamic waves

The approach to elastodynamic waves we have in mind [20] belongs to linear elasticity, that is we assume that the displacements are small. Typically, the wave equations are written for the displacement field  $\mathbf{u}(\mathbf{r}, t)$ . Again, we have to combine the general equations of motion relating in this case the stress tensor  $\vec{\sigma}$  to the displacement field  $\mathbf{u}$ :

$$\text{div } \vec{\sigma}(\mathbf{r}, t) = \rho(\mathbf{r}) \ddot{\mathbf{u}}(\mathbf{r}, t) \quad (1.15)$$

with Hooke's law, but this is in general done more conveniently in the usual tensor notation.

$$\begin{array}{ll}
\sigma_{ij,j} = \rho \ddot{u}_i & \text{EULER EQUATION; } A_{ij\dots,k\ell\dots} \text{ stands for } \partial_k \partial_\ell \dots A_{ij\dots} \\
\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) & \text{DEFORMATION TENSOR - SYMMETRIC} \\
\sigma_{ij} = c_{ijkl} \epsilon_{kl} & \text{HOOKE'S LAW} \\
\left. \begin{array}{l} c_{ijkl} = c_{ijlk} \\ c_{ijkl} = c_{klij} \end{array} \right\} & \text{SYMMETRIES OF THE MODULI} \\
\boxed{(c_{ijkl} u_{k,l})_{,j} = \rho \ddot{u}_i} & \text{WAVE EQUATION - FINAL RESULT}
\end{array} \tag{1.16}$$

For clarity, the arguments of all quantities are suppressed, but, of course, the displacement  $u$ , the stress tensor  $\sigma$ , and the strain tensor  $\epsilon$  are functions of  $(\mathbf{r}, t)$ , the material constants are functions  $c_{ijkl}(\mathbf{r})$ ,  $\rho(\mathbf{r})$  of position. In the wave equation, the moduli are also subject to differentiation, and so the random fields cannot be reduced to just one position dependent velocity of sound. Much of the comments on the wave equation for light apply here without change. The gradient term cannot be left out, because that would change the structure of the equation in a dangerous way: it would cease to be self-adjoint, and, in consequence, energy conservation would be violated. These terms are also important for properly taking into account coupling between waves of different local polarisation.

## 1.5 Scalar wave equations

While a quantitative treatment of any realistic problem would require the use of the full vector wave equation, many of the salient features of the wave propagation in random media can be understood already from the much simpler case of a single scalar wave equation. This section will be devoted to a discussion of the options which are at hand when selecting a standard equation for the future work.

### 1.5.1 Sound waves revisited

As the first try, we will obtain the equation for sound propagation in an ideal fluid as a limit of the elastodynamic equations [20]. For an alternative derivation starting from the fluid dynamics see [21]. An ideal fluid is represented, in the context of linear elastodynamics, as an isotropic medium with a vanishing shear resistance. Thus, it has only one of its elastic moduli, namely the bulk modulus  $\kappa$ , different from zero, and its stress tensor is isotropic, i.e., purely compressive; its principal component is  $-p(\mathbf{r})$ , the negative of the local pressure. The general eqs. of Sec. 1.4.2 reduce to

$$\begin{array}{ll}
\sigma_{ij} = -p \cdot \delta_{ij} & \text{STRESS = PURE PRESSURE} \\
\epsilon_{ii} = u_{i,i} \equiv \theta & \text{DILATION} \\
c_{ijkl} = -\kappa \cdot \delta_{ij} \delta_{kl} & \text{ONLY BULK MODULUS NON-ZERO} \\
\left. \begin{array}{l} \sigma_{ij} = c_{ijkl} \epsilon_{kl} \\ p = -\kappa \cdot \theta \end{array} \right\} & \text{HOOKE'S LAW} \\
\boxed{(\kappa u_{k,k})_{,i} = \rho \ddot{u}_i} & \text{WAVE EQUATION - FINAL RESULT}
\end{array} \tag{1.17}$$

Note that even this equation is not scalar. Dividing by  $\rho$  and taking the divergence of both sides, we get, however, a single scalar equation for the dilation. Its solution plays the role of a scalar potential, because the whole displacement field can be reconstructed by inserting the known dilation into the original wave equation. Equivalently, an equation for the pressure serves the same purpose. The two equations, in vector form, read

$$\begin{aligned}
\text{div}(\rho^{-1} \text{grad}(\kappa \theta)) &= \ddot{\theta} \\
\text{div}(\rho^{-1} \text{grad} p) &= \kappa^{-1} \ddot{p}
\end{aligned} \tag{1.18}$$

Comparing this with the equation for  $\theta$  we used in Sec. 1.2, we may conclude that the simple guess used there was not quite correct; we used it for its simplicity, and also to have later the chance to point out its limitations.

### 1.5.2 A model scalar equation

Instead of following Lord Rayleigh, who used the pressure equation given above, we will select a model equation as our starting point. In doing so, we follow the practice, as it appears in many theoretical papers, cf. [14]. Namely, we define an artificial scalar "displacement" field  $u(\mathbf{r}, t)$ , which will satisfy a wave equation structurally analogous to the elastodynamic wave equations of Sec. 1.4.2, but with only one elastic modulus, which we denote  $\kappa$ , although its meaning may be very different from the real bulk modulus. Hence, we postulate

$$\boxed{\rho(\mathbf{r})\ddot{u}(\mathbf{r}, t) = \text{div}(\kappa(\mathbf{r})\text{grad}u(\mathbf{r}, t))} \quad (1.19)$$

It is instructive to compare this equation with the pressure equation for a fluid; the structure of both equations is identical, but the material parameters have interchanged their placement, but also appear as reciprocal in the pressure equation, so that in the homogeneous case, the phase velocity comes out identical for both. We may thus preserve for  $\kappa$  its interpretation of an elastic ("bulk") modulus. Although we did not show this in detail, it is clear that in 1D, the present wave equation corresponds to the continuum limit of the 1D chain discussed in Sec. 1.3. In that case, we have presented a precise interpretation of  $\kappa$ . Extending this interpretation also to 3D, we may say that  $\kappa$  controls the off-diagonal disorder, insofar it is random, while  $\rho$  keeps its natural relation to the diagonal randomness.

In conclusion, we will show that the model wave equation satisfies a relation, which can be interpreted as a differential (local) conservation of energy. Such conservation laws are very important for the consistency of the theory and indeed, the Schrödinger equation, Maxwell equations, and elastodynamic equations all satisfy well known conservation laws of this type. Note that we do not assume any specific form of the energy density, it will emerge by itself. It is enough to multiply the wave equation by  $\dot{u}$ :

$$\rho \dot{u} \ddot{u} = \text{div}(\kappa \text{grad} u) \dot{u} = \text{div}(\dot{u} \kappa \text{grad} u) - \text{grad} \dot{u} \cdot \kappa \text{grad} u \quad (1.20)$$

We obtain finally

$$\underbrace{\left(\frac{1}{2}\rho\dot{u}^2 + \frac{1}{2}\kappa|\text{grad}u|^2\right)}_{\text{ENERGY DENSITY}} + \text{div}\left(\underbrace{-\dot{u} \kappa \text{grad} u}_{\text{ENERGY CURRENT DENSITY}}\right) = 0 \quad (1.21)$$

with a very suggestive interpretation summarized in

$$\dot{w} + \text{div} \mathbf{J}_w = 0 \quad (1.22)$$

with obvious definitions.

## 1.6 General properties of wave propagation

Let us state several properties of wave propagation important for understanding the case of random media. As a representative example we take the equation

$$\rho(\mathbf{r})\ddot{u}(\mathbf{r}, t) = \text{div}(\kappa(\mathbf{r})\text{grad}u(\mathbf{r}, t)) \quad (1.23)$$

1. The *wave equation* itself has the following characteristics:

- ◇ it is linear
- ◇ second order in time (and also in coordinates)
- ◇ the coefficients of the equation (expressed in terms of  $\rho$  and  $\kappa$  and their derivatives) are functions of coordinates, but not of time
- ◇ it is selfadjoint, so that it has a positive energy density  $w(\mathbf{r}, t) \geq 0$  satisfying the differential conservation law  $\dot{w} + \text{div} \mathbf{J}_w = 0$

2. The *boundary conditions* have to specify that the system is either infinite, or closed
3. From this, the following basic properties of a solution  $u(\mathbf{r}, t)$  follow:
  - ◊ reciprocity in space (not discussed here)
  - ◊ *time reversal property* stating that also the field  $u(\mathbf{r}, -t)$  is a solution of the wave equation with the boundary conditions
  - ◊ global conservation of energy

$$W[u] \equiv \int d^3\mathbf{r} w = \text{const} \quad (1.24)$$

4. This in turn implies that

- ◊ The solution to an initial value problem specified by  $u(\mathbf{r}, t = 0)$  and  $\dot{u}(\mathbf{r}, t = 0)$  is unique
- ◊ During propagation, full coherence of the field is preserved and the distinction between two fields  $u, v$  (as measured by  $W[u - v]$ ) does not deteriorate
- ◊ Reconstruction of an initial field by time reversal of a signal registered at later times is possible [22]
- ◊ In frequency domain, the preservation of coherence is expressed by the fact that frequencies do not mix, that is, the wave equation goes over into a single frequency Helmholtz equation

$$\omega^2 \rho(\mathbf{r}) U(\mathbf{r}, \omega) + \text{div}(\kappa(\mathbf{r}) \text{grad} U(\mathbf{r}, \omega)) = 0 \quad (1.25)$$

To this, we want to add three general comments

**sound and other fields** The above properties are positively valid – as a matter of mathematical structure of the wave propagation. Of course, as mentioned already in 1.2, the Schrödinger field, for example, cannot be measured, only its modulus. On top of that, in the quantum realm, the measurement itself destroys the coherence and there is no way of measuring the wave function over a time interval other than repeating the experiment on an ensemble . . . Among the classical fields, which can in principle be measured without limitations, it is sound which is particularly suited for experiments concerning an individual sample: this is given by the favorable interplay of the frequency and wavelength ranges and by the availability of efficient amplitude sensitive detectors, among other things.

**random media and phase coherence** It would seem that all this cannot be true for random media, where the waves get splintered into an apparently chaotic mess, and our experience tells us that the waves propagate diffusively and eventually vane out. In fact, this may be true *from the point of view of an observer*. A coarse-graining of the signal received is implicit to our senses. It might seem impossible to measure the scattered field with absolute precision, of course, but, in fact, this is not necessary. A signal with a finite spectral content can be captured by an appropriate sampling, which may be extensive, but need not be infinitely detailed.

**implicit but crucial assumptions** There are three basic assumptions for the above discussion:

*The system in question must be ◊ linear, ◊ closed, ◊ non-dissipative.*

A non-linear system damages coherence by mixing frequencies, and it may assume a chaotic behavior, that is the solutions may be oversensitive to initial conditions; retracing our steps may be impossible. The other two conditions have something in common, namely the "energy" leaking out into the unknown. This results in several things, irreversibility, decoherence of the signal, that is phase breaking, and, finally, a complete decay of the field. These three threats to coherence are omnipresent, of course. The essence of any experimental design lies to a great degree just in finding conditions favorable for keeping the coherence during the observation time.

## 1.7 Dissipation

A closer look at the effect of dissipation will be useful later. A consistent way of introducing dissipation depends on the details of the system. For example, the fluid of 1.5.1 may be assumed to be viscous, more specifically e.g. Maxwellian [21]. In our scalar equation, the same effect is obtained by adding a linear dissipative term characterized by a single relaxation time  $\tau$ :

$$\begin{aligned}
 \rho \ddot{u} + \rho \tau^{-1} \dot{u} &= \text{div}(\kappa \text{grad} u) && \text{WAVE EQUATION WITH LINEAR DAMPING} \\
 \dot{w} + \text{div} \mathbf{J}_w &= -\rho \tau^{-1} \dot{u}^2 && \text{ENERGY DISSIPATED INTO THE R.H.S. SINK} \\
 \rho \omega^2 U + i \rho \tau^{-1} \omega U + \text{div}(\kappa \text{grad} U) &= 0 && \text{HELMHOLTZ EQUATION WITH LINEAR DAMPING} \\
 \rho (\omega + i(2\tau)^{-1})^2 U + \text{div}(\kappa \text{grad} U) &= 0 && \text{HELMHOLTZ EQUATION IN THE LIMIT } \omega \tau \gg 1 \\
 \rho (\omega + i0)^2 U + \text{div}(\kappa \text{grad} U) &= 0 && \text{FOR } \tau \rightarrow \infty, \text{ RETARDED UNDAMPED SOLUTION SELECTED}
 \end{aligned} \tag{1.26}$$

This chain of equations is self-explanatory, but we may elaborate on the notion of complex frequencies by considering plane waves in a homogeneous medium, that is take  $\kappa$ ,  $\rho$  as constants and make the ansatz

$$u(\mathbf{r}, t) = A \cdot e^{-i(\omega t - \mathbf{k} \cdot \mathbf{r})}, \quad \mathbf{k} = k \mathbf{e}, \quad \mathbf{e} \cdot \mathbf{r} \equiv x \tag{1.27}$$

with the sign convention customary in physics, and in agreement with the Helmholtz equation above. A secular equation follows:

$$(\omega + i(2\tau)^{-1})^2 = c^2 \cdot k^2 - \underbrace{(2\tau)^{-2}}_{\approx 0 \text{ for } \tau \rightarrow \infty}, \quad c^2 = \kappa \rho^{-1} \tag{1.28}$$

Two types of solutions correspond to  $\omega$  real (and positive) and  $k$  complex, or conversely.

$$\begin{aligned}
 k \text{ real} \quad \omega &= c \cdot k - i(2\tau)^{-1} && u = A \cdot e^{-i c k t} \cdot e^{-t/(2\tau)} \cdot e^{i k x} \\
 \omega \text{ real} \quad k &= \omega/c + i(2\tau c)^{-1} && u = A \cdot e^{-i \omega t} \cdot e^{i \omega c^{-1} x} \cdot e^{-x/(2\ell_{\text{in}})}
 \end{aligned} \tag{1.29}$$

By this, an *inelastic mean free path* is introduced as

$$\ell_{\text{in}} = \frac{1}{\tau c} \tag{1.30}$$

The two types of solution correspond to a standing wave decaying with the relaxation time  $\tau$ , and to a running wave attenuated at a rate  $\ell^{-1}$ . The factors of 2 at  $\tau$  and  $\ell$  are easily understood: they disappear on going from amplitudes to intensities by  $I = |u|^2$ .

# Chapter 2

## Lecture two: Multiple scattering in random media

### 2.1 Born approximation

We start with the simplest problem, scattering of a plane wave on a finite and weak obstacle, adapting to our wave equation the procedure due to Lord Rayleigh [1, pp. 149–154]. The analogy with quantum scattering is striking (cf. [3], but any textbook will do). Surprisingly enough, for some reason there was a tendency to "simplify" the task by leaving out some of the gradient terms with disastrous consequences, as described in [23].

Let the whole space be filled by a homogeneous medium with constant  $\bar{\kappa}$  and  $\bar{\rho}$ , except for a bounded region  $K$  centred at the origin of coordinates, where weak inhomogeneities appear:

$$\left. \begin{aligned} \kappa(\mathbf{r}) = \bar{\kappa} + \tilde{\kappa}(\mathbf{r}) &= \bar{\kappa} (1 + \tilde{\kappa}(\mathbf{r})/\bar{\kappa}) \equiv \bar{\kappa} (1 + \hat{\kappa}(\mathbf{r})), & \hat{\kappa} \ll 1 \\ \rho(\mathbf{r}) = \bar{\rho} + \tilde{\rho}(\mathbf{r}) &= \bar{\rho} (1 + \tilde{\rho}(\mathbf{r})/\bar{\rho}) \equiv \bar{\rho} (1 + \hat{\rho}(\mathbf{r})), & \hat{\rho} \ll 1 \end{aligned} \right\} \mathbf{r} \in K \quad (2.1)$$

The total field will have two parts, the incident ("free") plane wave  $\bar{u}$  and the scattered wave we have to determine. In the time-independent formalism,

$$U(\mathbf{r}) = \bar{U}(\mathbf{r}) + \tilde{U}(\mathbf{r}), \quad \bar{U}(\mathbf{r}) = U_0 e^{i\mathbf{k}_i \cdot \mathbf{r}}, \quad \mathbf{k}_i = k \mathbf{e}_i, \quad k = \frac{\omega}{c}, \quad c^2 = \frac{\bar{\kappa}}{\bar{\rho}} \quad (2.2)$$

The Helmholtz equation with the  $U(\mathbf{r})$  standing for  $U(\mathbf{r}, \omega)$

$$\omega^2 \rho(\mathbf{r}) U(\mathbf{r}) + \text{div}(\kappa(\mathbf{r}) \text{grad} U(\mathbf{r})) = 0 \quad (2.3)$$

can be rearranged to

$$(\omega^2 \bar{\rho} + \bar{\kappa} \Delta) \tilde{U}(\mathbf{r}) = -\omega^2 \tilde{\rho}(\mathbf{r}) U(\mathbf{r}) - \text{div}(\tilde{\kappa}(\mathbf{r}) \text{grad} U(\mathbf{r})) \quad (2.4)$$

This equation is exact. On the l.h.s., the differential operator corresponds to the unperturbed medium, and, hence, it yields zero when applied on the incident plane wave. Only  $\tilde{U}$  remains. The right hand side of the equation is also at least of first order in the disturbance.

Now, we have to impose the boundary conditions:

- ◇ infinite space
- ◇ retarded boundary condition (the scattered wave must obey causality and must be leaving the scattering region)
- ◇ the incident wave must select the correct solution.

All this is achieved by converting the differential equation into an integral one, which is then solved by iteration. The first iteration will be just the Born approximation. The procedure is standard, and in this particular case the needed expressions are all well known. The Green function of free space is defined by an inhomogeneous wave equation with a point source of unit strength,

$$((\omega + i0)^2 \bar{\rho} + \bar{\kappa} \Delta) G_0(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (2.5)$$

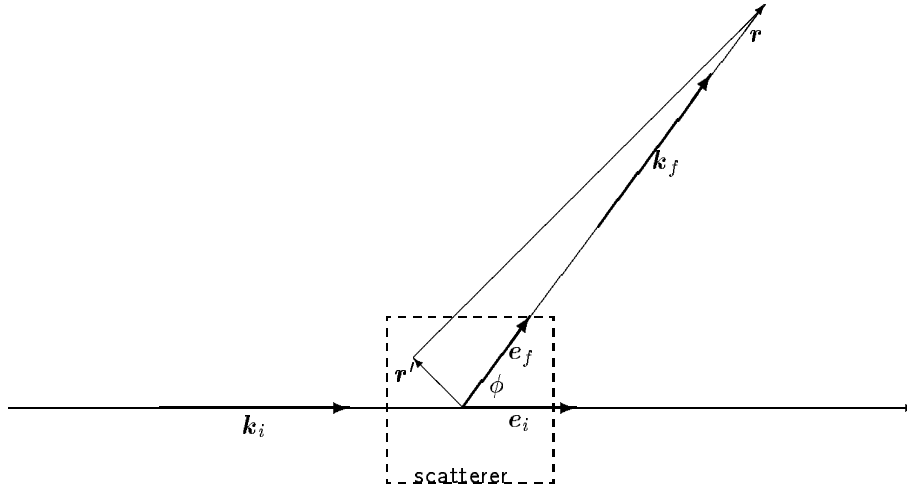
We indicate symbolically, in the sense of Sec. 1.7 that the solution needed is retarded. The appropriate solution, the well-known "retarded potential", reads

$$G_0(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi\tilde{\kappa}} \frac{e^{ikR}}{R}, \quad R = |\mathbf{r} - \mathbf{r}'| \quad (2.6)$$

Considering the right hand side of the above equation for  $\tilde{U}$  as a formal source, we obtain at once:

$$\tilde{U}(\mathbf{r}) = \int_{(\mathbf{K})} d^3\mathbf{r}' G_0(\mathbf{r}, \mathbf{r}') \cdot \{-\omega^2 \tilde{\rho}(\mathbf{r}') U(\mathbf{r}') - \text{div}'(\tilde{\kappa}(\mathbf{r}') \text{grad}' U(\mathbf{r}'))\} \quad (2.7)$$

#### FAR FIELD GEOMETRY FOR SCATTERING OF A PLANE WAVE



Now, to avoid the straightforward, but clumsy intermediate steps, we shall make two steps at once:

**1. Born approximation** In the integrand, the zeroth order approximation for  $U$  will be

$$U \xrightarrow{\text{BA}} U^{(0)} = \bar{U} \quad (2.8)$$

**2. Far field asymptotics** As shown in the sketch, we want to determine the scattering amplitude far from the scatterer in a direction  $e_f$ . There, the scattered wave becomes practically planar, with a wave vector  $\mathbf{k}_f = k e_f$ . This follows from the expansion in the exponent of the Green function,

$$R = |\mathbf{r} - \mathbf{r}'| \approx r - e_f \mathbf{r}', \quad \mathbf{r} = r e_f \quad (2.9)$$

The final result for the scattered wave becomes

$$\tilde{U}(r e_f) = \frac{\omega^2 U_0 e^{ikr}}{4\pi c^2 r} \cdot \left\{ \underbrace{\int d^3\mathbf{r}' \tilde{\rho}(\mathbf{r}') e^{i\mathbf{q} \cdot \mathbf{r}'} }_{\substack{\text{DIAGONAL DISORDER} \\ s\text{-wave}}} + \overbrace{(\mathbf{e}_i \cdot \mathbf{e}_f) \cos \phi}^{\text{OFF-DIAGONAL DISORDER}} \int d^3\mathbf{r}' \tilde{\kappa}(\mathbf{r}') e^{i\mathbf{q} \cdot \mathbf{r}'} \right\}, \quad \mathbf{q} = \mathbf{k}_i - \mathbf{k}_f \quad (2.10)$$

The following features of the scattered amplitude are to be noted:

- ◇ linearity in the incident amplitude  $U_0$ : the whole theory is linear
- ◇  $\omega^2$  dependence of *both* contributions, resulting in an  $\omega^4$ , that is  $\lambda^{-4}$  dependence of the intensity ...signature of the glorious RAYLEIGH SCATTERING



- ◇ linearity in the scattering potentials . . .signature of the Born approximation
- ◇ the decisive quantities are the *relative amplitudes* of the scattering potentials,  $\hat{\rho} = \tilde{\rho}/\bar{\rho}$ ,  $\hat{\kappa} = \tilde{\kappa}/\bar{\kappa}$
- ◇ the scattering amplitude is linear in the *structure factors*, that is, in the Fourier components of the scattering potentials. Only the *momentum transfer*  $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$  is important
- ◇ the  $\mathbf{q}$  - dependence includes the additional  $\omega$  dependence through the norm  $q \propto k = \omega/c$ , and the angular, or  $\phi$ , dependence. The denominations Rayleigh scattering, *s* - wave, and *p* - wave all correspond to the long wavelength limit. What we call the *s*-wave is, at small  $q$ , scattered isotropically, while the *p*-wave is, due to the cos factor, scattered preferentially in the forward and back directions. (The names are taken over from quantum theory, where they appeared first in connection with analogous symmetries of wave functiond in the hydrogen atom.)

**In the following, we shall consider only the diagonal scattering on the density fluctuations so as to keep the equations simple.**

So far, no specification was made about the nature of the scatterers. We have in mind a random medium. That means that, however small may the region  $\mathbf{K}$  be compared to the whole scattering setup, it still is assumed to be composed of many scattering centers, or, more generally, to be macroscopic with respect to the random potential fluctuations, and to be statistically homogeneous. These concepts would require a more cautious analysis, but their intuitive meaning is clear. The intensity of the scattered wave

$$|\tilde{U}(\mathbf{r}\mathbf{e}_f)|^2 = \frac{\omega^4 U_0^2}{16\pi^2 c^4} \cdot \frac{1}{r^2} \cdot \int d^3\mathbf{r}' \int d^3\mathbf{r}'' \hat{\rho}(\mathbf{r}') \hat{\rho}(\mathbf{r}'') e^{i\mathbf{q}\cdot(\mathbf{r}'-\mathbf{r}'')} \quad (2.11)$$

then becomes

$$|\tilde{U}(\mathbf{r}\mathbf{e}_f)|^2 = \frac{\omega^4 U_0^2}{16\pi^2 c^4} \cdot \frac{1}{r^2} \cdot \int d^3\mathbf{r}_d B(\mathbf{r}_d) e^{i\mathbf{q}\cdot\mathbf{r}_d} \quad (2.12)$$

where  $\Omega[\mathbf{K}]$  denotes the volume of the disordered region, and where we introduce a *dimension-less static density density correlation function*

$$B(\mathbf{r}_d) = \frac{1}{\Omega[\mathbf{K}]} \cdot \int d^3\mathbf{r}' \hat{\rho}(\mathbf{r}' + \mathbf{r}_d) \hat{\rho}(\mathbf{r}') \quad (2.13)$$

Is is apparent that this construction makes sense only in the case that the *correlation radius* of the disorder, beyond which the correlation function will be negligible, will be small compared to the size of the sample, so that the surface regions would play no role, and the sample will appear as statistically homogeneous. It is also apparent that in this manner, a new element is introduced into the description, namely the notion of *averaging*. The details of the local structure are not important, only the overall character of the disorder. The question, under which conditions this is permissible, and what is getting lost, will be among the central questions we intend to address.

## 2.2 Green function of the wave equation

### 2.2.1 Definition and basic properties

In principle, the method of the preceding section could be extended also to better approximations than a mere first iteration. There are important reasons, however, for introducing Green functions and work with them rather than with the wave fields themselves. The procedure is standard in the theory of partial differential equations and we will again just quote a few crucial points. A standard reference is [24]. In fact, we had a respectable Green function already, but now we assume a slightly different starting point, based on the following considerations:

#### REQUIREMENTS ON A PROPER GREEN FUNCTION

requirement	serves purpose
GF of the <i>true</i> wave equation	universal solver for all initial conditions
defined in <i>time domain</i>	allows to study pulses, transients, echos
satisfies prescribed <i>boundary conditions</i>	defines the "setup": resonator, waveguide,...
select the <i>retarded</i> GF	causality with the "natural" arrow of time

The prescription for getting the GF is then as follows:

- 1. equation of motion** Only the normalisation requires some thought; ours is such that the frequency dependent GF reduces for free space to the expression in the Sec.2.1. Otherwise, it is the wave equation with a point source:

$$\rho(\mathbf{r})\partial_{tt}G(\mathbf{r}, t; \mathbf{r}', t') - \operatorname{div}(\kappa(\mathbf{r})\operatorname{grad}G(\mathbf{r}, t; \mathbf{r}', t')) = \delta(t - t')\delta(\mathbf{r} - \mathbf{r}') \quad (2.14)$$

The Green function has *two* space-time arguments, the other referring to the position of the source. It is thus rather a continuous matrix, or a kernel of an integral operator than a function proper.

- 2. boundary conditions** The GF is defined on a space-time domain  $(\mathbf{r}, t) \in \mathbf{D} \otimes \mathbb{R}$ , where  $\mathbf{D}$  may be a finite or infinite connected region of space satisfying some "normality conditions". The boundary conditions should be homogeneous and time-independent; the simplest, but by no means obvious, such condition would be

$$G(\mathbf{r}_s, t; \mathbf{r}', t') = 0, \quad \text{for all times } t, t' \text{ and } \mathbf{r}_s \in \partial\mathbf{D}, \mathbf{r}' \in \mathbf{D} \quad (2.15)$$

- 3. retarded boundary condition** It is required that for all  $\mathbf{r}, \mathbf{r}'$ :

$$G(\mathbf{r}_s, t; \mathbf{r}', t') = 0, \quad \text{for } t \leq t' \dots \text{RETARDED GF} \quad (2.16)$$

For a second order equation, we also need to know about the time derivative, i.e., the velocity of the field. The boundary condition together with the equation of motion yields

$$\partial_t G(\mathbf{r}, t = t' + 0; \mathbf{r}', t') = -\delta(\mathbf{r} - \mathbf{r}')\rho^{-1}(\mathbf{r}'), \quad \text{INITIAL BOOSTER} \quad (2.17)$$

It can be checked directly that this GF solves the initial value problem, that is for initial field and field velocity,  $u(\mathbf{r}, 0), \dot{u}(\mathbf{r}, 0)$ , the solution of the wave equation for all positive times is

$$u(\mathbf{r}, t > 0) = - \int d^3\mathbf{r}' \{ \partial_t G(\mathbf{r}, t; \mathbf{r}', 0)u(\mathbf{r}', 0) + G(\mathbf{r}, t; \mathbf{r}', 0)\dot{u}(\mathbf{r}', 0) \} \rho(\mathbf{r}') \quad (2.18)$$

Other problems, like injection of a pulse through the boundary, volume sources, etc., can be expressed with the help of the GF as well ([20]).

## 2.2.2 Fourier transformation

[NOTE] The convention used in these notes is the usual one in physics, thus:

$$\begin{aligned} f(t) &= \int \frac{d\omega}{2\pi} F(\omega) e^{-i\omega t} & \longleftrightarrow & & F(\omega) &= \int dt f(t) e^{i\omega t} \\ f(\mathbf{r}) &= \int \frac{d^3k}{(2\pi)^3} F(\mathbf{k}) e^{-i\mathbf{k}\mathbf{r}} & \longleftrightarrow & & F(\mathbf{k}) &= \int d^3\mathbf{r} f(\mathbf{r}) e^{i\mathbf{k}\mathbf{r}} \end{aligned} \quad (2.19)$$

The Green function depends in principle on two times and two positions. That would mean in general a double Fourier transform. We are concerned only with time invariant systems, whose properties do not change with time. By this, the GF depends only on the time difference  $t - t'$  and the FT can be performed with respect to this difference. Of course, an inhomogeneous Helmholtz equation results, generalizing the homogeneous case of Sec. 2.1:

$$(\omega + i0)^2 \rho(\mathbf{r}) G(\mathbf{r}, \mathbf{r}'; \omega + i0) + \text{div}(\kappa(\mathbf{r}) \text{grad} G(\mathbf{r}, \mathbf{r}'; \omega + i0)) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.20)$$

For convenience, we repeat here the equation defining the GF for the homogeneous ("unperturbed") medium:

$$((\omega + i0)^2 \bar{\rho} + \bar{\kappa} \Delta) G_0(\mathbf{r}, \mathbf{r}'; \omega + i0) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.21)$$

The situation is different for space coordinates: our system is inhomogeneous indeed, and two  $k$ -vectors have to be introduced, which makes sense only if  $\mathbf{D}$  is extended anyhow. We will not do it. Only for a homogeneous medium with translational invariance in space, a single FT with respect to the position difference yields

$$((\omega + i0)^2 \bar{\rho} - k^2 \bar{\kappa}) G_0(\mathbf{k}; \omega + i0) = 1 \quad (2.22)$$

Writing this equation as

$$G_0(\mathbf{k}; \omega + i0) = \frac{1}{(\omega + i0)^2 \bar{\rho} - k^2 \bar{\kappa}} \quad (2.23)$$

we see two things. First, the poles of this expression for the GF give us the dispersion law in the form  $\omega^2 = (ck)^2$ . If not for the infinitesimal imaginary part of the frequency the expression for GF would be indefinite. Being positive, it interprets the pole in the retarded sense. In other words, the *poles* acquire small negative imaginary parts, and we know already from Sec. 1.7 that this corresponds to a weak dissipation and to the retarded solution, as required.

## 2.3 Operator form of the Green function equations

### 2.3.1 Integral equations for GF

The advantage of using  $G_0$  in Sec. 2.1 was that it took care of the boundary conditions automatically. We want to extend this and convert the equations for the GF into *integral equations*. It is easier to follow the process in the frequency domain. It should be borne in mind that there is the one-to-one correspondence with the time domain, and all equations in one domain can be mapped isomorphically onto the other domain. Repeating almost step by step what we did in Sec. 2.1, we transform the equation for  $G(\mathbf{r}, \mathbf{r}'; \omega + i0)$  to the integral form:

$$G(\mathbf{r}, \mathbf{r}'; \omega + i0) = \int d^3\mathbf{y} G_0(\mathbf{r}, \mathbf{y}; \omega + i0) \cdot \{ \delta(\mathbf{y} - \mathbf{r}') + [-\omega^2 \tilde{\rho}(\mathbf{y}) - \text{div}(\tilde{\kappa}(\mathbf{y}) \bullet)] G(\mathbf{y}, \mathbf{r}'; \omega + i0) \} \quad (2.24)$$

The heavy dot indicates the place within the differential operator, where the  $G$  function should be inserted. This is already the desired equation. We will rewrite it once more, defining a new function of two arguments, representing the *perturbation*, which may alternatively be also called "scattering potential, random field," etc.

$$V(\mathbf{y}, \mathbf{z}) = [-\omega^2 \tilde{\rho}(\mathbf{y}) - \text{div}(\tilde{\kappa}(\mathbf{y}) \bullet)] \delta(\mathbf{y} - \mathbf{z}) \quad (2.25)$$

The equation now becomes

$$G(\mathbf{r}, \mathbf{r}'; \omega + i0) = G_0(\mathbf{r}, \mathbf{r}'; \omega + i0) + \int d^3\mathbf{y} \int d^3\mathbf{z} G_0(\mathbf{r}, \mathbf{y}; \omega + i0) \cdot V(\mathbf{y}, \mathbf{z}) \cdot G(\mathbf{z}, \mathbf{r}'; \omega + i0) \quad (2.26)$$

We noticed already that  $G$  looks like the kernel of an integral operator, and indeed, we see that it functions precisely that way, resembling entirely a continuous matrix. It is then very economical to use this analogy and spare ourselves the effort of writing the integrals explicitly. Using the rule (of matrix multiplication)

$$C = AB \iff C(\mathbf{r}, \mathbf{r}') = \int d^3\mathbf{y} A(\mathbf{r}, \mathbf{y}) B(\mathbf{y}, \mathbf{r}') \quad (2.27)$$

we get finally the following equation, which is the real starting point for all formal work with Green functions:

$$G(\omega + i0) = G_0(\omega + i0) + G_0(\omega + i0) V G(\omega + i0) \quad (2.28)$$

We did not indicate the  $\omega$ -dependence of  $V$ , but its argument can be (and in our case really is) just  $\omega$  again. This is the advantage of the frequency domain: the frequency is simply one and the same in all quantities entering one equation. In the time domain, the form of the equations is less pleasant, although it is intuitively appealing. On Fourier transforming a product of two functions of frequency, a time convolution of both transforms results:

$$\begin{aligned} C(\mathbf{r}, \mathbf{r}'; \omega) &= \int d^3\mathbf{y} A(\mathbf{r}, \mathbf{y}; \omega) B(\mathbf{y}, \mathbf{r}'; \omega) \\ &\downarrow \\ C(\mathbf{r}, \mathbf{r}'; t - t') &= \int ds \int d^3\mathbf{y} A(\mathbf{r}, \mathbf{y}; t - s) B(\mathbf{y}, \mathbf{r}'; s - t') \end{aligned} \quad (2.29)$$

In the equation for  $G$ , we would have two subsequent convolutions, and so on. From now on, we will use the convention that

**wherever possible, the GF equations will be written in the symbolic, or algebraic form. Depending on the choice of representation, the above rules permit an unequivocal recovery of the fully explicit equations involving all arguments.**

The *integral equation for the Green function* then reads

$$\boxed{G = G_0 + G_0 V G} \quad (2.30)$$

We may go even further and draw very suggestive pictures:

DIAGRAM REPRESENTATION OF THE INTEGRAL EQUATION FOR GF

$$\text{====} = \text{---} + \text{---} \bullet \text{====}$$

Meanings of all symbols follow from a comparison with the equation above.

[NOTE] The operators, as we have defined them form an *algebra*. This means that there are two binary operations, *addition* and *multiplication*, and an unary operation, multiplication by a number, which give again an operator. There exists also an *operator zero*  $O$  and an *operator unity*  $1$ . With that, the *negative* of  $A$  is defined by  $A + (-A) = O$ , and the *inverse operator* by  $AA^{-1} = A^{-1}A = 1$ . All these operations and objects have the usual properties, and for that reason it is possible to perform the manipulations on a formal level. Care should be taken of two properties of multiplication:

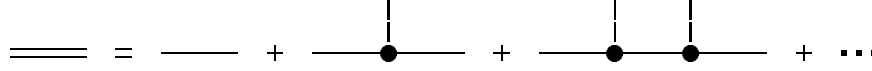
- ◊It is not commutative, that is, in general,  $AB \neq BA$
- ◊It is not always invertible, just like it is not allowed to divide by zero.

## 2.4 Born expansion, $T$ -matrix

Eq. (2.30) is a closed exact *equation*. The most common way how to generate its (approximate) explicit solution  $G$  is to make an expansion in terms of a small parameter. Depending on the situation, this might be, for example, the density of scatterers, or just on the contrary, the average separation between them, provided that the random potential is composed of individual scattering centers, of course. In general, the most obvious idea is to expand in terms of the strength of the scattering potential  $V$ . The expansion is easily obtained by iterating (2.30):

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots \quad \text{BORN EXPANSION OF } G \quad (2.31)$$

or, in the diagrammatic form,



The first two terms of the expansion correspond to the Born approximation of Sec. 2.1. The higher order terms correspond to repeated scatterings on the potential  $V$ , and in this sense, it is sometimes said that the Born approximation corresponds to single scattering, while the full Green function corresponds to a *multiply scattered wave*. It should be remembered, however, that the GF is a coherent superposition of the amplitudes corresponding to *all* orders, and that something like a "triple scattered wave" has only a very limited significance.

Inspecting the Born series, we see that all terms have a symmetric structure, and the unidirectional structure of (2.30) has disappeared. In fact, we get that the same series is obtained also by expanding the equation

$$G = G_0 + G V G_0 \quad (2.32)$$

which is a second equivalent form of (2.30).

A very important form of  $G$  results, if the symmetry of the Born expansion is kept, and the so-called *scattering matrix*, or *T-matrix* is introduced:

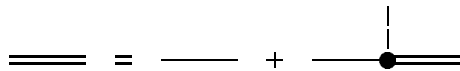
$$\begin{aligned} G &= G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots \\ &= G_0 + G_0 (V + G_0 V G_0 V + \dots) G_0 \\ &\equiv G_0 + G_0 T G_0 \quad \text{T-MATRIX DEFINED} \end{aligned} \quad (2.33)$$

The T-matrix is another very important formal tool of the theory. As we see, it gives the GF a form resembling the Born approximation, but it incorporates the scattering to all orders. We have derived presently two exact closed equations on the basis of rearranging the Born expansion. It can be objected that the series may not converge at all, and the derivations are then spurious. In fact, the procedure adopted *is* legitimate, and in a common use. Let us, however, arrive at the expression for the  $T$ -matrix in a formally impeccable way:

$$\begin{aligned} T G_0 &= V G && \text{DEFINITION OF THE T-MATRIX} \\ T G_0 &= V (G_0 + G_0 T G_0) && \text{REINSERTED ON THE R.H.S.} \\ \boxed{T = V + V G_0 T} &&& \text{INTEGRAL EQUATION FOR } T \end{aligned} \quad (2.34)$$

In diagrams:

DIAGRAM REPRESENTATION OF THE INTEGRAL EQUATION FOR THE T MATRIX



$$\equiv \text{---} + \text{---} \overset{T}{\blacksquare}$$

$$\overset{T}{\blacksquare} = \overset{|}{\bullet} + \overset{|}{\bullet} \text{---} \overset{T}{\blacksquare}$$

## 2.5 Multiple scattering expansion

A very important expansion of the total Green function, or, equivalently, of the scattering matrix may be developed, if we assume that

*the scattering potential  $V$  is composed of contributions from a number of individual scatterers:*

$$V = \sum_i V_i \tag{2.35}$$

This general assumption can be made more specific by prescribing the nature of the scatterers, their distribution in space and their quantitative characteristics. In an alloy, the scatterers are atoms of different species. In an emulsion, the scatterers will be the inclusions, that is, droplets of a fluid with properties different from the host liquid.

It is very suggestive to insert the Eq. (2.35) into (2.30) with the following interpretation:

$G$	=	$G_0$	$+G_0 V G$
TOTAL WAVE	=	INCIDENT WAVE	SCATTERED WAVE
$G_0 V G = \sum_i G_0 V_i G$			
SCATTERED WAVE	=	SUM OF $i$ -CONTRIBUTIONS	
$G_0 V_i \qquad G$			
$i$ -TH CONTRIBUTION	=	WAVELET FROM THE $i$ -TH SCATTERER	IRRADIATED BY TOTAL WAVE
? ? ?			

Only the part of interpretation marked by question marks is not satisfactory, because the self-irradiation of the centers is not prevented. At the same time, we have  $V_i$  as the strength of the last scattering off the  $i$ -th center, while the correct measure of that event should be *the one center scattering matrix*, which takes care of all multiple scatterings on the  $i$ -th potential:

$$T_i = V_i + V_i G_0 T_i \tag{2.37}$$

The correct multiple-scattering formulation is then given by the following chain of equations, conveniently

employing the  $T$ -matrix instead of  $G$ :

$$\begin{aligned}
G &= G_0 + G_0 T G_0 \\
T &= \sum_i Q_i \\
Q_i &= V_i (G_0 + G_0 \sum_j Q_j) \\
&= V_i \times \text{TOTAL FIELD (as before)}
\end{aligned} \tag{2.38}$$

$$\begin{aligned}
Q_i &= T_i (G_0 + G_0 \sum_{j \neq i} Q_j) \\
&= T_i \times \text{TOTAL FIELD WITH } i\text{-TH CONTRIBUTION EXCLUDED !!!}
\end{aligned}$$

The crucial *technical* step is to solve the third equation for  $Q_i$  and to employ the definition (2.37) of  $T_i$ . *Physically*, this means that a so-called *local field* acting at the center in question is introduced, very much like the Lorentz field in the theory of dielectric polarisation.

The so-called *multiple-scattering exclusions* make the resulting system of equations harder handle, but they provide a very satisfactory picture from the physical point of view. They are free of the previous contradictions. The scatterer is only weakly statistically correlated with the acting local field and this provides the starting point for the whole family of mean field theories including the CPA. When iterating these equations, the multiple scattering exclusions appear at each step: never does the wave scatter twice in a row on the same center:

$$T = \sum_i T_i + \sum_i \sum_{j \neq i} T_i G_0 T_j + \sum_i \sum_{j \neq i} \sum_{l \neq j} T_i G_0 T_j G_0 T_l + \dots \tag{2.39}$$

*The sum for  $T$  can be rearranged into a sum over all distinct scattering paths. Each path is given by an oriented connected graph having an initial point and an end point and an arbitrary number of steps in between.* Some of the paths may be "self-avoiding", but that is not a rule, and the path may have loops of arbitrary complexity. We should not mistake such a graphical representation for a classical random walk. One path means a succession of Huyghens wavelets propagating in succession from one center to the other. This leads to complicated phase relations dependent on the topological structure of the path, and just this wave property of the multiple scattering of waves gives rise to "non-classical" phenomena like localisation.

To illustrate the qualitative importance of multiple scattering, we indicate its link to the phenomenon of *speckles*. In the scattering of waves in random media, the speckles are a rule rather than an exception. This can be understood as follows. The scattered wave is a superposition of partial waves coming from all paths. Because of the multiple scattering effect, the wave is said to be *incoherently* scattered, and we will give an interpretation of that slightly misleading term later. As we have stressed in Lecture 1, the coherence of the wave undergoing a purely elastic scattering is, in fact, fully preserved. However, the total phase becomes extremely sensitive to small variations in, say, the angle of reception of the scattered wave, the spectral composition of the wave, etc., and this leads to an irregular, but fully deterministic oscillation of the intensity of the scattered wave. This is the speckle behavior. The variation of the intensity is not infinitely fast with the changing parameter, because there always exists a correlation in the values of the signal within a *coherence zone*, which depends on the wavelength of the scattered wave. Still, it is justified to speak about a statistical distribution of the speckle intensities. We want to show, following [25], that assuming bluntly than a random distribution of the phase of the partial waves coming from different paths, it may be derived that the statistical dispersion of the intensity in a speckle pattern equals to its mean value. Let us write the measured amplitude in the form

$$E = \sum_{\text{PATHS}} f e^{i\phi} \quad (2.40)$$

$$E_R + iE_I = \sum_{\text{PATHS}} f \cos \phi + i \sum_{\text{PATHS}} f \sin \phi \quad (2.41)$$

Assuming that the phase of each path varies greatly and that the paths are not correlated (this assumption *is* an oversimplification because of the crossing paths), the sum of cosines and the sum of sines are two uncorrelated Gaussian variables, as is known from elementary statistical theory. We will be interested in the statistics of the intensity  $I = |E|^2 = E_R^2 + E_I^2$ . With our assumptions, the statistical averages obey

$$\langle E_R^2 \rangle = \langle E_I^2 \rangle = \frac{1}{2} \langle I \rangle, \quad \langle E_R E_I \rangle = 0 \quad (2.42)$$

The joint two-dimensional statistical distribution is then

$$p(E_R, E_I) = \frac{1}{\pi \langle I \rangle} e^{-(E_R^2 + E_I^2)/\langle I \rangle} \quad (2.43)$$

From this, the distribution for the intensity is exponential,

$$p(I) = \int dE_R dE_I p(E_R, E_I) \delta(E_R^2 + E_I^2 - I) = \frac{1}{\langle I \rangle} e^{-I/\langle I \rangle} \quad (2.44)$$

and an easy integration yields that the intensity fluctuations are as large, as they can be:

$$\langle (I - \langle I \rangle)^2 \rangle = \langle I \rangle^2 \quad (2.45)$$



## 2.6 Configuration Averaging

So far, our Green functions were related to *one sample*. At various places, it was clear that it should not be completely arbitrary, but that it should be "typical", possessing some kind of regularity on a statistical level. In fact, we have already performed an averaging in Sec. 2.1 in order to define the pair correlation function of the random scattering potential. We may repeat the equation (2.13) here:

$$B(\mathbf{r}_d) = \frac{1}{\Omega[\mathbf{K}]} \cdot \int d^3\mathbf{r}' \hat{\rho}(\mathbf{r}' + \mathbf{r}_d) \hat{\rho}(\mathbf{r}') \quad (2.46)$$

Two points were essential for this definition to be of reasonable validity:

- ◇ The correlation range had to be small compared to the size of the sample
- ◇ The sample was assumed to be statistically homogeneous

When this was valid, the integration was in fact a way of scanning the sample at a statistically significant number of different places. The local properties of the sample were fluctuating in space, but at the same time the gradually accumulated integral converged to a limit in statistical sense.

A similar reasoning leads to computing such characteristics of the sample as the average density and the average modulus:

$$\rho_{\text{Ave}} = \frac{1}{\Omega[\mathbf{K}]} \cdot \int d^3\mathbf{r}' \rho(\mathbf{r}'), \quad \kappa_{\text{Ave}} = \frac{1}{\Omega[\mathbf{K}]} \cdot \int d^3\mathbf{r}' \kappa(\mathbf{r}') \quad (2.47)$$

This, of course, is still not *configuration averaging*, which plays such an important role in all Green function investigations. This has to be done differently. In order to talk about a configuration average, we have first to specify the statistical ensemble, to which our sample(s) belong(s). The whole idea is very similar to a careful preparation of experimental samples:

### ABOUT THE DEFINITION OF CONFIGURATION AVERAGE

concept	operational meaning
configuration	sample
configuration ensemble	protocol for preparation of samples
external parameters	control values for sample characterisation

A *configuration average* is thus a kind of statistical average over all samples ("configurations") representative of a given instance of disorder. Intuitively, the notion is obvious. A precise definition and an operational interpretation are rather subtle tasks, and we say a few words about this problem, because an ample use of configuration averages is to come below, and, as said, it is central to most of the theoretical work.

Suppose a physical quantity  $\Phi$  is a functional of configuration  $\mathbf{c}$ . To find the configuration average, we have to know the probabilities  $p(\mathbf{c})$  defining the statistical ensemble of configurations. The configuration average is then defined by

$$\langle \Phi \rangle \equiv \sum_{\mathbf{c}} p(\mathbf{c}) \Phi[\mathbf{c}] \quad (2.48)$$

We may rewrite this by introducing a distribution for  $\Phi$ :

$$\langle \Phi \rangle = \int d\varphi \sum_{\mathbf{c}} p(\mathbf{c}) \delta(\varphi - \Phi[\mathbf{c}]) \cdot \varphi \equiv \int d\varphi W_{\Phi}(\varphi) \cdot \varphi \quad (2.49)$$

Configuration average makes sense only if  $W_{\Phi}$  is sharp enough. In that case, the average may be found either from the definition, or by finding a "typical configuration"  $\mathbf{c}^*$ ,

$$\langle \Phi \rangle = \Phi[\mathbf{c}^*], \quad \delta W_{\Phi}(\Phi[\mathbf{c}]) / \delta \mathbf{c} |_{\mathbf{c}=\mathbf{c}^*} = 0 \quad (2.50)$$

Either definition has serious practical problems, but in any case we have first to justify the idea of configuration averaging. The theory has been developed for infinite samples. The analogy with ensembles of statistical mechanics is apparent. Indeed, of the two requirements which we have discussed already :  
 $\diamond$  spatial homogeneity of the sample  $\diamond$  finite range of statistical correlations in the ensemble, the latter condition coincides with what appears also in statistical mechanics, while the former one is more subtle: it replaces the temporal homogeneity required for (quasi)ergodic behavior by a sort of "ergodicity in space". With these two assumptions, extensive quantities can be shown to be macroscopically additive, and their densities  $\langle \Phi \rangle / \Omega$  to possess a thermodynamic limit, as the volume of the sample  $\Omega$  tends to infinity:

$$\frac{\langle (\Phi - \langle \Phi \rangle)^2 \rangle}{\langle \Phi \rangle^2} \xrightarrow{\Omega \rightarrow \infty} 0 \quad (2.51)$$

This thermodynamic limit can be calculated by the space-averaging procedure described above, provided the sample used is one of the "typical" configurations  $\mathbf{c}^*$ . Such quantities are called *self-averaging*, while the others, in particular various local characteristics, lead to no thermodynamic limit and are thus termed *non-self-averaging*.

For our purposes, it is important to state that completely random substitutional alloys, arrays of completely randomly distributed point-like scatterers in homogeneous space, and other reasonable systems satisfy the above two conditions. The whole subject of self-averaging got a proper treatment mainly thanks to the Kharkov school and a competent and definitive account can be found in [26] [27].

## 2.7 Averaged Green function: Coherent wave

### 2.7.1 Dyson equation

So far, the picture of wave propagation in a random medium was that introduced in Sec 2.1. There existed a reference homogeneous medium, and an incident wave propagating through it. The wave hit on a scatterer and the total wave then consisted of the incident wave plus the scattered wave. There emerge two flaws in this description, once we become concerned with a wave propagating in an extended sample, which for practical purposes may appear as basically *infinite*.

1. There is no well defined *asymptotic region* with no scatterers, which would permit to uniquely specify the reference "free propagation" medium, and the corresponding incident wave
2. Even if we settled for some choice about these two things, the separation into an incident and a scattered wave would remain operationally meaningless. On the one hand, it would depend on the subjective choice made. On the other hand, and more significantly, if anything propagates in a "macroscopically coherent" fashion through the medium at all, it is bound to be an attenuated wave, which gradually decays because of the scattering losses.

In a random medium, which satisfies the conditions for configuration averages (which we will from now on tacitly assume), the *coherent wave* can be conveniently defined by

$$u_{\text{coh}}(\mathbf{r}, t) \equiv \langle u(\mathbf{r}, t) \rangle \quad \text{DEFINITION OF COHERENT WAVE} \quad (2.52)$$

We will show in Sec. 2.8.3 that the coherent wave defined in this way has a self-averaging character and, consequently, it is meaningful even for one configuration.

This definition is in a natural way transferred on the Green function as well, and this allows to select the *effective medium* for the averaged propagation as well. We will use rather an overbar than the subscript "coh" to denote the averaged GF:

$$\overline{G} \equiv \langle G \rangle \quad \text{COHERENT WAVE} \quad (2.53)$$

$$G = G_0 + G_0 V G \quad G \text{ FOR ONE CONFIGURATION} \quad (2.54)$$

$$\overline{G} = G_0 + G_0 \langle V G \rangle \quad \text{CONFIGURATION AVERAGE OF A PRODUCT} \quad (2.55)$$

$$\langle V G \rangle = \Sigma \langle G \rangle \quad \text{DEFINITION OF SELF-ENERGY } \Sigma \quad (2.56)$$

$$\overline{G} = G_0 + G_0 \Sigma \overline{G} \quad \text{DYSON EQUATION} \quad (2.57)$$

By these definitions, we have replaced a (possibly local) real random scattering potential  $V$  by the self-energy  $\Sigma$ , which describes a translationally invariant (i.e., homogeneous) effective medium. Because this effective medium has to capture the effect of the random fluctuations of  $V$ , the self-energy  $\Sigma$  cannot be just a number like  $\rho$ , say,  $\langle \rho \rangle$ . In fact, the self-energy has in general a rather complex structure. The same properties appear in various representations as follows:

REPRESENTATION	PROPERTY OF $\Sigma$
$(\mathbf{r}, t)$	non-local in space non-local ( <i>retarded</i> ), in time, just like the GF
$(\mathbf{r}, \omega)$	non-local in space <i>and</i> frequency dependent complex-valued ( <i>retarded</i> ... $\omega + i0$ -dependence)
$(\mathbf{k}, \omega)$	wave vector <i>and</i> frequency dependent complex-valued ( <i>retarded</i> ... $\omega + i0$ -dependence)

## 2.7.2 Pole Green function

Before entering any specific approximation, we want to discuss a widely used approximate form of the Green function. It consists in replacing the true GF with the self-energy really  $\omega$ ,  $\mathbf{k}$ -dependent by a function having simple poles in the frequency dependence, whose location depends only on  $\mathbf{k}$ . This is the *pole Green function*, and it corresponds to the *quasiparticle states* of the microscopic solid state theory.

The imaginary part of the self-energy is responsible for the attenuation of the coherent wave. In the  $(\mathbf{k}, \omega)$  representation, the Dyson equation (2.57) reads

$$((\omega + i0)^2 \bar{\rho} - \bar{\kappa} k^2 - \Sigma(\omega + i0, \mathbf{k})) G_0(\omega + i0, \mathbf{k}) = 1 \quad \text{REFERENCE GF} \quad (2.58)$$

$$((\omega + i0)^2 \bar{\rho} - \bar{\kappa} k^2 - \Sigma(\omega + i0, \mathbf{k})) \bar{G}(\omega + i0, \mathbf{k}) = 1 \quad \text{AVERAGED GF} \quad (2.59)$$

$$(2.60)$$

This does not tell too much in general, but it may be shown that, for the retarded GF,  $\text{Im}\Sigma(\omega + i0) \leq 0$ . Suppose now, as is often the case, that  $\Sigma$  does not vary too fast around the pole  $\omega = ck$  of the reference medium. Then the full GF will also have a pole given (in a rough estimate) by

$$\bar{\rho} \omega_{\text{pole}}^2 + i|\text{Im}\Sigma(ck + i0)| - \bar{\kappa} k^2 - \text{Re}\Sigma = 0 \quad (2.61)$$

For real  $k$ , the pole will be complex. The real part of the  $\omega_{\text{pole}}(k)$  dependence describes the *renormalisation of the phase velocity* of the waves. We will not be much concerned with this effect. The imaginary part, if it is not too large, may be neatly combined with  $\omega^2$ , just like we did in Sec. 1.7. There, we found that the pole had an imaginary part

$$\omega_{\text{pole}} = \text{Re}\omega_{\text{pole}} - i \frac{1}{2\tau_{\text{inel}}}, \quad \text{REAL DISSIPATION} \quad (2.62)$$

Here, we obtain an analogous result,

$$\omega_{\text{pole}} = \text{Re}\omega_{\text{pole}} - i \frac{1}{2\tau_{\text{el}}}, \quad \text{ATTENUATION OF THE COHERENT WAVE} \quad (2.63)$$

if we interpret  $\text{Im}\Sigma$  as follows:

$$|\text{Im}\Sigma(ck + i0)| = \bar{\rho} \omega \frac{1}{\tau_{\text{el}}}, \quad \text{ELASTIC SCATTERING TIME} \quad (2.64)$$

This analogy is not superficial; in both cases the coherent wave is attenuated due to losses. In the inelastic case, the loss is irrecoverable. In the elastic case, the losses are within the wave field, whose incoherent component grows at the expense of the coherent wave. In fact, both scattering times may be combined,

$$\frac{1}{\tau_{\text{tot}}} = \frac{1}{\tau_{\text{el}}} + \frac{1}{\tau_{\text{inel}}} \quad (2.65)$$

In the  $(\mathbf{r}, \omega)$  representation, the pole GF generalizes the free GF (2.6) of Sec. 2.1. We have to define the *mean free path* in the usual manner,

$$\begin{aligned}\ell_{\text{tot}} &= c \tau_{\text{tot}} \\ \ell_{\text{el}} &= c \tau_{\text{el}} \\ \ell_{\text{inel}} &= c \tau_{\text{inel}}\end{aligned}\tag{2.66}$$

In general, these mean free paths are  $\mathbf{k}$  dependent, but if this dependence can be neglected, the Green function becomes an attenuated spherical wave,

$$\overline{G}_{\text{pole}}(\mathbf{r}, \mathbf{r}'; \omega + i0) = -\frac{1}{4\pi\kappa} \frac{1}{R} e^{i\omega R/c} e^{R/(2\ell)}, \quad R = |\mathbf{r} - \mathbf{r}'|\tag{2.67}$$

### 2.7.3 Approximations for the self-energy

It should be realised that the Dyson equation is a defining identity relating the Green function and the self-energy, rather than a real equation. To turn it into an equation, we have to make a *physical approximation for the self-energy*. It may be asked, why introduce the self-energy at all, because we could approximate the GF just the same. The answer is that an approximation of the same quality is much more efficient when applied on the self-energy than on the GF. For example, no finite iteration of the Green function will ever give rise to a relaxation time, which, as we have seen, comes out naturally from the properties of the self-energy. An understanding from a different angle can be achieved when formally iterating the Dyson equation:

$$\overline{G} = G_0 + G_0 \Sigma \overline{G}\tag{2.68}$$

$$= G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0\tag{2.69}$$

A *finite* order approximation for  $\Sigma$  gives rise to an *infinite* series for  $G$ . (To be sure, this is not a proof that such an approximation is sufficient.)

After these remarks, we may proceed to describe first the so-called *non-selfconsistent method* of generating approximations. We have, on the one hand,

$$\overline{G} = G_0 + G_0 \Sigma \overline{G}\tag{2.70}$$

but on the other hand also

$$\overline{G} = G_0 + G_0 \langle T \rangle G_0\tag{2.71}$$

as follows by averaging the identity between  $G$  and  $T$ . Comparing both equations, we obtain an equation expressing the self-energy in terms of  $\langle T \rangle$ :

$$\Sigma = \langle T \rangle - \langle T \rangle G_0 \Sigma\tag{2.72}$$

Now, the  $T$ -matrix can be expanded in powers of a small parameter, like the strength of the scatterers, or their concentration; to the lowest order, we recover the *Born approximation*, or obtain the *dilute limit*, respectively. Because then  $\Sigma \approx \langle T \rangle$ , the latter limit is also called *the averaged T-matrix approximation*. We will not go into any details.

In the context of any *(energy) transport theory*, it is much more important to develop and apply the alternative *self-consistent method* of approximating  $\Sigma$ . It is based on the observation that in the non-selfconsistent approach the quality of an approximation depends also on the choice of the reference medium. Clearly, the best choice would be to guess directly the true effective medium and to use  $\overline{G}$  for  $G_0$ . This is not practicable, of course, but we may arrange that the equations will pick up the true effective medium, or, strictly speaking, an approximation to it, while being solved. This is the self-consistency idea. To formalize it, we write down the unaveraged integral equation and the Dyson equation in its alternative form,

$$G = G_0 + G_0 V G\tag{2.73}$$

$$\overline{G} = G_0 + \overline{G} \Sigma G_0\tag{2.74}$$

Substituting for  $G_0$  from the second equation into the first one, we obtain a neat result

$$G = \overline{G} + \overline{G}(V - \Sigma)G \quad (2.75)$$

According to this equation, the total wave in a sample has two parts, the *coherent wave* and the rest, which must be considered as the *incoherently scattered wave*. This denomination is justified, because this second term has a zero configuration average. The scattering potential for this equation is the difference between  $V$  and  $\Sigma$ , so that the reference medium drops out of the final equation completely (it cannot be avoided entirely: we have to start from somewhere).

The beauty of the equation (2.75) is marred by the fact that  $\Sigma$  is not known. We will proceed to introduce a whole class of quantities  $\Sigma_{\text{trial}}$  with properties analogous to the true  $\Sigma$ , so that any of them would do in the formal sense. They define a *trial effective medium*, with a Green function  $\mathcal{G}_{\text{trial}}$  satisfying an equation generalizing the Dyson equation (2.7.1). The true unaveraged GF  $G$  then satisfies an integral equation analogous to (2.75). The trial equations are just an extension of the equations involving the true effective medium:

$$\begin{aligned} G &= G_0 + G_0 V G \\ \mathcal{G}_{\text{trial}} &= G_0 + \mathcal{G}_{\text{trial}} \Sigma_{\text{trial}} G_0 \\ G &= \mathcal{G}_{\text{trial}} + \mathcal{G}_{\text{trial}} (V - \Sigma_{\text{trial}}) G \end{aligned}$$

We introduce in a natural way a new scattering matrix corresponding to the additional scattering with respect to the "trial" medium.

$$\begin{aligned} G &= \mathcal{G}_{\text{trial}} + \mathcal{G}_{\text{trial}} T[\Sigma_{\text{test}}] \mathcal{G}_{\text{trial}} \\ T[\Sigma_{\text{trial}}] &= V - \Sigma_{\text{trial}} + (V - \Sigma_{\text{trial}}) \mathcal{G}_{\text{trial}} T[\Sigma_{\text{trial}}] \end{aligned} \quad (2.76)$$

Configuration averaging yields the following equation:

$$\overline{G} = \mathcal{G}_{\text{trial}} + \mathcal{G}_{\text{trial}} \langle T[\Sigma_{\text{trial}}] \rangle \mathcal{G}_{\text{trial}} \quad (2.77)$$

The trial medium will become the true effective medium just when  $\overline{G} = \mathcal{G}_{\text{trial}}$  will hold, which is obviously the same like to require that the following condition be satisfied:

$$\boxed{\langle T[\Sigma_{\text{trial}}] \rangle = 0} \quad \text{SELF-CONSISTENT EQUATION FOR SELF-ENERGY} \quad (2.78)$$

To obtain a practically useful equation, we have now to decide about a specific approximation for the scattering matrix. Two main classes of approximation schemes have been developed:

**self-consistent perturbation expansion** In this approach, the  $T$ -matrix is expanded by iteration, and the series is configuration averaged term by term. A closed equation for  $\Sigma$  results, and can be solved. We will do this in the lowest possible order, the Self-consistent Born approximation, in the next Section. This expansion has the obvious advantage that it is applicable to any scattering potential, if it is not too strong. Because it extrapolates the usual Born approximation beyond its nominal validity range, the solution procedure may be based on a gradual "turning on" of the perturbation. The main disadvantage is the limited convergence range: scattering resonances, including the Mie resonances, are not tractable by this method.

**self-consistent concentration expansion** This approach requires that the potential be a sum of individual scatterers. Beyond the dilute limit, where the approach is called the *averaged  $T$ -matrix approximation*, the whole scheme is best exemplified by the Coherent potential approximation. This is a *single center approximation*, that is, the condition (2.78) is replaced by a similar equation, formulated, however, for just one random center. A single center scattering matrix is introduced, which describes the additional scattering caused by a random scatterer replacing at a given place the effective medium. On average, the effective medium should be restored, if the statistics of the center corresponds to the randomness of the medium. Thus, *the single center scattering matrix should give zero on average*. This single scatterer condition is often called the Soven equation. The method works surprisingly well considering its simplicity, and much thought has been devoted to

the question, why? Without going into details, we may say that it is the self-consistent nature of the approximation in the first place, which makes it so powerful. There is a problem. In crystalline alloys, it is easier to formalize, what it means, to replace the effective medium by one true scatterer. In systems with topological disorder, many proposals have been made, but in fact the success of the CPA has been quite limited there. When the name "coherent potential" is used for classical waves in statistically homogeneous media, it usually means just another name for the self-energy (of the coherent wave), which may be obtained by a number of various methods [15].

## 2.8 Self-consistent Born approximation

This part should illustrate more explicitly, how things can be done in practice. We select the easiest situation and solve it by the simplest approximation. It is important to realize that the case which will be considered is truly "generic" and that it demonstrates many of the salient aspects of the theory.

### 2.8.1 Basic relations

Let us first obtain the formal equation for the self-energy in the *selfconsistent BA*. We expand in (2.76) to the lowest possible order, and then average:

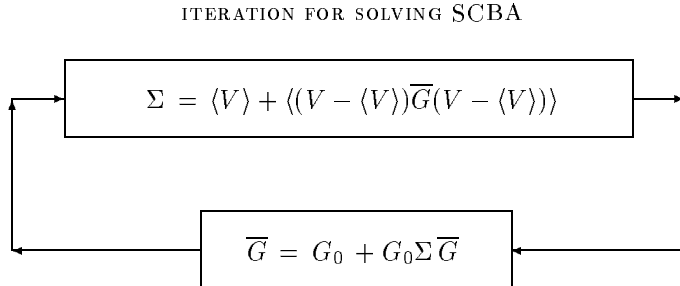
$$\begin{array}{llll}
 & \text{1st order} & \text{2nd order} & \text{all higher orders neglected -BA} \\
 T = & V - \Sigma & + (V - \Sigma)\overline{G}(V - \Sigma) & + (V - \Sigma)\overline{G}(V - \Sigma)\overline{G}T \\
 \langle T \rangle = & \langle V \rangle - \Sigma & + \langle (V - \Sigma)\overline{G}(V - \Sigma) \rangle & 
 \end{array} \quad (2.79)$$

Now, we use the self-consistency condition (2.78) to get zero on the l.h.s., and further take into account that we do not go beyond the formal second order in  $V - \Sigma$ . In this manner, we get the following sequence:

$$\begin{array}{ll}
 \text{1st order} & \Sigma = \langle V \rangle \quad \text{AVERAGED MEDIUM} \\
 \text{2nd order} & \Sigma = \langle V \rangle + \langle (V - \langle V \rangle)\overline{G}(V - \langle V \rangle) \rangle \quad \text{SELF-CONSISTENT BORN APPROXIMATION}
 \end{array} \quad (2.80)$$

It is remarkable that the self-consistent first order gives the averaged medium all by itself. There are reasons to guess that this may be the best choice among *constant self-adjoint operators*. In particular,  $\langle V \rangle$  minimizes the functional  $\langle (V - X)^2 \rangle$ . This optimized self-adjoint scattering potential then appears in the second order term. the same would still be possible in the 3rd order, but NOT beyond. One of the difficulties of the non-self-consistent expansions was the use of this insufficiently renormalized interaction.

Equation (2.80) would be pretty hard to solve for  $\Sigma$  directly even if this would not be hidden also inside the Green function. But it is, and the only way of getting a solution is a numerical iteration:



Independently of the original choice of  $G_0$ , in the first iteration, the GF will correspond to the averaged medium. Next iteration will give self-energy corresponding to the non-self-consistent Born approximation. Very often, for weak disorder, the next iteration induces only minor changes, and in most cases the whole process ends after a few iterative cycles.

## 2.8.2 Density fluctuations in the scalar wave equation

Now, we will apply the above equations more explicitly to the wave equation(2.20) in the special case, already considered before, for which only the density  $\rho$  is fluctuating, while the elastic modulus is constant. Furthermore, we will, on the basis of the preceding subsection, set the constant values of the material parameters in the free wave equation equal to those of the average medium, so that

$$\bar{\rho} = \langle \rho \rangle, \langle \tilde{\rho} \rangle = 0; \quad \kappa \equiv \bar{\kappa}, \tilde{\kappa} = 0 \quad (2.81)$$

With this, our wave equation (2.20) assumes the form

$$((\omega + i0)^2 \bar{\rho} + \bar{\kappa} \Delta) G(\mathbf{r}, \mathbf{r}'; \omega + i0) - \{-(\omega + i0)^2 \tilde{\rho}(\mathbf{r})\} G(\mathbf{r}, \mathbf{r}'; \omega + i0) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.82)$$

so that our scattering potential is local,

$$V(\mathbf{r}, \mathbf{r}') = -\omega^2 \tilde{\rho}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \quad (2.83)$$

while the equation (2.21) for the homogeneous ("unperturbed") medium does not change formally:

$$((\omega + i0)^2 \bar{\rho} + \bar{\kappa} \Delta) G_0(\mathbf{r}, \mathbf{r}'; \omega + i0) = \delta(\mathbf{r} - \mathbf{r}') \quad (2.84)$$

Introducing all necessary quantities into (2.80) and integrating trivially over the delta functions, we get an explicit expression for the self-energy

$$\begin{aligned} \Sigma(\mathbf{r} - \mathbf{r}'; \omega + i0) &= \langle \omega^2 \tilde{\rho}(\mathbf{r}) \overline{G}(\mathbf{r} - \mathbf{r}'; \omega + i0) \omega^2 \tilde{\rho}(\mathbf{r}') \rangle \\ &= \omega^4 \bar{\rho}^2 B(\mathbf{r} - \mathbf{r}') \overline{G}(\mathbf{r} - \mathbf{r}'; \omega + i0) \\ B(\mathbf{r} - \mathbf{r}') &= \langle \tilde{\rho}(\mathbf{r}) \tilde{\rho}(\mathbf{r}') \rangle \end{aligned} \quad (2.85)$$

where the pair correlation function is in fact the same as in the old definition (2.13), due to its self-averaging property.

This self-energy is non-local; to get an idea, it may be useful to set the model GF (2.7.2) for  $\overline{G}$  in (2.85). It is apparent that three different lengths come into play: the correlation radius of  $B$ , the wavelength  $2\pi c/\omega$ , and the mean free path  $\ell$ . There is one possibility, which may seem unnatural, but has a reasonable meaning. We make the self-energy local by assuming that  $B$  is local:

$$B(\mathbf{r} - \mathbf{r}') = b^2 \delta(\mathbf{r} - \mathbf{r}'), \quad b^2 \dots \text{MEASURES POTENTIAL STRENGTH} \quad (2.86)$$

This correlation function represents the well-known and so frequently employed *white noise model* for disorder. It looks rather artificial, because it implies that the density fluctuations may become arbitrarily large and also infinitely rapid in space. Introducing (2.86) into (2.85), we obtain that  $\text{Re } \Sigma = \infty$ . Such artifacts can be overcome, if it is realized that it is only required that  $B$  appear as a delta function when sampled by waves which are not excessively short. Such waves do not feel the far Fourier components of  $B$ , and a regularisation is achieved by putting an appropriate cut-off on the Fourier expansion of  $B$ .

We are, in fact, interested more in the imaginary part of the self-energy, which is regular, because  $\text{Im } \overline{G} \sim -\sin(R)/(4\pi\bar{\kappa}R)$  for  $R \rightarrow 0$ :

$$\text{Im } \Sigma(\mathbf{r} - \mathbf{r}'; \omega + i0) = \delta(\mathbf{r} - \mathbf{r}') \cdot (-\bar{\rho}\omega) \frac{b^2\omega^4}{4\pi c^3} \quad (2.87)$$

The expression is written in such a form that a comparison with the general relation between  $\text{Im } \Sigma$  and the elastic scattering time, Eq. (2.64), yields directly

$$\frac{1}{\tau_{\text{el}}} = \frac{b^2\omega^4}{4\pi c^3} \quad \text{WHITE NOISE ELASTIC SCATTERING TIME} \quad (2.88)$$

$$\frac{1}{\ell_{\text{el}}} = \frac{b^2\omega^4}{4\pi c^4} \quad \text{WHITE NOISE ELASTIC MEAN FREE PATH} \quad (2.89)$$

The following observation can be made. These results have the general features of the Born approximation, as we have seen them in Sec. 2.1. In particular, we obtain the Rayleigh  $\omega^4$  dependence, and the Born  $b^2$  dependence. The result has been obtained in the non self-consistent Born approximation, but it would not be changed by iteration, because the  $R \rightarrow 0$  asymptotics will not be changed. It is the final result, therefore, in this simple case.

### 2.8.3 Coherent wave is self-averaging in the Born approximation

This final comment on coherent waves is intended to elucidate in which sense the configuration averaged coherent wave has a direct meaning also for one configuration, that is, a single sample.

The coherent wave, in accordance with the Dyson equation, satisfies

$$u_{\text{coh}} = u_0 + G_0 \Sigma u_{\text{coh}} \quad (2.90)$$

where  $u_0$  is an incident plane wave. In the  $(\mathbf{k}, \omega)$  representation, this is an algebraic relation

$$u_{\text{coh}} = [1 - G_0(\mathbf{k}, \omega)\Sigma(\mathbf{k}, \omega)]^{-1}u_0 \quad (2.91)$$

in which  $\mathbf{k}$  corresponds to the incident wave.

Let us now turn to one configuration. The full wave will be written as

$$u = A u_0 + u' \quad \text{NOT } u_0 + \tilde{u} \quad (2.92)$$

Factor  $A$  takes into account the part of  $u$  which is scattered "forward", that is, which adds to the incident wave. We hope to identify  $A u_0 \leftrightarrow u_{\text{coh}}$ . For  $u$ , we have, cf. (2.30),

$$u = u_0 + G_0 V u \quad \text{AVERAGED MEDIUM} \dots \langle V \rangle = 0 \quad (2.93)$$

$$u = u_0 + G_0 V u_0 + G_0 V G_0 V u \quad (2.94)$$

$$A u_0 + u' = u_0 + G_0 V u_0 + G_0 V G_0 V (A u_0 + u') \quad (2.95)$$

where the wave equation was first iterated once, and then the decomposition of  $u$  introduced.

These general and, up to now, exact relations will now be specialized to our wave equation (2.82) with the disorder entering only through density fluctuations. To obtain the factor  $A$ , it is necessary to compute the  $\mathbf{k}$  Fourier component of the last equation. This can be done, if  $u'$  on the r.h.s. is neglected ... which is the Born approximation. On the l.h.s., the second term gives zero because  $u'$  was defined so that it does not contain any  $\mathbf{k}$ -component. Our sample has a volume  $\Omega$ . We get, with the shorthand  $g$  for  $G_0(\mathbf{k}, \omega)$ ,

$$A \Omega = \Omega - g \int d^3 \mathbf{r} \omega^2 \tilde{\rho}(\mathbf{r}) + g \omega^4 \int d^3 \mathbf{r} \int d^3 \mathbf{r}' e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \tilde{\rho}(\mathbf{r}) G_0(\mathbf{r} - \mathbf{r}') \tilde{\rho}(\mathbf{r}') \quad (2.96)$$

The result is already coming, it is sufficient to recall the identification

$$\langle \dots \rangle = [\dots]_{\text{Ave}}$$

for self-averaging quantities introduced in Sec. 2.6. The first integral is, by this, equal to zero, while the second becomes the  $\mathbf{k}$  component of the self-energy in the Born approximation, as obtained in Sec. 2.8, Eq. (2.80). This completes the whole identification, and shows that the coherent wave does indeed propagate, and is detectable, in a disordered sample. It may be added that this result is bound to the use of the Born approximation, or, as a more general statement, to the use of perturbation theory.



# Chapter 3

## Lecture three: Wave diffusion and beyond

In this lecture, we want to address two questions about wave propagation in a random medium:

- ◇ how to reconcile the wave propagation, which preserves coherence of the waves, and is time-reversible, on the one hand, with the diffusive spreading of the wave energy, which is irreversible, on the other hand;
- ◇ how to improve the basic picture of diffusive propagation by taking into account wave interference phenomena

### 3.1 Incoherent wave and energy spreading

We want to state these questions in a more explicit and systematic manner now, and it may be useful first to restate here a few basic relations from the previous lectures. We will proceed on two levels. On the general level, our approach will be based on a selfconsistently constructed division of the wave field into its coherent and incoherent parts. On the level of working equations, we will consider the scalar wave equation with random  $\delta$ -correlated density fluctuations treated in the Self-consistent Born approximation.

Here is a short summary of the equations.

#### A. General relations

$$\begin{aligned} u &= u_{\text{coh}} + u_{\text{incoh}} && (3.1) \\ u_{\text{coh}}(\mathbf{r}, t) &\equiv \langle u(\mathbf{r}, t) \rangle && \text{COHERENT WAVE DEFINED (2.52)} \quad (3.2) \\ \langle u_{\text{incoh}}(\mathbf{r}, t) \rangle &= 0 && (3.3) \\ G &= G_0 + G_0 V G && \text{INTEGRAL WAVE EQUATION (2.30)} \quad (3.4) \\ \overline{G} &\equiv \langle G \rangle && \text{COHERENT WAVE (2.53)} \quad (3.5) \\ \overline{G} &= G_0 + G_0 \Sigma \overline{G} && \text{DYSON EQUATION (2.57)} \quad (3.6) \\ G &= \overline{G} + \overline{G}(V - \Sigma)G && \text{SELF-CONSISTENT WAVE EQUATION (2.75)} \quad (3.7) \\ \langle T[\Sigma_{\text{test}}] \rangle &= 0 && \text{SC EQUATION FOR SELF-ENERGY (2.78)} \quad (3.8) \end{aligned}$$

NEW CONVENTION

$$\boxed{\omega^+ \equiv \omega + i0, \quad \omega^- \equiv \omega - i0} \quad (3.9)$$

$$((\omega^+)^2 \bar{\rho} + \bar{\kappa} \Delta) G(\mathbf{r}, \mathbf{r}'; \omega^+) - \{-(\omega^+)^2 \tilde{\rho}(\mathbf{r})\} G(\mathbf{r}, \mathbf{r}'; \omega^+) = \delta(\mathbf{r} - \mathbf{r}') \quad (3.10)$$

$$\bar{\rho} = \langle \rho \rangle, \langle \tilde{\rho} \rangle = 0; \quad \kappa \equiv \bar{\kappa}, \tilde{\kappa} = 0 \quad (3.11)$$

$$V(\mathbf{r}, \mathbf{r}') = -\omega^2 \tilde{\rho}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \quad (3.12)$$

$$((\omega^+)^2 \bar{\rho} + \bar{\kappa} \Delta) G_0(\mathbf{r}, \mathbf{r}'; \omega^+) = \delta(\mathbf{r} - \mathbf{r}') \quad (3.13)$$

$$\dot{w} + \text{div } \mathbf{J}_w = 0 \quad \text{ENERGY CONSERVATION (1.22)} \quad (3.14)$$

$$w = \frac{1}{2} \rho \dot{u}^2 + \frac{1}{2} \kappa |\text{grad } u|^2 \quad \text{ENERGY DENSITY} \quad (3.15)$$

$$\mathbf{J}_w = -\dot{u} \kappa \text{grad } u \quad \text{ENERGY CURRENT DENSITY} \quad (3.16)$$

$$\Sigma = \langle V \rangle + \langle (V - \langle V \rangle) \bar{G} (V - \langle V \rangle) \rangle \quad \text{SELF-CONSISTENT BA (2.80)} \quad (3.17)$$

$$\Sigma(\mathbf{r} - \mathbf{r}'; \omega^+) = \omega^4 \bar{\rho}^2 B(\mathbf{r} - \mathbf{r}') \bar{G}(\mathbf{r} - \mathbf{r}'; \omega^+) \quad (3.18)$$

$$B(\mathbf{r} - \mathbf{r}') = \langle \hat{\rho}(\mathbf{r}) \hat{\rho}(\mathbf{r}') \rangle = b^2 \delta(\mathbf{r} - \mathbf{r}'), \text{UNCORRELATED POINT-LIKE DISORDER (2.86)} \quad (3.19)$$

$$\text{Im } \Sigma(\mathbf{r} - \mathbf{r}'; \omega + i0) = \delta(\mathbf{r} - \mathbf{r}') \cdot (-\bar{\rho} \omega) \frac{b^2 \omega^4}{4\pi c^3} \quad \text{SCBA FOR (2.86), SEE (2.87)} \quad (3.20)$$

$$\frac{1}{\tau_{\text{el}}} = \frac{b^2 \omega^4}{4\pi c^3} \quad \text{ELASTIC SCATTERING TIME (2.88)} \quad (3.21)$$

$$\frac{1}{\ell_{\text{el}}} = \frac{b^2 \omega^4}{4\pi c^4} \quad \text{ELASTIC MEAN FREE PATH (2.89)} \quad (3.22)$$

◇◇◇

So far, we did not study the incoherent wave in much detail, except for looking at its qualitative link with *speckle patterns*. Now, we will center our attention on the incoherent wave. Namely, we will study the global characteristics of the evolution in space and time of the energy density associated with a wave process in our random medium. From a single configuration, we go over to the *configuration averaged properties*. It might seem that such an approach does not have much value, because  $u_{\text{incoh}}$  with its speckles does not seem to be exactly self-averaging. We have pointed out, however, already in Sec. 1.6 the role of the observer, or more precisely, in this purely classical domain, of the averaging properties of the measuring devices. It is clear from the discussion of configuration averages in Sec. 2.6 that the sampling of an area sufficiently larger than the correlation range of the disorder may give values close to the corresponding configuration averages. This procedure is known as *coarse graining*, or, in a more traditional context, *Lorentz averaging*. In other words, *if the wave in the random medium has a small overall variation, its coarse grained properties can be identified with the local configuration averages*. It is expected that any wave disturbance, arbitrarily sharp at its start, will spread later, and in the asymptotics of large times and distances its mean gradients will be small (*hydrodynamic limit*). This asymptotics we want to study. In actual fact, real systems seem to achieve this limiting behavior rather fast.

To study the energy spreading, it is convenient to start from Eq. (3.13), which can be averaged, and a conservation law for the averaged quantities of same form follows:

$$\partial_t \langle w \rangle + \text{div } \langle \mathbf{J}_w \rangle = 0 \quad (3.23)$$

In the present case, it is easy to see, when combining Eqs. (3.1), (3.3), and (3.15), that

$$\langle \mathbf{J}_w \rangle = \mathbf{J}_{w,\text{coh}} + \langle \mathbf{J}_{w,\text{incoh}} \rangle \quad (3.24)$$

where the two currents are obtained by substituting the respective waves into the expression (3.15). The coherent wave is attenuated, and, for this reason, after a sufficiently long time, all current will be carried only by the incoherent field.

In our case, the total current  $\langle \mathbf{J}_w \rangle$  can be written as

$$\langle \mathbf{J}_w \rangle = \bar{\kappa} \cdot \sum_i \frac{\partial}{\partial x_i} \frac{\partial}{\partial x'_i} \langle u(\mathbf{r}, t) u(\mathbf{r}', t) \rangle \Big|_{\mathbf{r}=\mathbf{r}'} \quad (3.25)$$

We were explicit about this to show that the physically important information about the incoherent propagation is contained in *configuration averages of bilinear combinations* of the field amplitudes. In the last equation, the two fields are taken at the same time, but at different positions. Altogether, there are the following possibilities:

name	function	describes
two-point correlation function	$\langle u(\mathbf{r}, t) u(\mathbf{r}', t') \rangle$	amplitude correlation spectroscopy
distribution function	$\langle u(\mathbf{r}, t) u(\mathbf{r}', t) \rangle$	amplitude spatial correlation equival. to distribution function of RTE [2] mean values of non-local quantities
autocorrelation function	$\langle u(\mathbf{r}, t) u(\mathbf{r}, t') \rangle$	temporal speckle autocorrelation
intensity	$\langle u(\mathbf{r}, t) u(\mathbf{r}, t) \rangle$	intensity spreading

The distribution function is no doubt the right starting point for any systematic transport theory, but we will consider only the intensity spreading, which is directly related to the diffusion problem. Just as before, it is convenient to express field amplitudes in terms of the Green functions. Remembering the initial value problem and its solution (2.18), and considering the case of a point pulse initial kick  $u(\mathbf{r}', t_0) = u_0 \delta(\mathbf{r}_0 - \mathbf{r}')$ , we obtain the simplest possible quantity to be studied,

$$P(\mathbf{r}, t; \mathbf{r}_0, t_0) = \langle |G(\mathbf{r}, t; \mathbf{r}_0, t_0)|^2 \rangle \quad (3.26)$$

This function describes the field intensity spreading from the initial point kick. In the early stage of evolution, the pulse propagates with the velocity of sound and rapidly expands. Scattering makes the spreading to slow down, and, after a long time, we might expect  $P$  to obey the diffusion equation. This is far from being certain. The P.W.Anderson's paper [5] is entitled: "On the absence of diffusion . . .".

## 3.2 Intermezzo: diffusion equation

Here, we concentrate the necessary background information about the diffusion equation. The energy balance equation (3.23) is not a closed equation; to close it, a second relation between both densities is needed. This is provided by a phenomenological "second Fick's law"

$$\langle \mathbf{J}_w \rangle = -D \text{grad} \langle w \rangle \quad (3.27)$$

$$D \quad \dots \quad \text{DIFFUSION CONSTANT} \quad (3.28)$$

Combining both, we get the *diffusion equation*

$$\partial_t \bar{w} - D \Delta \bar{w} = 0 \quad \bar{w} \equiv \langle w \rangle \quad (3.29)$$

This equation could be discussed at length, just as we did for the wave equation in Sec. 1.6. The solutions have unidirectional character in time, in contrast to those of the wave equation. They depend on the boundary conditions, etc., and an initial value problem has a unique solution, which can be expressed in terms of a Green function  $P_0$ , which satisfies the inhomogeneous diffusion equation with a  $\delta$  source. We write directly the Fourier transform:

$$(-i\omega + D|\mathbf{q}|^2) P_0(\mathbf{q}, \omega) = 1 \quad (3.30)$$

The signature of the diffusive behavior is the so-called *diffusive pole*

$$\omega = i q^2, \quad q = |\mathbf{q}| \quad (3.31)$$

In these lectures, the role of space dimension was not considered in a systematic way, but at this point, we want to make a small digression. It is obvious that the form of the diffusion equation does not depend on the dimension  $d$ . Solving (3.30) for  $P$  and performing the inverse Fourier transformation, we obtain

$$P_0(\mathbf{r}_0 - \mathbf{r}', t - t') = \frac{1}{(4\pi Dt)^{d/2}} e^{-|\mathbf{r}-\mathbf{r}'|/4Dt} \quad (3.32)$$

It is seen that the "particle" leaves the origin slower in lower dimensions. This does not mean localisation, of course, but it is remarkable that  $d = 2$  has a special position, because for  $d \leq 2$  the return probability  $\int dt P_0(0, t)$  diverges.

We used here the word "particle" to turn the attention to the fact that the diffusion equation corresponds to classical particles performing a completely random walk. If they move with a velocity  $c$  and their mean free path is  $\ell$ , the diffusion constant, as is shown in the elementary kinetic theory, is  $D = c\ell/d$ . If we were able to reproduce these results starting from the wave equation, that would mean that under some circumstances the waves behave like classical particles.

### 3.3 Asymptotic behavior of the spreading intensity

To study the asymptotics of  $P$ , Eq. (3.26), it is convenient to work with its time Fourier transform. We do it in two steps. In the first step, we introduce along with the *retarded GF* also the corresponding *advanced GF*. In the time domain, it is zero for positive time differences, in the frequency domain, it acquires a *negative imaginary part of frequency*. To introduce it into the Fourier transformation, we employ the following relation:

$$G(\mathbf{r}, \mathbf{r}', \omega - i0) = [G(\mathbf{r}', \mathbf{r}, \omega + i0)]^* \quad (3.33)$$

$$P(\mathbf{r} - \mathbf{r}', t) = \left\langle \int \frac{d\omega}{2\pi} e^{-i\omega t} G(\mathbf{r}, \mathbf{r}', \omega^+) \int \frac{d\omega'}{2\pi} e^{i\omega' t} G(\mathbf{r}', \mathbf{r}, \omega'^-) \right\rangle \quad (3.34)$$

Next, an "outer frequency" will be introduced by

$$\omega - \omega' = \Omega, \quad \omega = \eta + \Omega/2, \quad \omega' = \eta - \Omega/2 \quad (3.35)$$

with the result, where we write  $\omega$  for  $\Omega$  again:

$$P(\mathbf{r} - \mathbf{r}', t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} P(\mathbf{r} - \mathbf{r}', \omega) \quad (3.36)$$

$$P(\mathbf{r} - \mathbf{r}', \omega) = \int \frac{d\eta}{2\pi} \langle G(\mathbf{r}, \mathbf{r}', \eta + \frac{1}{2}\omega + i0) G(\mathbf{r}', \mathbf{r}, \eta - \frac{1}{2}\omega - i0) \rangle \quad (3.37)$$

It is qualitatively clear that the asymptotics of long times translates into the asymptotics  $\omega \rightarrow 0$ . This can be formalized by the following "regularisation":

$$\lim_{t \rightarrow \infty} f(t) = \lim_{\delta \rightarrow 0^+} \delta \int dt e^{-\delta t} = \lim_{\delta \rightarrow 0^+} \delta F(\omega = i\delta) \quad (3.38)$$

where  $F$  is the Fourier transform of  $f$ . In our case,

$$\lim_{t \rightarrow \infty} P(\mathbf{r} - \mathbf{r}', t) = \lim_{\delta \rightarrow 0^+} 2\delta P(\mathbf{r} - \mathbf{r}', \omega + i\delta) \quad (3.39)$$

From this, we may conclude that this limit decides about the basic distinction between waves which are  
 ◊ extended and spreading ... (3.39)  $\rightarrow 0$   
 ◊ localized and confined ... (3.39) has a non-zero limit.

In the extended case, there comes the finer classification: when is the spreading diffusive, and when do deviations from the diffusion behavior occur? We will show that in our simple situation specified by Eqs. (3.9 – 21), the diffusion approximation is valid.

## 3.4 Intensity spreading in Self-consistent Born approximation

### 3.4.1 Bethe-Salpeter equation

First, we have to develop a general formalism, which would permit to solve these newly posed questions. On this formal level, we have to develop a technique for configuration averaging a product of two Green functions. By product we mean the *direct product* in this case, and we write

$$K = \langle G \otimes G \rangle \quad (3.40)$$

$$K(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2 | \omega_1, \omega_2) = \langle G(\mathbf{r}_1, \mathbf{r}'_1; \omega_1) G(\mathbf{r}_2, \mathbf{r}'_2; \omega_2) \rangle \quad \text{EXPLICIT NORMALSIZE } (r, \omega) \text{ FORM} \quad (3.41)$$

We want to develop an expansion for  $K$  which would be parallel to that for  $G$ . We will start right from the self-consistent equation (3.7), so that everything pertaining to a single Green function will already be included. Of course, for the left GF in (3.41), we will use (3.7) directly, while for the right one, it is advantageous to use the alternative form (cf. (2.32)). This gives

$$K = \overline{G} \otimes \overline{G} + \overline{G} \langle (V - \Sigma) G \otimes G (V - \Sigma) \rangle \overline{G} \quad (3.42)$$

$$K_0 = \overline{G} \otimes \overline{G} \quad (3.43)$$

In the second line, we define the *coherent part of K*. The full  $K$  contains, in addition, the term involving all "incoherent scattering" which is of considerable complexity. We have to convert it, just as has been done in the case of the Dyson equation, into a closed equation for  $K$  by making a physical approximation. We want to use an analog to the Self-consistent Born approximation. This leads to the approximation

$$G \otimes G \approx \langle G \otimes G \rangle = K \quad (3.44)$$

This choice may be motivated in various ways. On the one hand, when scattering is weak, as we assume here, and this leads to a *perturbation theoretic* rationalisation of the approximation. We may also think of (3.44) as of a *mean field approximation*, in which random fluctuations of the unaveraged product are neglected. Whatever the reasons, with this approximation, relation (3.43) becomes an equation for  $K$ :

$$K = K_0 + \underbrace{\overline{G} \langle (V - \Sigma) K (V - \Sigma) \rangle \overline{G}}_{\approx 0} \quad \text{SCBA BETHE-SALPETER EQ.} \quad (3.45)$$

As indicated,  $\Sigma$  can be left out, just like in (3.16), because we have  $\langle V \rangle = 0$ .

The Bethe-Salpeter equation can be solved by iteration, and an infinite series results with the first terms

$$K = K_0 + \quad (3.46)$$

$$\overline{G} \langle V K_0 V \rangle \overline{G} + \quad (3.47)$$

$$\underbrace{\overline{G} \langle V \overline{G} \langle V K_0 V \rangle \overline{G} V \rangle \overline{G}}_{\text{LADDER EXPANSION}} + \dots \quad (3.48)$$

As indicated by the underbraces, the averaging proceeds in pairs of the scattering potentials, and one average is inserted into the other. This type of expansion is called the *ladder expansion*, because its topological structure is reminiscent of a collection of longer and longer ladders. In fact, it can be drawn diagrammatically in the ladder form [15], but we will not introduce the diagrammatic representation here.

### 3.4.2 Solution of the Bethe-Salpeter equation for the model scalar equation

Comparing (3.37) with (3.41), we see that

$$P(\mathbf{r} - \mathbf{r}', \omega) = \int \frac{d\eta}{2\pi} K(\mathbf{r}, \mathbf{r}; \mathbf{r}', \mathbf{r}' | \eta + \frac{1}{2}\omega + i0, \eta - \frac{1}{2}\omega - i0) \quad (3.49)$$

It is thus sufficient to know the two-point reduced quantity

$$\mathcal{K}(\mathbf{r} - \mathbf{r}' | \omega_1, \omega_2) = K(\mathbf{r}, \mathbf{r}; \mathbf{r}', \mathbf{r}' | \omega_1, \omega_2) \quad (3.50)$$

From the general structure of the Bethe-Salpeter equation (3.45) it is easy to see that, while in general, we would have to cope with the four-terminal structures appearing as a result of the direct product of two GF, in our case the task becomes much simpler. Namely, the choice of the local potential (3.11) with the short range correlation (3.17) reduces the whole task directly to an equation for  $\mathcal{K}$ . Introducing also  $\mathcal{K}_0$ , we get

$$\mathcal{K}(\mathbf{r} - \mathbf{r}') = \mathcal{K}_0(\mathbf{r} - \mathbf{r}') + \int d\bar{\mathbf{r}} \mathcal{K}_0(\mathbf{r} - \bar{\mathbf{r}}) b^2 \bar{\rho}^2 \omega_1^2 \omega_2^2 \mathcal{K}(\bar{\mathbf{r}} - \mathbf{r}') \quad (3.51)$$

$$\mathcal{K}(\mathbf{q}) = \mathcal{K}_0(\mathbf{q}) + \mathcal{K}_0(\mathbf{q}) b^2 \bar{\rho}^2 \omega_1^2 \omega_2^2 \mathcal{K}(\mathbf{q}) \quad (3.52)$$

We have left out the frequency arguments for brevity, and in the second line, the equation was Fourier transformed. This yields an algebraic relation, which can be solved:

$$\mathcal{K}(\mathbf{q}) = \frac{1}{\mathcal{K}_0^{-1}(\mathbf{q}) - b^2 \bar{\rho}^2 \omega_1^2 \omega_2^2} \quad (3.53)$$

What we get here is, of course, but the sum of a geometrical series corresponding to the ladder expansion. It remains to calculate  $\mathcal{K}_0(\mathbf{q})$ . This is just an integral,

$$\mathcal{K}_0(\mathbf{q}) = \int d^3\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \bar{G}(\mathbf{r}, \eta + \frac{1}{2}\omega + i0) \bar{G}(\mathbf{r}, \eta - \frac{1}{2}\omega - i0) \quad (3.54)$$

but it is very important to insert there the full SCBA Green functions:

$$\mathcal{K}_0(\mathbf{q}) = \int d^3\mathbf{r} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{(-1)}{4\pi\bar{\kappa}r} e^{+i(\eta+\omega/2)r/c} e^{r/(2\ell_+)} \frac{-1}{4\pi\bar{\kappa}r} e^{-i(\eta-\omega/2)r/c} e^{r/(2\ell_-)} \quad (3.55)$$

where the two mean free paths have the form (3.21) with  $\eta + \omega/2$ ,  $\eta - \omega/2$  substituted for  $\omega$  respectively. In the limit of long times, long distances, which means

$$(\omega/c)\ell \ll 1, \quad q\ell \ll 1 \quad (3.56)$$

where

$$\ell^{-1} = \frac{1}{2}(\ell_+^{-1} + \ell_-^{-1}) \approx \ell^{-1}(\eta) \quad (3.57)$$

we get

$$\mathcal{K}_0^{-1} \approx 4\pi\bar{\kappa}^2 \ell^{-1} + 4\pi\bar{\kappa}^2 c^{-1}(-i\omega + (\ell c/3)q^2) \quad (3.58)$$

and this finally gives the *diffusion form* of  $\mathcal{K}$ ,

$$\mathcal{K} = \frac{c/4\pi\bar{\kappa}^2}{-i\omega + (\ell(\eta)c/3)q^2} \quad (3.59)$$

If we make the identification according to Sec. 3.2,

$$D(\eta) = \frac{\ell(\eta)c}{3} \quad (3.60)$$

and introduce (3.59) into (3.49), we get for  $P$  the final expression

$$P(\mathbf{q}, \omega) = \int \frac{d\eta}{2\pi} \frac{c/4\pi\bar{\kappa}^2}{-i\omega + D(\eta)q^2} \quad \text{SCBA DIFFUSION LIMIT} \quad (3.61)$$

This is a natural result telling us that the spreading of a point kick proceeds asymptotically so that excitations of different frequencies diffuse with their frequency dependent diffusion constant. Because of the strong frequency dependence of the mean free path, we have to deal with a *dispersive diffusion* in contrast to the simple diffusion treated in Sec 3.2. For properly chosen experimental conditions, it may be possible to introduce an (experiment dependent) average diffusion rate.

Let us return to the fact that the diffusion approximation came out as a result of seemingly miraculous cancellations of terms in (3.53). They were not a miracle: the reason for the success was in *using consistent approximations for the single Green function  $\bar{G}$  and for the direct product  $\langle GG \rangle = K$ .*

This notion of consistency, based on the so-called *conserving approximations* (in our case ... conserving energy), and expressed in general in terms of the so-called *Ward identities*, is one of the most important and powerful tools in generating approximate theories free of basic inconsistencies. All this has been well known for decades; in the context of classical waves an extensive discussion appears in [15].

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# Sound in granular matter:

A case of wave propagation in random media

## Part II.

Lecture notes to a course given by

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## NOTE

This second part of the lecture notes concludes the whole writeup. The text corresponds to the actual subject matter presented in the course, although it gives more details than was possible to cover in the short time available for the lectures. The second part should have first concluded the general comments on wave propagation in random media by an elementary introduction to localisation of classical waves, in which the special properties of a  $\delta$ -correlated disorder are employed to derive most of the results without explicit use of diagrammatic technique. This segment is not included into the written form presently for several reasons.

It seemed to be more important to present a summary to problems for which no systematic and sufficiently simple account appears to be available. Under the heading of Lecture four, I give a two-part discussion of sound in granular matter structured as follows. The first part considers general questions of confined granular samples, in particular the inhomogeneous stress distribution and its consequences for the macroscopic elastic moduli. The second part describes in some detail the significance of several recent experimental studies of sound propagation in granular matter.

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## Chapter 3

# Lecture III: Wave diffusion and beyond *Continued from Part I.*

*This part of the lecture notes is not included. The interested reader may consult two recent references [28], [29], in particular the first one, which utilizes the case of randomly distributed  $\delta$ -scatterers to extract the results about localisation in a physically appealing manner similar to the method which has been used in the oral presentation of the present lecture.*

# Chapter 4

## Lecture IV: Sound in confined granular media

This part of the lectures is very different in its nature as compared with the previous lectures. There, we took the liberty to consider several model systems of a rather diverse nature and to demonstrate various aspects of wave propagation in random media always on a system which appeared to be conveniently suited for a given question. Now, we will be bound to a specified class of systems, namely the granulars. Actually, such systems consisting of, or containing as a principal constituent, "grains" are abundant in real life, and only their complexity slowed down their systematic exploration, especially from a physical point of view. Presently, the interest paid to granular matter is growing explosively, and a number of general reviews of the subject are available, [30], [31]. Other useful references will be quoted below.

Actually, granular matter as a whole is not a research subject any more today, as it has split already into a number of subfields. Our concern will be one special case, namely sound in a confined granular medium. The two introductory sections of this lecture are more general, however, and they serve to sum up the salient facts about granular matter in general, and to single out the basic characteristics of the physical problem we are going to address in the last two sections of this course. Many of the currently debated questions concerning granular systems neglected in these notes are commented in an inspirational way in a recent review article [32]. Consulting the Bibliography at the end of this lecture, the reader will appreciate the particular attention paid by Rev. Mod. Phys. to granular media.

### 4.1 General characterisation of granular matter

It would not be easy to give an all-encompassing definition of a granular system, but we may list several characteristic properties, which it should possess. A **granular system** *is composed of a "sufficiently" large number of grains, which are disjoint macroscopic solid particles interacting through non-cohesive contact forces.* Thus, a sand dune or a stone avalanche are good granular samples, a swarm of debris particles flying alongside in the outer space, a composite or a tool made of a sintered metal powder are not. Our conception of the granular matter does not preclude additional forces between the grains, for example, they could be charged, as will often be the case in industrial flows. On the other hand, the grains can be immersed into a medium, like a gravel soaked with water in a rock bed. It may be asked whether granular media are necessarily random. If the grains themselves are irregularly shaped bodies, the answer is obvious, but if the grains are chosen to be nearly identical, the granular matter may tend to "crystallize", as will be discussed in Sec. 4.1.2. This type of metaphoric language refers to the fact that arrays of balls may in a geometrical sense resemble scaled-up assemblies of atoms, crystalline or amorphous. This analogy is quite useful, but it is important to keep in mind the macroscopic size of the grains. By this we mean two essential points:

◊ *Typical energies exchanged at contact interactions are much larger than the thermal energy  $k_B T$ , so that the temperature enters only as a macroscopic parameter determining, say, thermal dilation of the grains*

◊ *The granular system is **dissipative**.* The dissipation may have several origins: constitutive properties of the grains, which may be plastic or viscoelastic, viscosity of the medium. *The most important source*

of dissipation, however, is the frictional component of the contact forces which cannot be described by an intergrain potential.

Thus, a granular system in motion, say a granular flow, is sustained by a steady influx of energy from outside, and is thus inherently open. External forces are important for static granular media as well, however, although in a different sense. Because the granular matter is basically non-cohesive, the grains are kept together by external influences, like stresses due to a confinement, or, in the case of sand piles, by the effect of gravity pressing the pile against its support.

### 4.1.1 Geometrical structure of granular samples

From now on, we will assume that all grains are spherical balls with (at least approximately) the same radius  $\frac{1}{2}a$ , so that the minimum distance of two grains will be  $\approx a$ . To specify an instantaneous configuration of a given sample at the time  $t$ , it is enough to indicate positions of all grain centers,

$$\{\mathbf{r}_1(t), \dots, \mathbf{r}_n(t), \dots, \mathbf{r}_N(t)\} \tag{4.1}$$

This is a rather complete information, indispensable for certain tasks; but it may be also important to have some reduced characteristics which would give a more concise description and, at the same time, would be more informative by revealing explicitly the basic statistical behavior of the sample in question. Let us have a look into both possibilities.

The full knowledge of the individual particle (grain) trajectories is natural for a direct numerical solution of the dynamics of a given sample; less often it will be the subject of an experimental study, although we have to be cautious here. For a microscopic system composed of atoms, nobody expects that exact positions of all of them will be known from a measurement. The situation may be different for a macroscopic sample. It should be realized that a typical route to a set of starting particle coordinates in a numerical study is most frequently to measure the positions on an appropriate hand built model, rather than to generate them on a computer. Such balls-and-sticks models have been heavily used since the Bernal's famous work to study in a model way possible geometries first in liquids and later also in solid amorphous substances of various kinds [16], [33]. Only later it was realized that the same models can serve also in the studies of macroscopic granular assemblies [31]. Rather often, in particular in 2D, the same macroscopic set of disks is used first to find the grain positions and then to perform a physical measurement ...

One point of interest is that in the complete description the particles are labelled. When looking on the photographs of Bernal's models, it is apparent that to each ball a small sticker with its number is attached. This is natural for macroscopic grains, but the models were intended to depict atoms in a liquid, which can be thought to be identical and, consequently, could be permuted classically, or are indistinguishable quantumly. This point has been raised by Alexander [34] and we will not be able to discuss it in detail here. The essential point is that in reality the particles, even in the case of atoms, are well localized to their trajectories and, classically, their permutation is possible in a liquid, but it is prevented in a solid by immense energy barriers; similarly the permuted many particle wave functions are orthogonal and their symmetrized combination leads to an equivalent description. This stresses once more the close analogy between the atomic and the macroscopic cases.

The labelled trajectories have their role in a basic distinction of three types of granular media, "gaseous", "liquid", and "solid", as discussed in [30]. The distinction is based on the analogy with atomic systems. As the first step, we separate out the gaseous phase by defining it as a system in which the average separation between particles is larger than their radius.

**In detail:** The region  $K$  occupied by particles should be specified precisely enough so that we will be able to tell its **volume**  $\Omega[K]$ , and by this the average volume per particle,

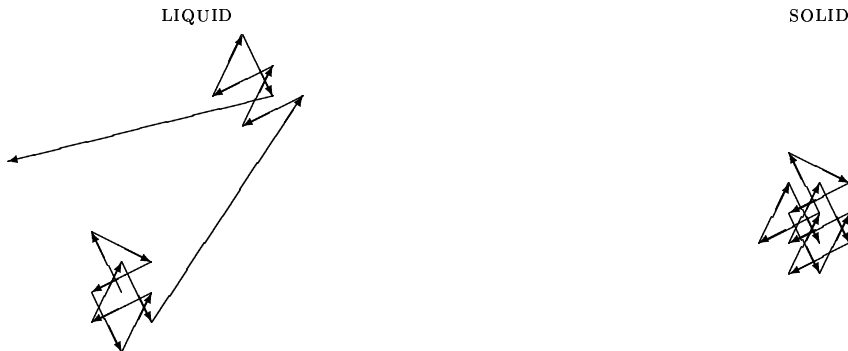
$$\frac{\Omega[K]}{N} \equiv \frac{4\pi}{3} \cdot \bar{R}^3 \tag{4.2}$$

which in turn defines the average interparticle distance. The criterion for the system to be dilute, that is "gaseous" is then

$$\frac{\bar{R}}{a} \gg 1 \quad \text{GASEOUS PHASE} \tag{4.3}$$

This reasoning is based, of course, on implicit assumptions about the statistical nature of the system, in particular about its homogeneity, something like assuming that we deal with a single homogeneous phase.

It is a more subtle question, how to distinguish between liquids and solids. Taking up first the "microscopic" approach, that is dealing with individual grains, we may loosely say that in a liquid each particle may and in a due time will stray away from any position within the system, while in a solid the particles fluctuate within a finite range, [33, p. 14], as may be sketched in the following manner:



These plots purport to be strobos of the successive positions of a selected particle. Obviously, it is essential to follow the trajectory of one labelled particle in this case. How could this be formalized?. Following [34], we may define a **solid** as follows. The positions of the particles at a given instant  $t_{\text{REF}}$  will be taken as reference positions and then deviations as a function of time may be defined,

$$\mathbf{r}_i \equiv \mathbf{r}_i(t_{\text{REF}}) \quad \text{REFERENCE POSITIONS} \quad (4.4)$$

$$\mathbf{u}_i = \mathbf{r}_i(t) - \mathbf{R}_i \quad \text{DEVIATIONS} \quad (4.5)$$

In order to evade the problem of the movements of the sample as a whole, we switch to the intergrain distances  $R_{ij} \equiv |\mathbf{R}_i - \mathbf{R}_j|$  etc., and write the condition for a sample to be solid as

$$\frac{[\mathbf{u}_{ij}^2]_{\text{A}}}{R_{ij}^2} < 1 \quad \text{FOR ALL } i, j \quad (4.6)$$

where the subscript A denotes a not clearly specified average over times in the spirit of Sec. 2.6 in the Part I, where the averages were taken rather over the positions, however. This condition is not very strong, yet it guarantees the basic rigidity of the sample. The condition which is usually taken is much stronger, namely  $[\mathbf{u}_i^2]_{\text{A}}/a^2 \ll 1$ , the well-known *Lindemann criterion*. This is all well, but in fact, such requirements would eliminate from consideration a vast class of objects, which we have good reasons to term solids. Most of the systems of real significance will undergo a **slow relaxation**, paramount to certain viscous behavior, and the above criterion would have to be modified appropriately, as discussed in [36, p. 5]. It appears that the microscopic criteria of the kind of (4.6) can only be linked with the macroscopic point of view, external forces are included. Thus, the condition (4.6) is equivalent to the existence of a finite shear modulus of the system. Its modification accounting for a possible slow relaxation involves a viscosity under an external (shear) stress, etc. While this macroscopic formulation has a global character, there is another important exception to (4.6). Namely, this criterion may be valid for most of the particles, but **not necessarily for all**  $i, j$ . Small mechanically unstable or loose regions are a signature of most of the amorphous substances. The existence of the so-called two level states which are thought to be responsible for the linear term in the specific heats of many non-crystalline materials is linked with these locally loose regions.

One final remark will concern the concept of the **long range order** (LRO). Often the distinction between a crystalline (periodically ordered) and non-crystalline, or amorphous, matter is put like loss of the LRO in the latter case. This is linked to a narrow definition of the LRO, based just on the lattice periodicity. In fact, even a non-crystalline solid sample obeying (4.6) possesses a strict and permanent mutual arrangement of the constituent particles (grains or atoms) and in this sense, it has a degree of LRO comparable with crystals. This is also related to a small configuration entropy of amorphous solids, as discussed from various points of view in the references given.

In conclusion of this subsection, we will quote the definitions of several more conventional characteristics of particle arrays for the sake of reference. The transition from individual trajectories to a

distribution of the particles is mediated by the **particle density**

$$\rho(\mathbf{r}, t) = \sum_{n=1}^N \delta(\mathbf{r}_n(t) - \mathbf{r}) \quad (4.7)$$

Assuming that the system is large and homogeneous, just as in Sec. 2.6, we may repeat the definitions of the averaged quantities, the mean particle density and the pair correlation function by

$$\bar{\rho}(t) \equiv [\rho(t)]_{\text{Ave}} = \frac{1}{\Omega[\mathbf{K}]} \cdot \int d^3\mathbf{r}' \rho(\mathbf{r}', t) \quad (4.8)$$

$$B(\mathbf{r}_d; t, \tau) = \frac{1}{\Omega[\mathbf{K}]} \cdot \int d^3\mathbf{r}' \rho(\mathbf{r}' + \mathbf{r}_d, t + \tau) \rho(\mathbf{r}', t) - \bar{\rho}(t + \tau) \bar{\rho}(t) \quad (4.9)$$

For a stationary system, both quantities are  $t$ -independent and for a static immobile array, also the  $\tau$ -dependence loses its meaning. We will discuss such static arrangements of balls in the next subsection. The *radial distribution function* will be introduced now for the case of static assemblies; it can be linked with the scattering factor appearing in the expressions for the diffraction intensities in the kinematic approximation. As we know, the general expression for the scattering factor is

$$S(\mathbf{q}) \sim \int d^3\mathbf{r}_d B(\mathbf{r}_d) e^{i\mathbf{q}\cdot\mathbf{r}_d} \quad (4.10)$$

where  $\mathbf{q}$  is called the *momentum transfer* or the *scattering vector* depending on the respective community and the proportionality factors are not indicated. In the case of a macroscopically (globally) isotropic medium, the correlation function can be written as a function of the length  $r$  of  $\mathbf{r}_d$  in the form

$$B(r) = \bar{\rho} \cdot (\rho_r(r) - \bar{\rho}) \quad (4.11)$$

Here, a new quantity is introduced, a radial (angle averaged) particle density  $\rho_r(r)$ . It is expected that  $\rho_r(r) \xrightarrow{r \rightarrow \infty} \bar{\rho}$ ; in fact this limit will be achieved within the distance of a few  $a$ . This makes the integral for  $S(\mathbf{q})$  convergent. The explicit integration in the isotropic case simplifies to

$$S(q) \sim \int dr 4\pi r^2 (\rho_r(r) - \bar{\rho}) \frac{\sin(qr)}{qr}, \quad q = |\mathbf{q}| \quad (4.12)$$

By this, several quantities are defined:

$J(r) = 4\pi r^2 \rho_r(r)$	RADIAL DISTRIBUTION FUNCTION
$J(r)_{\text{rnd}} = 4\pi r^2 \bar{\rho}$	"GAS" RADIAL DISTRIBUTION FUNCTION
$G(r) = (J(r) - J(r)_{\text{rnd}})/r$	REDUCED RADIAL DISTRIBUTION FUNCTION

The radial distribution function has a simple interpretation:  $J(r)dr$  gives the average number of particles in a spherical shell of a radius  $r$  and a thickness  $dr$ . The "reduced" RDF has the merit that its sine Fourier transform yields immediately the scattering factor  $S(q)$ .

### 4.1.2 Random close packings of spheres

The single most popular case among all granular systems and indeed a synonym for them in the mind of a general public are static assemblies of hard spheres. In order to be stable, such assemblies have to be as dense as possible, **close packed**. Regular close packings of one or several species of balls have been introduced long ago in physical crystallography to model crystal structures which did not involve covalent bonding: ionic crystals, metals and, more recently, the ideal case of rare gas crystals. The start of a systematic use of irregular arrays of spheres in modelling liquid and, later, amorphous structures can be associated with the work of Bernal; accounts of that and of other anecdotic episodes in the prehistory can be found in [16, 33, 36] and in the article by Finney in [31]. These references also provide an extensive discussion of the whole problem of irregular, **random close packings, RCP**. Here, we will only give a summary of the most important points.

From the purely geometrical point of view assumed presently, a sample will be fully, "microscopically", specified, if the positions and the radii

$$\{\mathbf{r}_1, \dots, \mathbf{r}_n, \dots, \mathbf{r}_N\}, \quad \{a_1, \dots, a_n, \dots, a_N\}$$

of all spherical grains will be known. On the basis of Euclidean considerations, simple in principle, we should be able to decide, if the array is a random close packing and find all its properties.

We should, of course, ask once more, how the coordinates can be obtained, but this question will be profitably deferred to the end of this section. At this moment, it is important to note that it has been established experimentally, that is as a hypothesis based on a vast experience with modelling close packed structures, that

**all 3D close packed structures fall into two classes:**

- ◇ **regular close packings** epitomized by an *fcc* crystal
- ◇ **random close packings** or the so-called *Bernal structures*

This might not seem as very surprising granted that an array of identical spheres can be made periodic, while an array of assorted balls can only be irregular. The interesting thing is that this division persists rather in a rather stable manner for balls whose sizes have a statistical dispersion varying in a fairly large range. That is, even balls with nearly equal diameters tend to form a random close packing under favorable conditions, while even a sizable dispersion in diameters does not preclude a formation of a regular packing. To explain the distinction between both types of packings and to give a more precise meaning to the statements just made, we have first to introduce some more characteristics of ball arrays and to look at the differences.

**Global characteristics** By this we mean such characteristics, which reflect the overall or summary properties of the assembly of balls.

*Ball composition* We illustrate the possibilities by a few examples. The simplest is the **monodisperse** case, that is all balls having the same radius  $a$ . A **binary mixture** will have balls distributed bimodally between two diameters  $a_A, a_B$  with weights  $c_A, c_B$ , satisfying the condition  $c_A + c_B = 1$ . A **polydisperse distribution** is such that the radii are distributed statistically around an average value  $\bar{a}$  with a dispersion  $\delta a$ , say. Etc.

*Packing ratio* (filling factor, ...) When defining the gaseous phase, Eq. (4.3), we could have said also that in a gas the fractional volume occupied by the grains (the van der Waals "excluded volume") is small. This fractional volume is termed the packing ratio  $P$ :

$$\begin{aligned} P &= \frac{1}{\Omega[\mathcal{K}]} \sum_{n=1}^N \frac{\pi}{6} a_n^3 \\ &= \frac{N}{\Omega[\mathcal{K}]} \frac{1}{N} \sum_{n=1}^N \frac{\pi}{6} a_n^3 \end{aligned} \tag{4.13}$$

and, finally, denoting the average volume of one ball by  $\varpi$ ,

$$P = \bar{\rho} \cdot \varpi \tag{4.14}$$

Obviously, the ball composition is an input, then there follows the model building, and the packing ratio comes at the end as an output. The distinction between regular and random close packings is based on the observation that the **packing ratio for all monodisperse or moderately polydisperse samples** has accumulated around two distinct values

$P \leq 0.740$	REGULAR CLOSE PACKING
$P \leq 0.637$	RANDOM CLOSE PACKING

This behavior is explained microscopically on the basis of topological considerations. Namely, a **connectivity matrix**  $\mathcal{C}$  can be constructed to each sample such that

- ◇  $\mathcal{C}(i, j) = 1$  BALLS  $i, j$  ARE NEIGHBORS
- ◇  $\mathcal{C}(i, j) = 0$  BALLS  $i, j$  ARE NOT NEIGHBORS

This matrix defines the topological structure of the sample. Now, it turns out that the regular and



the random close packings are topologically very different and that there is no "continuous" way of transforming one type of structure on the other. Recrystallisation of a glassy sample would involve simultaneous changes of large regions of the sample, very much in line with the first order character of the phase transition liquid–solid. There is, however, much more to this: the non-crystalline structures are not equilibrated, both in a geometrical, and, as will be seen later, in an energetical sense. In other words, they are metastable. The barriers to the more stable regular structures are so monstrously huge that the corresponding transition is very unlikely. The tectites, an instance of a natural glass, have a "geological age". The same goes, of course, for the granular samples, and this is at the bottom of the existence of the two clearly distinct structure types.

Of course, in order to give a real meaning to such statements about the topological structures, we have to be able to decide at least, who is a neighbor of a given ball in a sample. This is more easy in a regular sample. The close packing implies precisely 12 (nearest) neighbors, which all touch the central ball. The situation is less clear for a random close packing, which is less dense. This could happen in two ways: either the number of neighbors decreases on the average, or the distances between the nearest balls increase, and many of them do not touch each other. This latter possibility turns out to be correct. The neighboring balls are then defined on the basis of the so-called **Voronoi region** (known in solid state physics as the Wigner-Seitz cell). This is a polyhedron circumscribed around a given ball. Its faces are formed by intersections of planes perpendicular to connecting lines to all other balls and, in the simplest case of equally sized balls, bisecting the distance between their centers. Only some of the planes lead to a face at the end; these correspond to a neighbor. Here is an illustration in 2D:

Figure

This compound representation of a close packed structure shows the balls together with the two complementary ("dual") representations of the structure, the bonds (connecting lines) and the cells (the Voronoi regions). The cells fill without gaps the whole space (the plane in this case): they are said to be a **tesselation** of the space. The bonds form edges of complementary polyhedra (in 2D, sides of polygons), which all together form the **dual tesselation** of the space (or plane). These dual polyhedra are centered around the holes between the balls, in other words, they represent the structure from the point of view of the porous space. For one thing, some smaller balls can fit into the interstitial positions. Thus mixtures of balls with sufficiently different radii can achieve a much higher filling of the space than the monodisperse balls alone. The critical radii are easily obtained from considering the interstitial polyhedra. This has been done long ago in the crystallography by Goldschmidt and pursued further by Pauling, as summarized in the famous Pauling-Goldschmidt rules for stability of the ionic crystals. Similar considerations hold also for glasses, as shown in the example below. There, the theoretical RDF for a monodisperse random close packing is compared with experimental curves for a metal glass  $a - \text{Ni}_{76}\text{P}_{24}$ . The metalloid is light and does not show in the X-ray structure factor. The metal RDF is almost that of a monodisperse random close packing: the metalloid atoms are sitting in the interstitial spaces.

**Local characteristics** Knowing just the local neighborhoods of all balls, at least in a statistical sense, represents thus already a very detailed information about a given structure. This is discussed at some length in the references given above; some very interesting insights can be found especially in the articles by Finney and by Rivier in [31]. We may mention here three such characteristics.

*Coordination number*  $NN$  is the same like a number of nearest neighbors. It is thus given by the number of faces of the Voronoi region corresponding to a given site. As said, in regular close packed structures, it is 12 for all sites (balls). In random close packings, the average number of neighbors increases, at the expense of being more remote, of course. The coordination number is the principal local characteristic for a liquid, or for an amorphous solid, where the interparticle forces act even at distances larger than  $a$ , and it is informative also for the granular systems. The left panel of the following picture illustrates the distribution of coordination numbers in a random close packing.

*Number of contacts*  $NC$  that is of those nearest neighbors which are touching the central ball directly, has a principal importance for granular matter, because only the touching balls contribute to the force transfer and to the mechanical stability in a system with contact forces exclusively. Clearly, always  $NC_n \leq NN_n$ . The number of contacts cannot be too small in order to render the structure stable. We have to distinguish a local stability. This is guaranteed by  $NC_n \geq 4$ , as may be nearly obvious.

There is, however, also the far more sophisticated concept of a global stability, which can be achieved only for  $[NC]_{\text{Ave}} \geq 6$ . This inequality is a result of extremely interesting considerations of purely geometrical constraints for an amorphous structure, as discussed in [34], see also [35]. The right hand panel of the last figure gives the idea about the real situation. It is apparent that 6 appears to be the most probable,

and roughly the average number of contacts. Thus, in fact,  $[\text{NC}]_{\text{Ave}} \approx 6$ .

**In detail:** This can also be understood in geometrical terms, as noted in the last two references: There are  $3N$  coordinates of the ball centers, while the requirements of a close contact of the form  $|\mathbf{r}_i - \mathbf{r}_j| = \frac{1}{2}(a_i + a_j)$  lead altogether to  $[\text{NC}]_{\text{Ave}} \cdot \frac{1}{2}N$  constraints (each ball is counted twice). A regular situation requires that the number of constraints does not exceed the number of unknowns, otherwise the system would be overconstrained, i.e., *overdetermined*. Hence,  $[\text{NC}]_{\text{Ave}} \leq 6$ . The two opposing inequalities lead to the above result.

How about the exceptional overconstrained systems? It is important to realize that **all regular close packings are overconstrained**, because they have 12 rather than 6 contacts per ball on the average. Similarly in 2D, the hexagonal close packed plane has 6 contacts per site, in excess of the value of 4 expected on the basis of the above estimate. This is due to the special symmetry of these packings, of course. There are important consequences of these results, to which we will return in the next section.

*Pair correlation function* We have discussed already the significance of this quantity and now we may see its actual form for a random close packing. The quantity actually plotted is the radial particle density. We see that no particles appear for distances shorter than the intimate contact, the ensuing peak corresponds to the first coordination sphere. We see, how the distances are distributed. Integration of  $J(r) = 4\pi r^2 G(r)$  from zero to a variable upper limit would show a saturation to a value close to the average coordination number  $[\text{NN}]_{\text{Ave}}$  just before the onset of the next peak, which corresponds to the second coordination sphere, etc. It is obvious that the information contained in the first peak of the RDF is complementary to some extent to the statistics of the coordination numbers. The RDF is richer in that it also reaches beyond the first coordination sphere. In principle, it should provide information about the **intermediate range order**. In fact, it is this mesoscopic range of the structures which carries the most important defining properties of random structures, as will emerge below in another context. The related geometrical considerations and experimental evidence on glasses can be found in [36, Sec. 3.4].

### 4.1.3 Modelling granular matter

To conclude this part on the geometry of granular samples, we should make several comments concerning the question 'how do we know?'. As mentioned already, the original aim of generating macroscopic close packed arrangements of spheres was to model atomic structures of liquids and glasses. This was possible to do by hand building comparatively small clusters using the balls-and-sticks technique, measuring the coordinates optically and refining the positions on a computer. The models building has always been between the art and science, and human intuition helped to get across the difficulties in obeying all geometrical constraints and conditions. Locally, the requirement was to keep as close as possible to the close packed geometry. At the same time it was important to generate a model which could be continued to a larger size, if the need would arise. This implied the loose conditions of homogeneity, so that the cluster built would have no center, for example. This work has been successful, and, as we have seen, the model and the experimental RDF could be brought into agreement, including the correct average density.

The requirements on the macroscopic granular samples have sharpened up considerably, as soon as they were intended to "model themselves". First, they have had to involve many more grains in order to be relevant to the physical questions newly posed. Second, the method of generation of a granular sample could not have been detached from the actual system in question. New standards have been set up, which basically apply at present, but may still undergo an unforeseen development. To grasp the basic issues, it is advisable to scan the proceedings of specialized conferences, for example [37], [38], or [39].

Paradoxically enough, not only it is more difficult to get a good granular sample than to model a microscopic cluster, but at the same time, it is by no means easier to achieve an experimental information about the arrangement of the grains in a macroscopic granular matter than in a non-crystalline array of atoms. This may explain the prevalence of work done on 2D systems. Their advantages include a better control during their preparation, easier description and characterisation, and, finally, a possibility of a direct determination of the grain arrangement before, during, and after an experimental work on the system. This is rather favorable as far as these systems are studied for their own sake. On the other hand, there are all reasons to keep serious reservation about the use of 2D samples as models of "real" 3D situations. This emerges on all levels. Thus, waves in 2D and in 3D behave quite differently, and the localisation problem is posed in an entirely different way in both cases. As concerns directly the problem of the geometry of random close packings, in 2D, the bonds form a planar graph, whose topological

properties are rather special and care should be taken when transferring the results to 3D. There also emerge certain basic differences specifically between the 2D and 3D random close packings. There seems not to exist a 2D random close packing topologically distinct from the regular 2D structures similar to the 3D case, the 2D samples tend to recrystallize, etc.

As perspires from almost any remark made in the whole section on the geometry of granular matter, this question of grain arrangement cannot be detached from the question of the underlying forces, energetics, etc. In that sense, the discussion of the modelling procedures does not belong here; admittedly, there are theoretical techniques still in use, in which the grains are added one by one so as to satisfy reasonable geometrical conditions. A typical present day method of generation, however, is dynamical. Either the sample is physically produced under certain precisely defined conditions, that is, the **generation process follows a strict protocol**. Or the sample generation is simulated on a computer, in which case it proceeds again according to a well defined dynamical process. In either case, the specifications will include external forces acting, boundary conditions (free heap, vertical silo, a closed vessel?), the speed and the method of adding further grains, dissipative processes including the ambient medium (air, a liquid?, quiescent or flowing?). Another questions: ... will the sample be compactified by tapping, vibrations, or, to the contrary, will precautions be made to keep it loose? will it be left free, or will an external stress (hydrostatic, uniaxial, shear) be imposed? finally, it should be clear that the granular systems more than any other substance are susceptible to further modification during the experimental work, or even when they are left alone. In other words, the "sample preparation" never ends.

We may conclude this discussion by a brief summary, which will serve as a point of departure for the next section:

Any given granular sample at a given moment is the result of its own history and cannot be, as a rule, specified by any set of global equilibrium characteristics. This represents yet another, and deeper, analogy between the granular systems and the close packed amorphous substances.

## 4.2 Forces in granular samples

The geometry of a granular sample and the forces acting on it represent twin facets of one physical picture and cannot be approached in an independent way. Because of the non-cohesive nature of granular matter, it cannot be mechanically equilibrated without external forces, involving sometime the volume forces, like gravity, but always contact forces at the interface with a container or a support. Rather often, only the external forces, a pressure distribution underneath a grain heap, say, are accessible. Establishing the relationship between the external force distribution and the resulting force pattern inside the sample is thus one of the important tasks. It has been approached on the basis of rather varied models: microscopic – dealing with individual grains, phenomenological – with a "block" as a basic unit, and macroscopic – working with a continuum description. In fact, each of the approaches could be applied only in conjunction with some very strong assumptions, which could not have been verified beforehand. Thus, we have witnessed a parade of competing speculative theories, attempting at the best agreement with empirical data. Unfortunately, the data are often as uncertain as their attempted explanations, and the outcome so far has been undecisive [32]. Luckily for our intentions, the difficult questions mostly concern the comparatively loose granular systems with free surfaces, for example freshly created piles, while the situation seems to be more transparent for strongly confined samples, which are of a direct interest for us. This enables us to avoid this vast and confused ground.

We will proceed as follows. First, the problem of **multicontact equilibria** will be posed. Then the mechanics of an **individual contact** will be overviewed. From that we will proceed to the **assemblies of grains** and review what is known about the resulting microscopic force distributions. Finally, the transition to an **effective continuum** will be queried.

### 4.2.1 Multicontact equilibria

*Rigid grains with idealized contacts* It may be proper to recall first the textbook treatment of rigid bodies in contact according to [40, §38]. There will be made no assumption concerning the shapes of the contacting bodies – grains, except that they be smooth so that they might develop a well defined contact plane.

**Note:** Even this is not self-evident. The grains may have shapes close to singular, with edges, cusps and spikes. Goddard [41] has proposed that grains with spikes could account for the observed pressure dependence of the sound velocity.

The positioning of the grain is specified by the radius vector  $\mathbf{r}_n$  of its *center of inertia* and by the Euler angles or other coordinates determining its orientation in space. The connectivity matrix now specifies which grains are in a direct contact, and for these, the *points of contact*  $\mathbf{R}_n^m$  and the *contact forces*  $\mathbf{F}_n^m$  are defined. At each contact, there exists a well defined tangential plane and a normal to it. We denote by  $\mathbf{n}_n^m$  the *normal vector* pointing outwards. With this, there is a unique decomposition of the forces into their *normal* (compressive) and *tangential* (shearing) *components*

$$\mathbf{F}_n^m = \mathbf{N}_n^m + \mathbf{T}_n^m \quad \text{NORMAL AND TANGENTIAL FORCES} \quad (4.15)$$

Clearly, these contacts can be viewed from both sides, and there hold obvious relations

$$\begin{aligned} \mathbf{R}_n^m &= \mathbf{R}_m^n && \text{COMMON POINT OF CONTACT} \\ \mathbf{n}_n^m &= -\mathbf{n}_m^n && \text{COMMON NORMAL OF CONTACT} \\ \mathbf{F}_n^m &= -\mathbf{F}_m^n && \text{LAW OF THE ACTION AND REACTION} \end{aligned} \quad (4.16)$$

Now we are ready to write the **conditions of a static equilibrium** for each grain. There are two of them for each grain. If we omit for simplicity the volume forces and consider only the contact interactions, they have the form

$$\begin{aligned} \mathbf{F}_n &= \sum_{\text{CONTACTS } m} \mathbf{F}_n^m = 0 && \text{TOTAL FORCE EQUILIBRIUM} \\ \mathbf{L}_n &= \sum_{\text{CONTACTS } m} \mathbf{R}_n^m \times \mathbf{F}_n^m = 0 && \text{TOTAL MOMENT EQUILIBRIUM} \end{aligned} \quad (4.17)$$

**In detail:** The moment condition is originally written with respect to the center of inertia of the grain,  $\mathbf{L}_{n \text{ TRUE}} = \sum_m (\mathbf{R}_n^m - \mathbf{r}_n) \times \mathbf{F}_n^m = \mathbf{L}_n - \mathbf{r}_n \times \mathbf{F}_n = \mathbf{L}_n$ , because of the first equilibrium condition. The same is not true in the dynamical case, when the total force on a grain is typically non-zero.

Things may now seem simple, but in fact all the above equations do not define the forces uniquely as a function of the external forces in general. This is so, because the contact forces have a singular character and infinitesimal movements of the grains may be associated with large changes in the values and the directions of the forces:  $\diamond$  The normal components are the so-called *reaction forces* corresponding to the mutual constraints which the grains in contact impose on each other. when the contact is under a positive pressure, the force can be arbitrarily large. On the contrary, an infinitesimal negative normal displacement will make the non-cohesive reaction force vanish at once.  $\diamond$  The tangential components are due to *friction*. Within a pure mechanics of rigid bodies, two limiting situations are admissible: a *perfectly smooth* surface leading to a **perfect gliding** of the grains on each other, or a *perfectly rough surface* causing the grains to a **perfect rolling** over each other. In the gliding case, the tangential forces vanish identically and do not participate at the grain interactions. In the rolling case, the grains are constrained *geometrically* to make identical small displacements in the tangential direction, be they virtual or real. The corresponding tangential force is then also of a reactive nature and may be "arbitrary".

All this is known in technical mechanics rather well under the name of **hyperstatic systems** (also known as "statically undeterminate"). Attempts to "regularize" the forces lead typically to spurious results depending on the method of regularisation. In fact, the proper approach appears to be a *dynamical method*, in which the static equilibrium is a result of a dynamical evolution including a dissipation. In this case, the resulting force distribution can also vary continuously in a wide range, but a **given force distribution is truly a functional of the dynamical history of the sample**. Clearly, the geometry and the forces acting are determined simultaneously for a specific sample preparation run. Some examples

may be found, e.g., in [31], but a most illuminating, although terse, discussion is in the article by Radjai in [39, p. 305].

Rigid grains in a rolling contact move so that their instantaneous contact points have the same velocities. Thus, the constraint is formulated not in terms of the coordinates, but in terms of their time derivatives, and its form is a differential equation. There are then two principal possibilities. Either the equation is integrable, that is the velocities can be expressed as total derivatives of a function of coordinates, or it is not. These two cases bear the names:

*holonomous constraints* – the integrable case

*anholonomous constraints* – the non-integrable case

Here, we arrive at still another, and a very profound, difference between the 2D and the 3D cases. A 2D disk rolling down a line is holonomously constrained, as the velocity is given by the derivative of the total rolling angle. A 3D ball rolling down a plane is an anholonomous case (see in Ref. [40]). The same reasoning applies also in the multicontact case . . .

*Towards realistic grains: Hertz-Mindlin model* Now it will be admitted that the grains be deformable and the friction in the contacts obey a realistic force law. A typical model of the contact falling into this class is the so-called Hertz-Mindlin contact; it is also the only one, whose properties and consequences for granular matter have been explored to any depth. We will devote to this particular model the next two sections, so that we would be able later to discuss adequately the force distributions as they have been modelled already.

The *Hertz-Mindlin contact* is defined as elastic in the normal direction and as obeying the Coulomb law of friction in the tangential direction. The normal force is consequently purely repulsive and one-sided, it vanishes for arbitrarily small positive normal displacements of the grains. The Coulomb law postulates that no sliding occurs unless the tangential load reaches a *static threshold*. Beyond this threshold, sliding sets on, but it is dissipative due to a non-zero friction force. Let us assume that both power laws are sufficiently stiff with respect to the forces acting in the system (something we can always achieve at our will by reducing the external loads). For geometrical reasons the stresses concentrate around the contacts. The grains are locally responding according to the laws of elasticity and they are deformed around the contact points, while they preserve their overall shape as if they were rigid. The tangential forces arouse no sliding within certain range, which has to be observed in any case in order to keep the system static. The contact forces of both types act within the small contact regions, and, in fact, all of the above equations for equilibrium forces remain valid, if only an allowance is made for the deformation of the granular system resulting from the local deformations around the individual contacts. Rather clearly, the general picture of the static granular sample is not really different from the case of ideal rigid grains. There is certain regularisation introduced of the contact forces, but their nature is not deeply changed and all conclusions about the hyperstatic behavior of the granular assembly, and about the necessity to follow the life history of a sample, remain valid.

*Overview of the contact models* The Hertz-Mindlin contact is not the only possibility, and many variants can be devised, either by simplifying the Hertz-Mindlin assumptions, or, on the contrary, by improving the model by adding further realistic features. This has certainly not been done very systematically, although a number of various modifications in non-negligible. Here, we will give a sampling of this area by listing some references and adding just the necessary comments.

SOME CONTACT MODELS APPLIED TO ASSEMBLIES OF SPHERICAL BALLS

LEGEND: 2D . . . only 2D arrays; 3D . . . used also in 3D; XX . . . not utilized yet

friction law $\Rightarrow$ constitutive $\Downarrow$ law	ideally smooth	realistic friction law	Coulomb friction law	ideally rough
<b>rigid grains point contacts</b>	Tkachenko & Witten [35] [40] 2D	<i>N O T S T U D I E D</i>	Radjai et al. [37, p.169], [42] 2D	<i>ideal case</i> [40] XX
<b>elastic grains Hertz contacts</b>	J.-N. Roux, Melin [38, p.215] [43] 2D	Baumberger & al [44] [45] XX	Duffy & Mindlin, Goddard [46] [41] 3D	<i>N O T S T U D I E D</i>
<b>visco-elastic/ plastic grains</b>	<i>N O T S T U D I E D</i>	Baumberger & al [44] [45] XX	Schäfer & al, Lud- ing [47] [39, p. 285] XX	<i>N O T S T U D I E D</i>

A mechanical combination of various friction and constitutive laws yields 12 possibilities. Some are of little interest, and we have indicated these by the label "not studied". One of the four excluded cases might in fact be interesting for some problems of soft matter, namely the ideally viscoelastic balls. Perhaps I have just overlooked the work done in this direction. For the other entries, only one or two references are given, basically of a theoretical character. For some entries, this is just fair, for some other ones, many more references may exist, and I quote those of a special interest. The character of the works cited is not uniform. To some extent, this is indicated by the labels 2D, 3D, and XX. The XX label may deserve an explanation. It indicates a physical situation, for which a contact between two bodies has been studied, but the results were not confronted with the case of many grains. As concerns, the studies of granular assemblies, they ALL relate to systems of "BALLS", that is 2D or 3D bodies with a full rotational symmetry.

Let us now browse through the table column by column. It is natural to start with the *coulomb friction law*, and within that column with the Hertz-Mindlin model. Here, we quote, first of all, the Duffy&Mindlin classics from 1957. They were able to derive the effective elastic compliances for a close packed regular cubic array of balls and they were the first to derive analytically their history dependence: the results were different depending on the way the stresses were successively imposed on the sample. The work of Goddard [41] was concerned with the sound velocity in irregular granular samples and it was based on a kind of a mean field approximation; we will return to this paper later. Thus, while these studies dealt with the 3D granular matter in an impressive way, their scope was limited. It is significant that direct calculations of a stress distribution involving the Hertz-Mindlin contacts in an unrestricted way seem not to be published. The difficulty consists in the necessity to calculate explicitly the elastic displacements of the contacts as a part of finding the static equilibrium. It is then understandable that all effort was devoted to the case "one below", namely assuming the grains to be rigid. This is the top entry of the column, and the use of this model is associated with the calculations of F. Radjai, although we may see that a number of top theorists of the field contributed to disentangling at least this "simple" problem. As explained already, this case can be understood as the limit of extremely stiff Hertz contacts and it seems that all essential physics is represented by this model to a reasonable degree. This work will be at the focus of our attention in the next section.

Moving to the bottom of this column, we encounter two papers which deal in fact with the dynamical interaction of two grains during their collision. In order to make such collisions adequately dissipative (... the *restitution coefficient*), it appears as **important to make the grains inelastic**. It should be borne in mind, however, that it is barely possible to account properly for the *slow relaxation* of a static granular sample without admitting the time variable in the constitutive laws. As a consequence, the "viscoelastic Hertz-Mindlin contact" seems to be a proper model for a realistic view of granular systems. One objection comes to mind immediately, however. If we take for granted that the correct description of a contact interaction stand on two legs, the bulk constitutive law in the grain, and the friction law at the grain interface, it would seem inappropriate to have one leg of iron and the other of clay. It is obvious that the venerable historical Coulomb law is a very good, but at the same time also a truly schematical reflection of reality. We have to admit that, while processes like creep, hardening/weakening, etc. can take place inside the grain, a parallel roster of processes should be allowed for in the contact, which is not a simple geometrical structure with two nearby surfaces, but a complex object with its own existence. It is for that reason that the column with the heading "physical friction law" is included, although a situation of such degree of complexity was not considered so far at all in the connection with granular system. In the insert, some basic notions of the contemporary physical picture of dry friction are briefly summarized.

DRY FRICTION BETWEEN TWO BODIES

Having thus reached the apogee of complexity in the contact force laws, we retrace our steps and look at the two outermost columns of our table. They correspond to the two limiting cases treated by Landau & Lifshitz in [40], and this part of the problem has been discussed already. In particular, the case of ideally rough grains is a convenient limit of the Coulomb law. As a rule, this limit is not singular, insofar the static granular media are concerned, and by this we may conclude its discussion. Such is

not the opposite case of the ideally smooth gliding contacts, which leads to an exceptional behavior in many important respects. It should be noted that in spite of that, quite an important deal of all papers on forces in granular systems has been considering precisely this case. The reason: simplicity and tractability. Looking first at the gliding pure Hertz contacts, we may note that the absence of friction is not crucial for regular arrays with a high degree of symmetry of all local environments. On the other hand, the problems with overdermination become then dominant, and they have to be faced. In the quoted paper by J.-N. Roux, this is achieved by making a detailed study just of a carefully constructed and controlled overdetermined 2D ball array. The work of Melin [43] is "intermediate": the model assumes a frictional dissipative force, but it has a linear viscous character. As a result, it vanishes at zero velocities and it does not contribute to the static force fluctuations in the sense of the Coulomb law. To understand the problem from another side, we may notice that a granular system made of balls without friction involves only central forces. This is the so-called Cauchy model of interatomic forces, and it leads to the known consequences for the tensor of the macroscopic elastic moduli [?], whose components become heavily interrelated at variance with the moduli of real systems.

The unique properties of the grains without friction are made particularly clear in the paper [35], which concerns the simplest granular system ever, a 2D random array of gliding rigid balls. We have already looked into the question of the average number of contacts in such a system, but we made there a number of tacit assumptions, which will be spelled out now. The balls can freely rotate in their places and their placement in the space is fully specified by the positions of their centers alone. The conditions for their contact are also specified by the required distances between the centers, which we have employed in Sec. 4.1.1. Going over to the forces, we see that once the contact points are (geometrically) specified, the forces act along the respective radii, so that it is enough to know their magnitude to describe them completely. On the other hand, because their lines of action pass through the center of the ball, which is the center of inertia at the same time, it appears that the moment of the contact forces acting on each ball is strictly zero, so that the moment condition is satisfied identically, and only the total force condition remains in power. All this is peculiar just to the case of gliding spherical balls, and "normalcy" is renewed by either including the friction, or, even more simply, by considering non-spherical grains. The consequences of the singular situation are striking, as the reader can find in the paper quoted.

We conclude this longish section by stating that in what follows, we will assume the Coulomb friction law, and consider its consequences for individual contacts and for the multicontact force distribution in several model situations.

#### **4.2.2 Hertz contact**

#### **4.2.3 Mindlin contact with friction**

#### **4.2.4 Stress inhomogeneities**

### **4.3 Sound propagation in granular samples**

#### **4.3.1 Basic considerations**

#### **4.3.2 Experiments of Gilles and Coste**

#### **4.3.3 Experiments of Liu and Nagel**

#### **4.3.4 Experiments of Page and collaborators**

#### **4.3.5 Experiments of Jia**

### **4.4 Concluding remarks**

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