Random Green matrices: From proximity resonances to Anderson localization

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Universal properties of the spectra of certain matrices describing multiple elastic scattering of scalar waves from a collection of randomly distributed point-like objects are discovered. The elements of these matrices are equal to the free-space Green's function calculated for the differences between positions of any pair of scatterers. A striking physical interpretation within Breit-Wigner's model of the single scatterer is elaborated. Proximity resonances and Anderson localization are considered as two illustrative examples.

Scattering of scalar waves from various kinds of obstacles is rich of interesting and often unexpected physical phenomena. An example of such phenomenon is the case of fixed frequency sound incident on small identical air bubbles in water [1–3]. Electron or phonon scattering from defects or impurities in crystal lattices give another example. Multiple-scattering effects from such objects are nontrivial and require special conditions to manifest themselves in their whole beauty. Already for two scatterers placed together well within the wavelength of the scattered wave field extremely narrow proximity resonances can appear [4,5]. For three scatterers there is the possibility for Efimov's effect [6–8]. For very many scatterers we expect, for some range of parameters, that Anderson's localization can show up [9–11]. It would be nice to have a unified approach encompassing all mentioned effects and giving some more insight into them. We use random Green matrices as a tool to achieve this purpose.

The Green's function is one of the fundamental basic building blocks for constructing a self-consistent description of the multiple scattering. In the case of scalar waves the Green's function is something very simple. It describes the spherical outgoing s-wave centered at the scatterers position. In this paper we study the spectra of certain matrices describing multiple scattering of scalar waves from a collection of randomly distributed pointlike objects. The elements of these matrices are equal to the Green's function calculated for the differences between positions of any pair of scatterers. We discover several interesting properties of the spectra of such Green matrices including a striking phase-transition-like behavior when the number of scatterers increases. In the limit of the infinite medium the eigenvalues behave remarkably well in that they distribute themselves not all over the complex plane but only on a fixed line. According to our numerical experience these properties seem not to depend on the specific form of the Green's function used and thus appear to be truly universal.

The Breit-Wigner-type model of the single scatterer allows us to give a clear physical interpretation of the obtained results. In this particular case the real and imaginary parts of the eigenvalues of the Green matrix can be considered as first-order approximations to the relative widths and positions of the resonances. Thus it is possible to extract some qualitative information about the resonances just from the spectrum of the Green matrix without looking for resonance poles in a complex energy plane. This approximation works surprisingly well in many physically interesting cases. The remarkable examples are proximity resonances and Anderson localization.

Let us begin by recalling the basic concepts of single scattering. Consider single spherically symmetric scatterer placed at $\vec{r}=0$. The asymptotic form of the wave function can be written in the usual way,

$$\psi_{\vec{k}}(\vec{r}) \simeq e^{i\vec{k}\cdot\vec{r}} + f(\vec{k})\frac{e^{ikr}}{r} \quad \text{for} \quad |\vec{r}| \to \infty, \tag{1}$$

where $f(\vec{k})$ is the scattering amplitude. We restrict ourselves to scatterers that are small as compared to the wavelength and therefore only an s wave e^{ikr}/r persists in scattering. Thus we will call such scatterers s-wave scatterers. In this case the scattering is *isotropic* and the scattering amplitude depends only on $k=|\vec{k}|$. In the following we will assume that the scattering is *elastic*. Therefore the optical theorem holds,

$$|f(k)|^2 = \frac{1}{k}\operatorname{Im} f(k). \tag{2}$$

It is easy to verify that this requirement gives the following form of the *single* scattering amplitude:

$$f(k) = \frac{e^{2i\delta(k)} - 1}{2ik}. \tag{3}$$

The scatterers necessarily have an internal structure. Thus in general the phase shift δ should be regarded as a function of energy $E = k^2/2$. For example, to model a simple scatterer with one internal Breit-Wigner-type resonance one can write

$$\cot \delta = -\frac{E - E_0}{\Gamma_0}. \tag{4}$$

The total scattering cross section $k^2\sigma = 4\pi \sin^2\delta$ takes then the familiar Lorentzian form

$$k^2\sigma = \frac{4\pi\Gamma_0^2}{(E - E_0)^2 + \Gamma_0^2}. \tag{5}$$

In a more elaborate way the individual scattering amplitudes can be parametrized using the R-matrix formalism (see, e.g., [12]).

Let us now briefly recall the basic equations of the s-wave multiple-scattering theory (see, e.g., [13]). After integrating Eq. (1) over the energy shell $k=|\vec{k}|$ the scattering wave function for incoming wave ψ_0 can be written as

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \psi_0(0)f(k)\frac{e^{ikr}}{r}. \qquad (6)$$

The only significant difference to Eq. (1) is an extra factor $\psi_0(0)$ which multiplies the scattering amplitude. This observation gives a hint how to write a scattering wave function for a system of N identical s-wave scatterers placed at points $\vec{r}=\vec{r}_a$:

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \sum_{a=1}^{N} \psi'(\vec{r}_a)f(k)\frac{e^{ik|\vec{r}-\vec{r}_a|}}{|\vec{r}-\vec{r}_a|}. \qquad (7)$$

It turns out that the incoming wave calculated at the position of the scatterer $\psi^{(0)}(0)$ needs to be replaced by the sum of the incoming wave *and* waves scattered by all other scatterers:

$$\psi'(\vec{r}_a) = \psi^{(0)}(\vec{r}_a) + \sum_{b=1}^{N} \psi'(\vec{r}_b)\frac{e^{2i\delta}-1}{2}G_{ab}. \qquad (8)$$

The elements of the G matrix from Eq. (8) are equal to the Green function calculated for the differences between the positions of the scatterers:

$$G_{ab} = \begin{cases} \dfrac{e^{ik|\vec{r}_a-\vec{r}_b|}}{ik|\vec{r}_a-\vec{r}_b|} & \text{for } a \neq b, \\ 0 & \text{for } a=b. \end{cases} \qquad (9)$$

Equations (8) form a system of linear equations determining the wave function ''acting'' on each scatterer $\psi'(\vec{r}_a)$ for a given incoming wave $\psi^{(0)}(\vec{r}_a)$. If we solve it then we are able to find the wave function everywhere in space. A similar integral equation relating the stationary outgoing wave to the stationary incoming wave is known in the general scattering theory as the Lippmann-Schwinger equation [14].

A way of dealing with *resonances* in this formalism is to look for resonance poles in the complex k plane. Resonance poles are values of k for which it is possible to solve Eqs. (8) as a homogeneous equations, i.e., for the incoming wave $\psi^{(0)}$ equal to zero. The real and imaginary parts of the corresponding resonance energies $E=k^2/2$ determine then the positions and widths of the resonances. This method has been applied recently to the analysis of resonances in a system of $N=2$ s-wave scatterers [4,5]. It turned out that very interesting phenomena can arise for pair of identical scatterers placed very close together, well within one wavelength. An extremely narrow p-wave *proximity* resonance develops from a broad s-wave resonance of individual scatterers. A new s-wave resonance of the pair also appears [4].

It is seen from Eqs. (8) that for $\psi^{(0)}\equiv 0$ the latter system of equations is equivalent to the *eigenproblem* for the G matrix,

$$\sum_{b=1}^{N} G_{ab}\psi'(\vec{r}_b) = \lambda\psi'(\vec{r}_a), \quad a=1,\ldots,N \qquad (10)$$

where

$$\lambda = -1 - i\cot\delta. \qquad (11)$$

For fixed positions of the scatterers $\vec{r}_a$ the eigenvalues of the Green matrix from Eq. (9) still remain functions of energy $E=k^2/2$. Using an explicit model of the scattering phase shift $\delta(E)$ and solving Eq. (11) in a complex E plane it is possible to determine the positions and widths of the resonances. In the particular case of the Breit-Wigner type s-wave scatterers the real and imaginary parts of the eigenvalues of the G matrix have a nice physical interpretation: they are equal to the relative widths $(\Gamma-\Gamma_0)/\Gamma_0$ and positions $(E-E_0)/\Gamma_0$ of the resonances. Indeed, using the explicit form of the complex energy $E\to E-i\Gamma$ and substituting the Breit-Wigner model of the scattering into Eq. (11) we get

$$E-i\Gamma = E_0 - i\Gamma_0[1+\lambda(E-i\Gamma)]. \qquad (12)$$

This system of two-coupled nonlinear equations determines the values of the resonance poles $E-i\Gamma$. In many physically interesting cases Eq. (12) can be solved numerically by iteration. For instance, in solving it up to the first order in Γ_0 one substitutes $\lambda(E_0)$ for $\lambda(E-i\Gamma)$, getting

$$\text{Re}\,\lambda(E_0) \simeq \frac{\Gamma-\Gamma_0}{\Gamma_0}, \quad \text{Im}\,\lambda(E_0) \simeq \frac{E-E_0}{\Gamma_0}. \qquad (13)$$

In this paper we deal with resonances in systems of N Breit-Wigner-type s-wave scatterers placed randomly inside a sphere, with the constant uniform density ρ. Let us start with the simplest possible example of a system of $N=2$ scatterers separated by a distance d. In this case the G matrix from Eq. (9) has two eigenvectors: $[1,-1]$ corresponding to the eigenvalue $\lambda_1 = -e^{ikd}/(ikd)$, and $[1,1]$ corresponding to the eigenvalue $\lambda_2 = -\lambda_1$. They are related to p- and s-wave resonances, respectively. Using the Breit-Wigner model of the scattering phase shift and solving Eq. (12) in a complex E plane it is possible to determine the positions $E_{1,2}$ and widths $\Gamma_{1,2}$ of these resonances. We repeated this procedure for 10^3 different separations of the scatterers $k_0 d$. The only independent parameter left is the width of the resonance of a single scatterer which we have set to $\Gamma_0/E_0=0.01$. Equation (12) was solved numerically by iteration reaching the accuracy of $10^{-6}\Gamma_0$ already after five iterations. The resonance poles obtained in this way are depicted in Fig. 1. They form a characteristic two-arms spiral. We see that for scatterers very close to each other $(d\to 0)$ one arm of this spiral approaches the axis $\Gamma=0$. It corresponds to the very narrow p-wave resonance. On the other hand, in this limit the second arm tends asymptotically to the axis $\Gamma=2\Gamma_0$. This arm corresponds to the s-wave resonance of the pair which is about
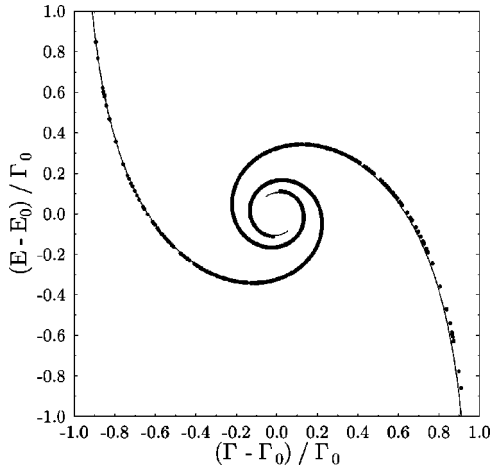
FIG. 1. Resonance poles calculated for 10^3 different systems of $N=2$ s-wave scatterers for $\Gamma_0/E_0=0.01$. Solid line corresponds to the approximate solution of Eqs. (12) up to the first order in Γ_0. The agreement is excellent.
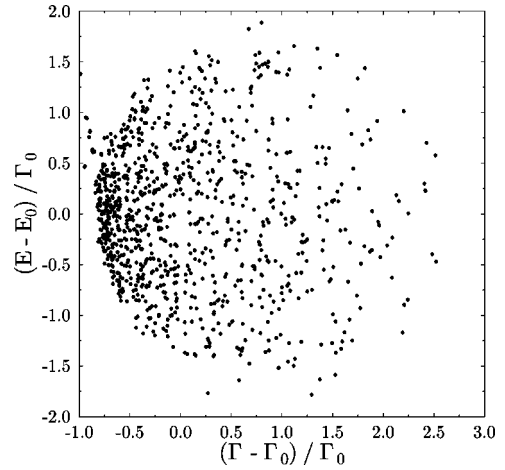

FIG. 2. Resonance poles corresponding to a certain specific configuration of $N=1000$ s-wave scatterers. The tail corresponding to p-type proximity resonances from Fig. 1 still persists. However, for $E\simeq E_0$ quite a lot of resonance poles are located near the $\Gamma=0$ axis.

twice as broad as the resonance of the single scatterer. For $d\rightarrow\infty$ both arms meet in the point $E=E_0$, $\Gamma=\Gamma_0$ reproducing the results of the single scattering. For comparison in the same figure we have the eigenvalues $\lambda(E_0)=\pm e^{ik_0d}/ik_0d$ plotted as a solid line ($k_0=\sqrt{2E_0}$). They can be considered as an approximate solution of Eq. (12) up to the first order in Γ_0. The agreement between the strict and approximate solutions is surprisingly good for $\Gamma_0/E_0=0.01$. It follows from inspection of Fig. 1 that the p-wave proximity resonance is shifted down in energy with respect to the resonance of an individual scatterer, i.e., $E_1<E_0$. For the s-wave resonance the opposite holds, i.e., $E_2>E_0$. It is interesting to note that this behavior is reversed for two-dimensional (2D) proximity resonances. In the latter case the eigenvalues of the G matrix can be expressed by the modified Bessel function of the second kind K_0, i.e., $i\pi\lambda=\pm 2K_0(-ikd)$.

As a second example let us consider a certain specific configuration of $N=1000$ scatterers placed randomly inside a sphere, with the uniform density $n=1$ scatterer per wavelength cubed l_0^3. The wavelength chosen l_0 corresponds to the resonance energy E_0 (i.e., $l_0=2\pi/k_0$ where $k_0=\sqrt{2E_0}$). In Fig. 2 we plot the positions of the resonance poles obtained after numerically iterating Eq. (12) five times. This has been done for each eigenvalue separately and required diagonalizing 4001 complex G matrices of size 1000 $\times$1000. Comparing Fig. 2 with Fig. 1 we see that the tail corresponding to p-type proximity resonances still persists in the case $N=1000$. On the other hand, the second arm of the spiral from Fig. 1 corresponding to the resonance of s-type between pairs of scatterers completely disappeared. It follows also from the inspection of Fig. 2 that new collective effects start to appear. They are visible especially for energies that are close to the resonance energy of a single scatterer, i.e., $E\simeq E_0$. For instance, in this range of energies quite a lot of resonance poles are located near the $\Gamma=0$ axis. They correspond to narrow resonances with width $\Gamma\simeq 0.25\Gamma_0$. As we will show in a moment the width of these resonances Γ decreases with an increasing number of scatterers N (while

keeping the density constant) and in the limit of the infinite medium $N\rightarrow\infty$ they become localized states. It is also seen from Fig. 2 that a few new broad (i.e., $\Gamma\simeq 2.5\Gamma_0$) resonances appeared for $E\simeq E_0$. In addition, in Fig. 3 we have the spectrum of the G matrix corresponding to the same configuration of the scatterers. It has been calculated for $E=E_0$ and may be considered as a first-order approximation to the resonance poles from from Fig. 2. We see that the agreement with the strict solution is not perfect, but nevertheless by using the approximate expressions Eq. (13) it is still possible to gain correct qualitative information about the resonances.

Looking for resonance poles in a complex energy plane turns out to be an enormous numerical problem for a large number of scatterers. Nevertheless, as we have seen, sometimes it is possible to extract some qualitative information
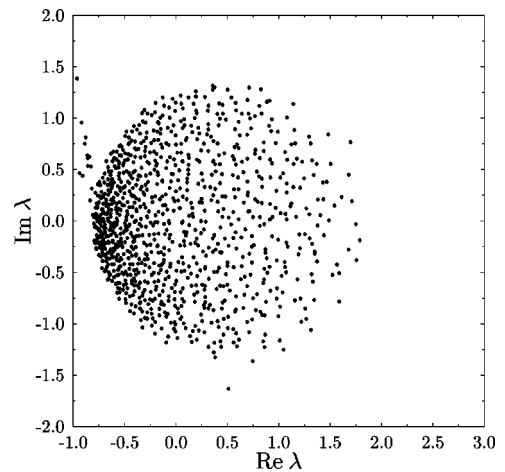

FIG. 3. Spectrum of the G matrix corresponding to the configuration of $N=1000$ s-wave scatterers from Fig. 2. It can be considered as an approximate solution of Eqs. (12) up to the first order in Γ_0. The agreement with Fig. 2 is not perfect but the approximate solution given by Eq. (13) still allows us to gain correct qualitative information about the resonances.
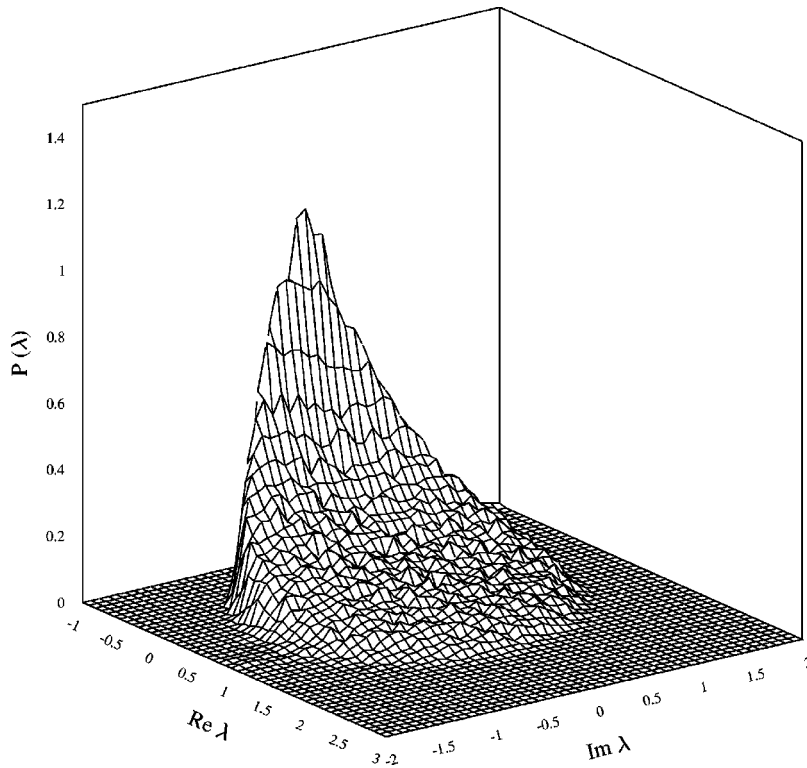
FIG. 4. Surface plot of the density of eigenvalues $P(\lambda)$ calculated for 100 different distributions of $N=1000$ s-wave scatterers. It shows clearly where the most weight of the $P(\lambda)$ distribution is located.

about the resonances just from the spectrum of the G matrix calculated for real values of energy. Moreover, what is even more interesting, a striking phase-transition-like behavior appears in the spectra of such a Green matrices when the number of scatterers increases. This transition may be interpreted as an appearance of the band of localized states emerging in the limit of the infinite medium. It is an interesting analog of the Anderson localization in noncrystalline solids such as amorphous semiconductors or disordered metals. To illustrate the appearance of the band of localized electromagnetic waves, emerging in the limit of infinite system, we have to study the properties of finite systems for increasing number of scatterers (while keeping the density constant).

For each distribution of the scatterers $\vec{r}_a$ placed randomly inside a sphere with the uniform scaled density $n=1$ scatterer per wavelength cubed we have diagonalized numerically the G matrix from Eq. (9) and obtained the complex eigenvalues λ. The resulting probability distribution $P(\lambda)$, calculated from several different distributions of N scatterers is normalized in the standard way $\int d^2\lambda P(\lambda)=1$. Let us now compare the surface plots of $P(\lambda)$ (treated as a function of two variables $\text{Re}\,\lambda$ and $\text{Im}\,\lambda$) calculated for systems consisting of $N=1000$ and 5000 scatterers. They are presented in Figs. 4 and 5, respectively. It is seen from inspection of all these plots that, for increasing size of the system (in our case it increased $\sqrt[3]{5}\simeq1.7$ times), at some $\text{Im}\,\lambda$ the probability distribution $P(\lambda)$ apparently moves towards the $\text{Re}\,\lambda=-1$ axis and simultaneously its variance along the $\text{Im}\lambda=\text{const}$ axes decreases. This tendency is easily seen, e.g., for values of $|\text{Im}\,\lambda|$ that are close to 0. Our numerical investigations indicate, that in the limit of an infinite medium, the probability distribution $P(\lambda)$ tends to the delta function in $\text{Re}\,\lambda$:

$$\lim_{N\to\infty} P(\lambda)=\delta(\text{Re}\,\lambda+1)f(\text{Im}\,\lambda). \qquad (14)$$

We have some numerical evidence that this fact is a general property of G matrices, not restricted to the considered case of one scatterer per wavelength squared $n=1$. Moreover, this mathematical property of random Green matrices seems to be fulfilled also in the 2D free-space case [15] and in the case of a 2D system with nontrivial boundary conditions [16] and thus appears to be truly universal.

Let us now consider an infinite system of identical Breit-Wigner-type s-wave scatterers located randomly with uniform physical density $\rho=k^3n/(2\pi)^3$. It follows from Eq. (14) that for almost any random distribution of the scatterers $\vec{r}_a$ (except maybe for a few special ones with measure zero) infinite number of eigenvalues λ of the G matrix satisfies the condition

$$\text{Re}\,\lambda_j=-1 \qquad (15)$$

(note that we added an index j which labels the localized waves). As pointed out before, this occurs not only for $n=1$ but for a whole range of n and therefore, for fixed physical density ρ, for a range of energies $E=k^2/2$. Therefore at real values of energy E_j determined by the equation

$$\text{Im}\,\lambda_j(E_j)=\frac{E_j-E_0}{\Gamma_0} \qquad (16)$$

these eigenvalues are solutions of Eq. (12) for $\Gamma=0$. Thus the corresponding eigenvectors $\psi'_j(\vec{r}_a)$ of the G matrix describe localized states which exist at *discrete* energies E_j. It seems reasonable to expect that the function f from Eq. (14)
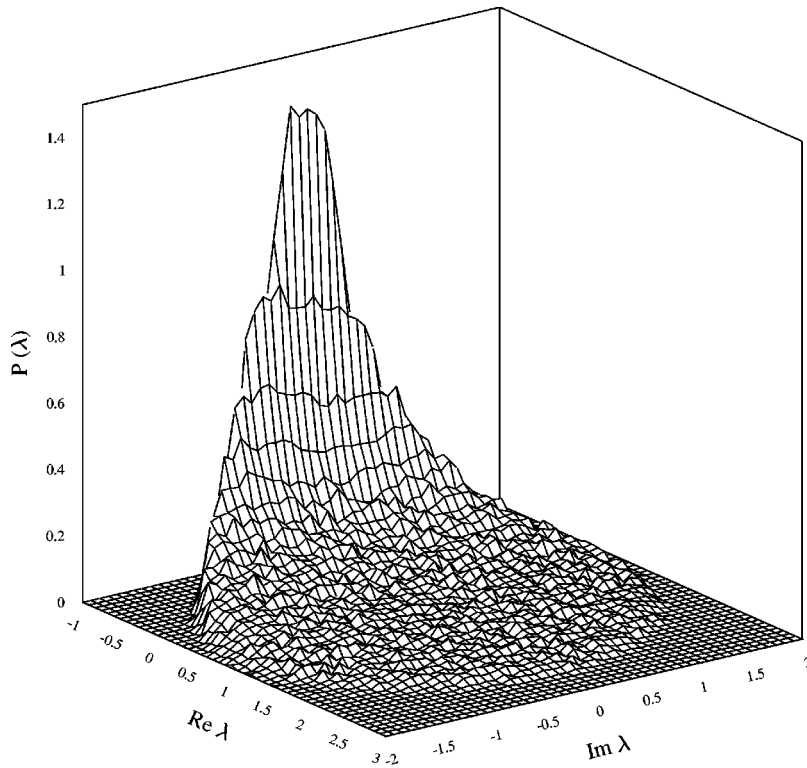
FIG. 5. Surface plot of the density of eigenvalues $P(\lambda)$ calculated for 10 different distributions of $N = 5000$ s-wave scatterers. For increasing values of N, the probability distribution $P(\lambda)$ apparently moves towards the Re $\lambda = -1$ axis and, simultaneously, its variance along the Im λ = const axes decreases.

has compact support, i.e., $f(\text{Im}\,\lambda) = 0$ for $|\text{Im}\,\lambda| > \text{Im}\,\lambda_{\text{cr}}$. This means that in the limit $N \rightarrow \infty$ a countable set of discrete energies E_j corresponding to localized states becomes dense in some finite interval $|E - E_0| < E_{\text{cr}}$. Therefore for random distribution of scatterers the distribution of resonance poles also seems to undergo a phase transition

$$\lim_{N \rightarrow \infty} P(E, \Gamma) = g(E)\delta(\Gamma) \quad \text{for } |E - E_0| < E_{\text{cr}}. \quad (17)$$

Thus an entire continuous *band* of spatially localized states appears in the limit of an infinite medium. Physically speaking this means that different realizations of a sufficiently large disordered system are practically (i.e., by a transmission experiment) indistinguishable from each other. Similarly, as pointed out by Anderson, in a sufficiently disordered solid an entire band of spatially localized electronic states can be formed [9,10].

Last but not least let us observe that the G matrix from Eq. (9) is a *traceless* matrix, i.e., $\Sigma_a \lambda_a = 0$. This means that it is impossible for all eigenvalues to fulfill the localization condition Eq. (15). The inspection of Fig. 2 suggest that these eigenvalues may be first approximations to very broad resonances responsible for enhanced coherent backscattering from a random medium. This so-called weak localization is usually considered as the precursor of strong (Anderson) localization. The property $\Sigma_a \lambda_a = 0$ serves also as a good test for the accuracy of our numerical procedures.

In summary, properties of the spectra of certain matrices describing multiple elastic scattering of scalar waves from a collection of randomly distributed pointlike objects have been discovered. The elements of these matrices are equal to the free-space Green's function calculated for the differences

between positions of any pair of scatterers. Physical interpretation of the obtained results within the Breit-Wigner's model of the single scatterer has been provided. For any distribution of the scatterers the real part of the eigenvalues of the Green matrix seems to be always greater (or equal) than -1. This means that metastable resonance states corresponding to the eigenvectors of the Green matrix decay in time. In the case of two scatterers the real part of one eigenvalue tends to -1 as the distance between the scatterers decreases. This corresponds to the appearance of an extremely narrow p-wave proximity resonance. The remaining eigenvector describes a broad s-wave resonance of the pair. Another property corresponds to the case of scatterers distributed randomly with fixed uniform density. In the limit of the infinite medium almost all eigenvalues condense to a smooth line Re $\lambda = -1$. This transition may be interpreted as an appearance of the band of localized states emerging in the limit of the infinite medium. The relation between the distribution of eigenvalues of an infinite matrix and its elements is mathematically a very complicated problem. It is therefore very surprising that the distribution exhibits such simple regularities which seem to apply under very general conditions. One cannot escape the feeling that there is a very simple basis underlying the properties of the spectra of the random matrices considered, which still has to be discovered.

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