EUROPHYSICS LETTERS 1 July 1991

Europhys. Lett., **15** (5), pp. 535-540 (1991)

Effect of Resonant Scattering on Localization of Waves.

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(received 10 January 1991; accepted in final form 16 April 1991)

PACS. 71.55J – Localization in disordered structures.
PACS. 42.20 – Propagation and transmission in inhomogeneous media.

Abstract. – We present a localization theory for scalar waves in three dimensions that incorporates off-shell contributions and repetitive scattering between the particles. We argue that localization may be difficult to reach for strong individual scattering efficiencies.

The possibility of localizing classical waves has attracted the attention of many experimentalists and theoreticians. Some workers claim to have approached the Anderson transition closely, but the experiments have not been conclusive as yet, although the theories published so far all predict intervals of energies within which localization should be observable [1]. These optimistic predictions are based upon extrapolation of results obtained in the low-disorder limit, and there is considerable suspicion that such extrapolation may not be justified. In fact, the corrections in the self-energy of the amplitude Green's function become as large as the leading term in a low-disorder expansion, when localization sets in.

One (experimental) strategy for achieving localization would be to take the strongest possible individual scatterers, and increase their density until localization occurs. When developing a theory for this limit, two complications immediately show up: i) the scattering particles interact, and cannot be treated as distributed independently and ii) the possibility that a wave visits one particular scatterer more than once, this is what we will call *dependent scattering*, can no longer be ignored. The latter correction has a general tendency to shift localization to higher disorders. This pessimistic expectations have led some authors to suggest alternative pathways for localization [2]. We have recently set up a theoretical framework to describe dependent scattering corrections in the amplitude Green's function [3].

In this paper we will describe the rather dramatic consequences in the weak localization theory, as developed by Vollhardt and Wölfe [4] and Götze [5], when applied to a model of point-scatterers in a scalar wave equation with inclusion of dependent scattering. All previous theories would predict the occurrence of localization for this model, provided the density or the individual scattering efficiency is sufficiently large. It turns out, however, that the resonating properties of the individual scatterers play a major role in the importance of dependent scattering. Intuitively, one might say that because the optical size of a resonating scatterer is larger than its physical size, the overlap of the optical volumes occurs at lower density than the one at which the scatterers start to touch physically. This will have drastic consequences for the *collective* amount of scattering, which determines, after all, the onset of localization.

The theory that we will present includes off-shell contributions. In the presence of disorder the wave will travel a finite distance, roughly equal to the scattering mean free path, before it gets scattered again. Thus, at successive scattering, the wave does not yet satisfy the dispersion relation, and the uncertainty in momentum is inversely proportional to the scattering mean free path. We will show that it is the neglect of this effect that makes it necessary to introduce an (*ad hoc*) momentum cut-off in the weak-localization correction of the diffusion coefficient [6-8]. If we incorporate the finite spectral width into the theory, we find that no cut-off is necessary. If one insists on sticking to such a cut-off, our work shows that it must be inversely proportional to the scattering mean free path. Finally, we use our point-models to obtain a simplified description of the localization of low-energy electrons. We demonstrate that the general belief that localization always sets in for sufficiently low energy is not influenced by dependent scattering.

We turn to the description of multiple scattering of scalar waves in the presence of topological disorder. The averaging over all possible configurations gives rise to the definition of a mass operator Σ [9]. The formal solution of the Dyson equation for the averaged, retarded, amplitude Green's function is, in momentum space,

$$G(E,p) = \frac{1}{(E/c_0)^2 - p^2 - \Sigma(E^+,p)}. \tag{1}$$

Here, c_0 is the speed of light, $E^+ \equiv E + i\varepsilon$. Its poles $p(E)$ in the upper sheet determine, by definition, the renormalized wave vector, and the scattering mean free path, according to $p(E) \equiv k(E) + i/2l_{\mathrm{sc}}(E)$, which can be solved once Σ is known. Localization, however, is associated with the vanishing of the diffusion constant, and thus is a property of the averaged *intensity* Green's function. The latter can be expressed in terms of an irreducible vertex via the Bethe-Salpeter equation [9]. Its application in combination with the Dyson equation yields a generalized Boltzmann equation for $\Phi_p(q,\omega|E)$, which is the averaged intensity Green's function, Laplace-transformed (variable ω) with respect to time and Fourier-transformed (variable $\boldsymbol{q}$) with respect to position. For details we refer to Kirkpatrick [6]. The variables E and $\boldsymbol{p}$ represent internal energy and momentum that may be fixed by initial conditions:

$$[-i\boldsymbol{q}\cdot\boldsymbol{p} + \operatorname{Im}\Sigma(E^+,p)]\,\Phi_p(q|E) = \frac{-c_0}{2E} S(E,p)\left[1 + \sum_{p'} U_{pp'}(E)\,\Phi_{p'}(q|E)\right]. \tag{2}$$

The summation over $\boldsymbol{p}'$ indicates the integral $\int \mathrm{d}^3\boldsymbol{p}'/(2\pi)^3$. We have let $\omega \to 0$ to describe steady-state transport. The spectral function is defined by

$$S(E,p) \equiv \frac{2E}{c_0}\,\frac{-\operatorname{Im}\Sigma(E^+,p)}{|(E/c_0)^2 - p^2 - \Sigma(E^+,p)|^2}, \tag{3}$$

which is positive and normalized to unity [10]. A Ward identity,

$$-\operatorname{Im}\Sigma(E^+,p) = \frac{c_0}{2E}\sum_{p'} S(E,p')\,U_{p'p}(E), \tag{4}$$

relates amplitude and intensity properties and guarantees the existence of an equation of continuity [10]. The density of states per unit volume [11] follows from $2\pi N(E) \equiv \sum_p S(E, p)$. We will expand eq. (2) and retain the lowest angular moments of Φ_p only,

$$\Phi_p(q|E) = \frac{S(E,p)}{2\pi N(E)}\left[P(q|E) + 3\frac{\sum_{p'} S(E,p')}{\sum_{p'} S(E,p')/p'}\,\frac{\hat{\boldsymbol{p}}\cdot \boldsymbol{J}(q|E)}{pv_\mathrm{E}} + \dots\right], \tag{5}$$

where $P \equiv \sum_p \Phi_p$ and $\boldsymbol{J} \equiv v_\mathrm{E} \sum_p \hat{\boldsymbol{p}}\Phi_p$ represent density and streaming. The latter definition differs from its electron analogue [4], because all energy is transported with a yet to be specified speed of light v_E. We multiply eq. (2) with $\hat{\boldsymbol{p}}/p$ and sum over $\boldsymbol{p}$. In the limit $q \to 0$ a constitutive relation between $\boldsymbol{J}$ and P is found. The factor of proportionality is associated with the energy-dependent diffusion coefficient,

$$-i\boldsymbol{q}P(q|E) = D(E)^{-1}\boldsymbol{J}(q|E). \tag{6}$$

If we define the *transport mean free path* according to the relation $D = v_\mathrm{E}\, l_\mathrm{tr}/3$ we find

$$l_\mathrm{tr}(E)^{-1} = \frac{1}{2}\,\frac{\sum_{pp'} S(E,p)\,U_{pp'}(E)\,S(E,p')\left(\dfrac{1}{p^2} - \dfrac{\hat{\boldsymbol{p}}\hat{\boldsymbol{p}}'}{pp'}\right)}{\sum_p S(E,p)\,E/pc_0}. \tag{7}$$

It is this length scale that is important in time-integrated transmission [12] and enhanced-backscattering experiments [13]. In such steady-state situations v_E is of no importance, and will therefore be discussed in a separate paper [14]. We remark here that it is fixed by the demand that P and $\boldsymbol{J}$ satisfy an equation of continuity. The Boltzmann result, $l_\mathrm{tr}^{(\mathrm{B})} = l_\mathrm{sc}/(1 - \langle\cos\theta\rangle)$, is readily obtained if we use «on-shell» contributions in the spectral distribution and approximate Σ and U by their lowest order in density.

In order to evaluate eq. (7) for large disorders we must make some further assumptions concerning the vertex $U_{pp'}(E)$ and the mass operator $\Sigma(E^+, p)$. We will assume from now on that $\Sigma(E^+, p)$ is independent of the momentum p. This was proven [3] to be an accurate result for short-range interactions. From eqs. (1) and (3) it is inferred that the regime $kl_\mathrm{sc} \leq 1/2$ no longer has a well-defined energy shell. In that case the spectral distribution (3) has most of its weight located at $p = 0$.

If we assume that strong localization is attributed to constructive interference of time-reversed waves, we add to the irreducible vertex the summation of the most-crossed diagrams. In the diffusion approximation [13] we adopt, for isotropic scatterers,

$$U_{pp'}^{(\mathrm{m.c.})}(E) = \frac{4\pi}{l_\mathrm{sc}(E)^2}\,\frac{3}{l_\mathrm{tr}^{(\mathrm{B})}(E)(\boldsymbol{p}+\boldsymbol{p}')^2}. \tag{8}$$

Insertion of eq. (8) into eq. (7) gives, after some algebra,

$$l_\mathrm{tr} = \frac{l_\mathrm{sc}}{G(\gamma)}\left[1 - \frac{3}{\gamma^2}F(\gamma)\right], \tag{9}$$

where we have introduced a Ioffe-Regel type parameter $\gamma \equiv kl_\mathrm{sc}$. We replaced the

Boltzmann transport length in eq. (8) by the exact transport (7) in a self-consistent way [4]. The function $F(\gamma)$ is given by

$$\begin{cases} F(\gamma) = H(\gamma) \int\limits_0^\infty \mathrm{d}x \int\limits_0^\infty \mathrm{d}y f_\gamma(x) f_\gamma(y) \left[\dfrac{x^2+y^2}{4xy} \log \left| \dfrac{x+y}{x-y} \right| - \dfrac{1}{2} \right], \\ H(\gamma) \equiv \dfrac{\gamma}{1/2 + \operatorname{arctg}(\gamma - 1/4\gamma)/\pi}, \quad f_\gamma(x) = \dfrac{2}{\pi} \dfrac{1}{[x^2 - \gamma + 1/4\gamma]^2 + 1}, \end{cases} \tag{10}$$

and $G(\gamma) = [1 + 1/4\gamma^2][1/2 + \operatorname{arctg}(\gamma - 1/4\gamma)/\pi]$ is, for $\gamma > 1/2$, a smooth function of order unity. We stress that eq. (9) implicitly uses the most-crossed diagrams as is the only angle-dependent contribution in the vertex. The rest is assumed to be isotropic and absorbed in l_{sc}, using the Ward identity on the isotropic term in eq. (7). The definition of $k(E)$ and $l_{sc}(E)$ is then used to set $\mathrm{Im}\,\Sigma(E^+) = k(E)/l_{sc}(E)$.

For low disorder, eq. (9) has the structure as found by Kaveh [15], Kirkpatrick [6] and others. However, we have not introduced a momentum cut-off q_0 to arrive at this result. If we compare our theory to the cut-off result we identify $F(\gamma)$ as the factor of proportionality between the cut-off and π/l_{sc}. This factor equals, for low disorder, $(\log 2\gamma - 1)/2$. The finite spectral width thus makes the cut-off proportional to π/l_{sc}, an *amplitude* property, rather than $\pi/l_{tr}^{(B)}$, a property of the *intensity* Green's function. This sheds new light on the exact choice of the cut-off, because it proves that no self-consistent renormalization procedure should be applied to this cut-off. Such an approach would naturally result if the cut-off is taken to be proportional to $\pi/l_{tr}^{(B)}$, notwithstanding the fact that $l_{sc} = l_{tr}^{(B)}$ for our isotropic point model.

Equation (9) locates the mobility edge ($l_{tr} = 0$) at $\gamma_c = 0.972$, valid for isotropic scatterers. This is close to the criterium (0.844) found by Zdetsis *et al.* [16] on the basis of the potential well analogy. For anisotropic scattering one should investigate whether a factor $4\pi/(l_{tr}^{(B)})^2$ enters in eq. (8) rather than $4\pi/l_{sc}^2$, leading to $kl_{tr}^{(B)} \sim 1$ near the edge. We suspect that the momentum cut-off must then still be π/l_{sc}.

Equation (9) provides a transport length scale once a solution for the amplitude Green's function is at hand. A diagrammatic calculation of the latter, in which multiple scattering from the same particle is taken into account, was recently presented [3]. We calculated the parameter γ for various individual scattering efficiencies, using an isotropic point-model [17]

$$t(k_0) = -\frac{4\pi}{1/\alpha - ik_0} \tag{11}$$

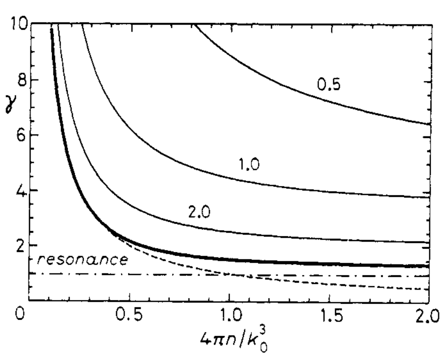

Fig. 1. – The Ioffe-Regel parameter $kl_{sc} \equiv \gamma$ for fixed (individual) scattering efficiency $S \equiv \alpha k_0$ (indicated by the numbers) *vs.* the disorder parameter (scaled density). The dashed line indicates the independent-scattering result for resonating particles. For details see [3].

with $k_0 = E/c_0$, to describe the scattering off one particle. Figure 1 displays the results of our calculations. Striking is the fact that large scattering efficiencies $S \equiv \alpha k_0$ have $\gamma > \gamma_c$ for *any* disorder, and no localization seems possible. This contradicts the intuitive feeling that localization is easiest to reach using strongly scattering particles. In fact what happens is that the optical volumes of the scatterers start to overlap. In that case it can be deduced that the collective cross-section is smaller than the sum of the individual cross-sections. For resonating scatterers the optical radius is roughly equal to the wavelength λ, so that overlapping occurs once $\rho\lambda^3 \sim 1/kl_{sc} > 1$. This proves that in the regime of localization this overlapping must be considerable. Our results disagree with the work of Sornette and Souillard [18], who maximalized the amount of scattering, but did not distinguish between the *individual* and *collective* amount of scattering.

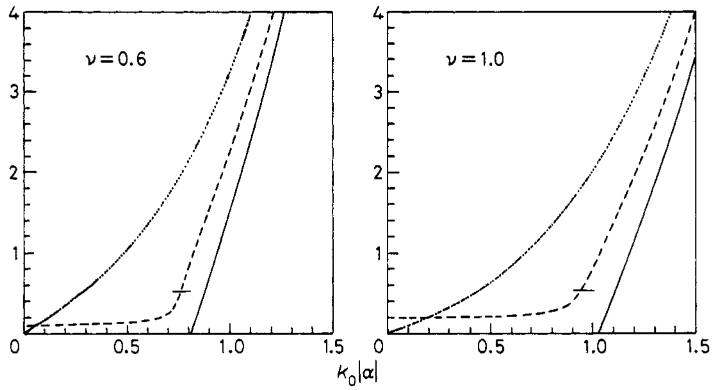

Fig. 2. – The transport mean free path (solid line), the scattering mean free path (dashed line) and the independent-scattering mean free path $l_{sc}^0 = 1/n\sigma$ (dotted line) as a function of energy, for spinless low-energy electrons. The parameter ν is proportional to the density of the scatterers according to $\nu = 4\pi n|\alpha|^3$, $\alpha < 0$ is the scattering length.

The T-matrix equation (11) can be used to model the localization of spinless low-energy electrons with scattering length α. The corresponding interaction is attractive for $\alpha < 0$. Figure 2 plots the Ioffe-Regel parameter as a function of the energy. It is demonstrated that localization sets in for sufficiently low energy [19]. Dependent scattering pushes the mobility edge towards larger energies than expected on the basis of the independent-scattering approximation, which is mainly due to a shift of the energy continuum. Although derived for classical waves, we applied eq. (9) to calculate l_{tr}. The disappearance of the shell at $kl_{sc} = 1/2$ is indicated by a horizontal bar.

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This work is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM) and was made possible by financial support from the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

REFERENCES

[1] CONDAT C. A. and KIRKPATRICK T. R., *Phys. Rev. B*, **36** (1987) 6783.
[2] JOHN S., *Comments Cond. Matter Phys.*, **14** (1988) 193; *Phys. Rev. Lett.*, **58** (1987) 2487.

[3] VAN TIGGELEN B. A., LAGENDIJK A. and TIP A., *J. Phys. C*, 2 (1990) 7653. (One of the internal lines in the diagrams was not renormalized in this reference. This has been corrected in this work.)
[4] VOLLHARDT D. and WÖLFE P., *Phys. Rev. B*, 22 (1980) 4666.
[5] GÖTZE W., *J. Phys. C*, 12 (1979) 1279.
[6] KIRKPATRICK T. R., *Phys. Rev. B*, 31 (1985) 5746.
[7] ECONOMOU E. N., SOUKOULIS C. M. and ZDETSIS A. D., *Phys. Rev. B*, 30 (1984) 1687.
[8] ZHANG Z. Q. and SHENG P., in *Scattering and Localization of Classical Waves in Random Media*, edited by P. SHENG (World Scientific, Singapore) 1990, p. 161.
[9] FRISCH U., in *Probabilistic Methods in Applied Mathematics*, Vol. I, edited by A. T. BARUCHA-REID (Academic Press, New York, N.Y.) 1968.
[10] MAHAN G. D., *Many-Particle Physics* (Plenum Press, New York, N.Y.) 1981.
[11] ECONOMOU E. N., *Green's Functions in Quantum Physics* (Springer-Verlag, New York, N.Y.) 1979.
[12] GENACK A., in *Scattering and Localization of Classical Waves in Random Media*, edited by P. SHENG (World Scientific, Singapore) 1990, p. 207.
[13] VAN DER MARK M. B., VAN ALBADA M. P. and LAGENDIJK A., *Phys. Rev. B*, 37 (1988) 3575.
[14] VAN ALBADA M. P., VAN TIGGELEN B. A., LAGENDIJK A. and TIP A., to be published.
[15] KAVEH M., *Philos. Mag. B*, 56 (1987) 693.
[16] ZDETSIS A. D., SOUKOULIS C. M., ECONOMOU E. N. and GREST G. S., *Phys. Rev. B*, 32 (1985) 7811.
[17] GROSSMANN A. and WU T. T., *J. Math. Phys.*, 25 (1984) 1742.
[18] SORNETTE D. and SOUILLARD B., *Europhys. Lett.*, 7 (1988) 269.
[19] FRÖHLICH J. and SPENCER T., *Commun. Math. Phys.*, 88 (1983) 51.