Random Elastic Scattering: Long-Range Correlation and Localization

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Low density of random elastic scatterers provides a long-range correlation between transmitted and incident wave functions in any dimensionality. Exact formulas prove it. They also demonstrate different localization lengths for different quantities. The experimental implications are strong localization in very pure wires at reasonable temperatures and periodical resonance-type minima and maxima of a residual resistance in a static magnetic field. The results are also true for any (e.g., electromagnetic wave) random scattering.

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The well-known peculiarity of random elastic scattering (RES), which makes it drastically different from inelastic scattering, is localization.[1-4] However, the phase randomization in RES is taken for granted.[4,5] In this paper I prove a strong long-range correlation in any dimensionality for an ensemble average[6] of a RES (when no inelasticity and incident-particle interaction are present): at low RES density, the average scattering matrices are almost diagonal. This reminds one of a one-dimensional (1D) one-channel situation, when a strong localization would be easily observable, and since resistance reduces to scattering characteristics,[4,7-13] it implies a new avenue for the experimental observation of strong localization.

While commonly used very dirty and very thin samples provide only a weak localization, very clean and perfect samples may provide a strong localization with all its unusual qualities: resistance irreproducibility[4-6] and exponential dependence on temperature and conductor length (cf. Refs. 12, 12a, and 13, where, as everywhere else, RES phase randomization was assumed). Consider a cylindrical wire (of an arbitrary length and cross section) with nonoverlapping impurity projections on the wire axis x, i.e., with low enough impurity density n_i: $n_i \ll (d_0 S)^{-1}$. [d_0 is an impurity size along x, and S is the wire cross-section area; the inequality is always true in a "nematic liquid crystal" of disk impurities. The jth impurity potential energy is $U \propto \delta(x - x_j)$, M_e is an incident particle mass, r is a transverse radius vector and δ is a delta function.] Such a wire can be separated into one-impurity-containing sheets, between which the potential energy (inside the wire) is zero, and where wave functions are 1D plain waves with amplitudes modulated in the cross section. This resembles a 1D multichannel situation. The relation between wave-function amplitudes on both sides of an impurity is provided by a "transfer" matrix, which is obviously multiplicative and reduces the total scattering to a single-impurity average (over all possible transverse positions) scattering. The latter, and thus the former, is almost diagonal (with the accuracy s/S, where s is the impurity cross section). This long-range correlation (which is rigorously proven later) implies "on average" the noninterference of different scattering channels and thus a 1D-type resistance (pseudo-1D case, with the localization length L_l of order of an elastic mean free path l) in a reasonable temperature interval, where an inelastic mean free path $l_i > l$.

All of these results are related to $n_i S d_0 \ll 1$ and to the possibility of introducing (in the absence of impurities) a local longitudinal wave vector k_x. They are valid for arbitrary cross section (constant or periodically changing along x; any irregular change in the cross section is an "impurity"), length, and boundary conditions (e.g., specular or transversely periodical ones). They are also valid in a static magnetic field, parallel or perpendicular to x, and applicable to any kind of an elastic scattering (e.g., of electromagnetic waves) in the absence of incident-wave interaction.

The main experimental problem is probably to match $n_i S d_0 \ll 1$ with the specular boundary reflection. In this aspect a large de Broglie wavelength (and therefore, e.g., semimetals Bi, As, Sb) is helpful.

A single-impurity transmission is inversely proportional to the final-state longitudinal wave vector k_x (and thus the major contribution to conductance is provided by $k_x \simeq k_F$, where k_F is the Fermi wave vector), and depends on its

minimal value $\tilde{k}$. The latter, for a given k_F, is determined by the (transverse) quantification. A weak magnetic field H affects the quantification and periodically provides[12,12a] $\tilde{k}=0$ at $eH/c\hbar \sim k_F^{1/2}d^{-3/2}$ (d is the wire thickness). When $\tilde{k}=0$, then the wave with $k_x=0$ is completely reflected, while the reflection, and thus the corresponding localization length, of $k_x \sim k_F$ decreases by a factor of $(k_F d_0)^{-1}$. This implies sharp resonance-type conductance maxima, with a possible change from a strong to a weak localization. The change starts when $\tilde{k}$ is of order of the inter-k_x distance $\hbar/d$, and dominates the reflection when $\tilde{k} \lesssim (Sk_F^{D-2})^{-1}$, D being a dimensionality. Temperature T^* smears k_F by $k_F(K_B T^*/\epsilon_F)$ and $k_x \equiv (k_F^2-\kappa^2)^{1/2}$ (in the vicinity of $k_x=0$) by $k_F(K_B T^*/\epsilon_F)^{1/2}$ (K_B is the Boltzmann constant, ϵ_F is the Fermi energy, and κ is the transverse wave vector). Thus, the localization length starts decreasing with H when $T^* < \epsilon_d \sim \hbar^2/2M_e d^2$, the relative decrease being $(K_B T^*/\epsilon_F)^{1/2}(Sk_F^2)^{-1}$, and is maximal when $T^* < \epsilon_d (dk_F)^{-2} \sim \epsilon_d^2/\epsilon_F$.

A strong strictly longitudinal ($\vec{H} \| \hat{x}$) magnetic field (with cyclotron radius $r_c \ll d$) simplifies experimental requirements (anisotropy may also be helpful): (i) Except for boundary effects in the vicinity r_c of wire surfaces, surface reflection becomes almost unimportant. (ii) In the transverse plane an electron remains within the area πr_c^2, so, if $n_i S d_0 \gg 1$, a large magnetic field may provide a transition to a strong localization. (iii) A magnetic field quantization replaces ϵ_d in the above inequalities by $\hbar\Omega_c$ (Ω_c is a cyclotron frequency; boundary effects are again neglected). In semimetals this may allow for the resonance ($\tilde{k}=0$) observation. (iv) The values of "quantum" magnetic field ($\hbar\Omega_c > \epsilon_F$), which leave only $k_x \simeq 0$, provide a resonance-type decrease in the localization length, and increase in the resistance, and thus may imply a transition to the localization. But note that boundary effects may become the major ones.

Now I derive analytical formulas for multiparticle scattering. According to Landauer,[7] a 1D conductance $G=(e^2/\pi\hbar)|T|^2/(1-|T|^2)$, with T being a conductance transmission matrix. The Landauer formula is applicable to current-carrying 1D one-channel wires (with insulated surfaces), imbedded in a cylindrical wire with a given arbitrary dimensionality resistance inside (far enough from 1D junctions). In this case, by Ref. 12, the total (1D) transmission matrix $T_t \simeq \tau_L T \tau_R$; τ_L, T, and τ_R are, correspondingly, the transmission matrices of the left junction, the given resistance, and the right junction. The calculation of τ_L and τ_R is simple and straightforward; the task is to evaluate T.

Suppose a wave function to the left and to the right of an arbitrary scatterer equals, correspondingly, $\alpha_+\psi_+ - \alpha_-\psi_-$ and $\alpha_+'\psi_+' - \alpha_-'\psi_-'$ (subscripts denote the direction of the wave: $+$ for a wave moving to the right, $-$ to the left; the ψ's form a complete set and, as well as α's, are the vectors in the space of quantum numbers). Then $\alpha_+' = \alpha_+\tau_+ - \alpha_-'\rho_-$ and $\alpha_-' = \alpha_+\rho_+ - \alpha_-'\tau_-$, ($\tau$ and ρ are transmission and reflection matrices), and (cf. Ref. 14) thus[15]

$$(\alpha_+, \alpha_-) = (\alpha_+', \alpha_-')\theta;$$
$$\theta = \begin{pmatrix} \tau_+^{-1} & -\tau_+^{-1}\rho_+ \\ \rho_-\tau_+^{-1} & \tau_- - \rho_-\tau_+^{-1}\rho_+ \end{pmatrix}. \quad (1)$$

Applying Eq. (1) to N consequent scatterers and to their total scattering (with reflection and transmission matrices R and T and $\alpha_-'=0$ for the transmitted wave), one obtains

$$(T^{-1}, -T^{-1}R) = (\hat{I}, \hat{0})\theta^{(N)};$$
$$\theta^{(N)} = \theta_N \theta_{N-1} \cdots \theta_1. \quad (2)$$

Here $\hat{I}$ and $\hat{0}$ are unity and zero matrices; $x_{j+1} > x_j$. If the jth impurity is situated at (x_j, r_j), then an obvious wave-function transformation reduces $\theta_j \equiv \theta(x_j, r_j)$ to $\theta_j^0 \equiv \theta(0, r_j)$:

$$\theta_j = \omega_j \theta_j^0 \omega_j^{-1}, \quad (\omega_j)_{\sigma s} = \sigma\delta_{\sigma s}\Omega_j^{\sigma},$$
$$\sigma, s = \pm 1, \quad \Omega_j = \exp(i\hat{k}x_j), \quad (3)$$

where $\hat{k}_{\nu\mu} = \delta_{\nu\mu}k_\nu$, $k_\nu = (k^2 - \kappa_\nu^2)^{1/2}$ is a longitudinal wave vector k_x for a given set of transverse quantum numbers ν ($\mathrm{Re}k_\nu, \mathrm{Im}k_\nu \geq 0$), and κ_ν is a transverse wave vector. Equations (2) and (3) reduce $\theta^{(N)}$ to an individual scattering.[15a]

Consider, for simplicity, an individual disk scattering, described by the Schroedinger equation $\Delta\psi + k^2\psi = \delta(x)V(r)\psi$. An incident wave $\psi_{s\nu} = \exp(isk_\nu x)\varphi_\nu$ {$s=\pm 1$; φ_ν's form a complete set of orthonormal transverse wave functions; $[A] \equiv \int A\, dr$; $\sigma, s = \pm 1$; a bar denotes a complex conjugation; $V(r) = V^0(r - r_j)$} provides

$$\theta_j = 1 + \theta_j', \quad (\theta_j')_{\sigma s} = \sigma\tilde{\Omega}_{\sigma j}\Gamma\tilde{\Omega}_{sj}^{-1}; \quad (4)$$

$$\tilde{\Omega}_{js} = \exp(is\hat{k}x_j + i\hat{\kappa}r_j),$$

$$\Gamma_{\nu\mu} = i(2k_\mu)^{-1}[\varphi_\nu\bar{\varphi}_\mu V^0], \quad (5)$$

where $\hat{\kappa}_{\nu\mu} = \delta_{\nu\mu}\kappa_\nu$.

By Eqs. (2) and (4), $\theta^{(N)} - 1 = \sum_j \theta_j' + \cdots$. In, e.g., $(\sum_j \theta_{j\sigma s}')_{\nu\mu}$, each term, by Eq. (5), is periodic with respect to x_j and r_j. Reducing all N scatterer positions to these periods and intro-

ducing the corresponding probability density, one obtains $\sum_j \theta_{j\sigma s'} \approx \langle \sum_j \theta_{j\sigma s'} \rangle$, where angular brackets denote an ensemble average. Similarly, $\theta^{(N)} \simeq \langle \theta^{(N)} \rangle$ (but cf. Ref. 6).

Still, the knowledge of an ensemble average for all impurity densities may allow one[12] to determine a typical value. First evaluate $\langle \theta^{(N)} \rangle$. According to Eq. (2), $x_{j+1} > x_j$; suppose $0 \leq x_j \leq L$. The corresponding probability density P (of any of N RES being at x_1; of any of the remaining $N-1$ being at $x_2 > x_1$, etc.) is[16]

$$P = (N/L)\{[(N-1)/L]\, t(x_2 - x_1)\} \cdots = N! L^{-N} \prod_{j=1}^{N-1} t(x_{j+1} - x_j), \quad (6)$$

with $t(x) = 1$ for $x > 0$ and $t(x) = 0$ for $x \leq 0$. (Thus, Abrahams-Stephen averaging[5] with $P = L^{-N}$ is approximately valid only for large interimpurity distances.) Equation (6) enables one to evaluate, e.g., the ensemble averages $\langle \theta^{(N)} \rangle$ and $\langle T^{-1} \rangle$.

According to Eqs. (2) and (6),

$$\langle \theta^{(N)} \rangle = N! L^{-N} a_N(L); \quad a_N(L) = S^{-1} \int_0^L [\theta(x)]\, a_{N-1}(x)\, dx, \quad a_0(x) = 1. \quad (7)$$

By Eq. (7), $A(\zeta; L) = \sum \zeta^N a_N(L)$ (sum from $N = 0$ to ∞) yields the equation $\partial A/\partial L = \zeta \bar{\theta}(L) A$, $A(\zeta; 0) = 1$. Thus, accounting for Eq. (3), $A(\zeta/L; L)$ equals

$$\sum_{N=0}^{\infty} (\zeta^N/N!) \langle \theta^{(N)} \rangle = \exp(iEL) \exp(-iEL + \zeta S^{-1}[\theta^0]), \quad (8)$$

where $E_{\sigma s} = \sigma \delta_{\sigma s} \hat{k}$; while Eq. (4) provides

$$[\theta^0]_{\nu\mu} = \delta_{\nu\mu} \{1 + i(2k_\nu)^{-1} [|\varphi_\nu|^2 V^0]\}. \quad (9)$$

Equations (8) and (9) complete the calculation of the average-generating S matrix of the scattering matrix θ for an *arbitrary* $V(r)$ and prove its diagonality (with respect to quantum numbers), i.e., the long-range correlation. The calculation of diagonal terms reduces to a 2×2 matrix and provides, e.g., the following $\langle T^{-1} \rangle_{mm}$ localization lengths:

$$\operatorname{Re} \ln \langle T^{-1} \rangle_{mm} \sim \begin{cases} [V^0] n_i k_m^{-2}, & \text{if } ak_m \gg c_i^{1/2}, \quad La^{D-2} \lesssim S, \quad (10) \\ n_i L [V^0]^2 / (S k_m^2)', & \text{if } ak_m \gg c_i^{1/2}, \quad La^{D-2} \gtrsim S, \quad (11) \\ La[V^0](n_i a^{-D})^{1/2}, & \text{if } ak_m \ll c_i^{1/2}, \quad L \gg a c_i^{-1/2}, \quad (12) \end{cases}$$

where D is a dimensionality, $a = \pi/k_F$, $c_i = a^D n_i$, and k_m is real. Thus, the $\langle T^{-1} \rangle$ localization length has a resonance dependence on the incident (real) k_m and rapidly changes in the region $ak_m \sim c_i^{1/2}$. A typical $k_m \sim k_F$ implies, when $D \geq 2$, no localization and no mobility edge in $\langle T^{-1} \rangle$. Small $k_m \ll a^{-1} c_i^{1/2}$ provide the $\langle T^{-1} \rangle$ localization in any dimensionality. All results are valid also for mirror wire boundaries, when $s \ll (S/Ln_i)^{1/2}$, s being an impurity cross-section area. A static magnetic field $\vec{H} \parallel \hat{x}$ and $\vec{H} \perp \hat{x}$ here and on changes only the quantization (i.e., ν, φ_ν).

To evaluate nonaveraged quantities, assume a transverse impurity size $d_t \ll a$. Since only ν and/or $\mu < d/d_t$ are of importance (when $\nu \sim d/d_t$, then $\kappa_\nu \sim \pi/d_t \gg k_F$; note that at the resonance only $\kappa_\nu = k_F$ matters), $[\varphi_\nu \bar{\varphi}_\mu V^0] \sim [\varphi_\nu V^0][\bar{\varphi}_\mu V^0]/[V^0] \equiv V_\nu \bar{V}_\mu / [V^0]$. The corresponding scattering is described by Eq. (5) with Γ replaced by Γ^*:

$$\Gamma_{\nu\mu}^* = i(2[V^0] k_\mu)^{-1} V_\nu \bar{V}_\mu. \quad (13)$$

The individual-scattering model (13) yields the unitary relation (i.e., current conservation) and allows one to evaluate any (nonaveraged) scattering quantity by virtue of the simplicity of the calculations with Γ^* (since, e.g., $\Gamma^{*2} = \Gamma^* \operatorname{Tr} \Gamma^*$, etc.; the details of these rather boring calculations will be presented elsewhere[17]). For instance,

$$T = 1 - \sum_{j,j'} \tilde{\Omega}_{j+} (1 + \operatorname{Tr} \hat{D})_{jj'}^{-1} \Gamma^* \tilde{\Omega}_{j'+}^{-1}; \quad D_{jj'} = \exp[i\hat{k} |x_j - x_{j'}| + i \hat{\kappa} (r_{j'} - r_j)] \Gamma^*. \quad (14)$$

Tr denotes the trace with respect to matrix indices ν and μ. Now one can also evaluate any averaged quantity. For instance, when the interimpurity distance is large enough, one can use Abrahams-Stephen averaging[5] with $P = L^{-N}$ and, similar to Refs. 12 and 17, obtain for a multichannel 1D wire $\langle T \rangle \sim [\tau^0]^N$, $\langle (T^+ T)^{-1} \rangle \sim [(\tau^{0+} \tau^0)^{-1}]^N$, and

$$-\operatorname{Re} \ln \langle T \rangle_{mm} \sim L k_m^{-1} n_i [V^0] t/(1 + t^2), \quad t = \sum_\mu |V_\mu|^2/(2k_\mu [V^0]) \propto [V^0]; \quad (15)$$

$$\operatorname{Re} \ln \langle (T^+ T)^{-1} \rangle \sim L [V^0]^2 n_i a^{3-D} K^*, \quad K^* = (a^{D-1}/S) \sum_m (ak_m)^{-2}. \quad (16)$$

Equations (15) and (16) provide the $\langle T \rangle$ and $\langle (T^+ T)^{-1} \rangle$ "resonance" at $\min k_\mu \equiv \tilde{k} = 0$, indicated

earlier—cf. also Refs. 12 and 12a. (The accurate calculation at $\tilde{k} \to 0$ accounts for a small difference between Γ^* and Γ.) In Eq. (15), $t \sim 1$ for $D=1$, $t \sim |V^0| \ln(a/d_0)$ for $D=2$, and $t \sim |V^0| d_t^{2-D}$ for $D \geq 3$. By Eqs. (10)–(12), (15), and (16), the localization lengths are very different for $\langle T \rangle$, $\langle T^{-1} \rangle$, $\langle (TT^+)^{-1} \rangle$, and resistance.[2,4]

If the impurity size is $d_0 \neq 0$ in all directions, then, to allow for the nonoverlapping impurity x projections, d_0 must be less than the average interimpurity distance $\tilde{d}_0 \sim 1/n_i S$. Until $\tilde{d}_0 > a$, i.e., until $n_i S a < 1$, the finite value of d_0 should not be important. But when $n_i S$ is large enough, $n_i S a \gg 1$, then the "allowed" impurity size $d_0 < (n_i S)^{-1}$ provides a single-impurity attenuation, which tends to zero when $d_0 \to 0$ (and $D \geq 2$). This may signal the crucial role for $D \geq 2$ of the assumed nonoverlapping of impurity projections. Another very important problem is how much the results of this section depend on the scattering model (13). The presented approach is straight-forwardly generalized to any (e.g., electromagnetic wave) scattering.

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[15]Matrices θ account for the states both with real and with imaginary wave vectors (the latter exponentially decay in the vicinity of the impurity).

[15a]In a periodic (along x) lattice, a band is determined by the eigenvalues $\exp(-i\tilde{k}a)$ of $\omega_j \omega_{j+1}^{-1} \theta^0$; $\tilde{k}$ is a quasi wave vector, and a is a period.

[16]Equation (6) is valid for $U \propto \delta(x)$. If the impurity size is d_0, then L in Eq. (6) should be replaced by $L - Nd_0$ and $x_{j+1} - x_j$ by $x_{j+1} - x_j - d_0$.

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Optical Structure near 20 meV in Valence-Fluctuation Compounds

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The first measurement is reported of low-energy (20 meV) structure in the low-temperature dielectric function of two valence-fluctuation materials: $CePd_3$ and $YbCu_2Si_2$. The structure is consistent with energy-dependent scattering of electrons off a resonant level whose width and position (relative to the Fermi level) are roughly comparable. No such structure is observed in the integral-valent materials YPd_3, $DyPd_3$, and $LuCu_2Si_2$. The valence-fluctuation compounds $CeCu_2Si_2$ and $CeAl_3$ do not show a resonance above 4 meV.

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In this Letter we report far-infrared optical-absorption measurements at photon energies between 4 and 40 meV in the valence-fluctuation compounds $CePd_3$ and $YbCu_2Si_2$. Both compounds show a broad absorption feature at low temperature, which we attribute to electron scattering

