Wave Functions for Open Quantum Systems and Stochastic Schrödinger Equations

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It is shown that evolution of an open quantum system can be exactly described in terms of wave function which obeys Schrödinger equation with randomly varying parameters whose statistics is universally determined by separate dynamics of the system’s environment. Corresponding stochastic evolution of the wave function is unitary on average, and this property implies optical theorem for inelastic scattering as demonstrated by the example of one-dimensional conducting channel with thermally fluctuating potential perturbation.

I. Generally, even simple quantum systems have no definite wave function and require the density matrix language instead [1]. But if the density matrix, \( \rho(t) \), evolves under von Neumann equation, still one can write

\[ R(t) = \sum_{\alpha} \Psi_{\alpha}(t) P_{\alpha} \Psi_{\alpha}^*(t) , \]  

with \( \Psi_{\alpha}(t) \) obeying the Schrödinger equation, and say that the system has random wave function whose randomness is determined by initial conditions only. This is not the case as soon as the system becomes open, i.e. constantly interacts with the rest of the nature, and therefore is governed by some kinetic equation. However, in the framework of the “stochastic representation” of quantum interactions [2, 3], or deterministic interactions at all [2, 4], we can again rehabilitate wave function if say that it is stochastic one being governed by a well-defined stochastic Schrödinger equation. Let us consider this potential convenience more attentively.

II. Suppose that (i) a composite quantum system “D+B”, with “D” being a dynamic subsystem under direct interest and “B” its environment (“thermal bath” or “all the Universe” or some other), has the bilinear Hamiltonian

\[ H(t) = H_d(t) + H_b + B_j D_j \]  

(repeated indices imply summation over them), where operators \( H_d, D_j \) relate to “D” while \( H_b, B_j \) to “B”; (ii) common density matrix of “D+B”, \( \rho(t) \), obeys the von Neumann equation, \( d\rho(t)/dt = i[H(t), \rho(t)]/\hbar \), and (iii) in the old days “D” was statistically independent of “B”, \( \rho(t_0) = \rho_D(t_0) \times \rho_B(t_0) \) (where e.g. \( t_0 \to -\infty \)).

Then marginal density matrix of the subsystem “D”, \( \rho_D(t) \equiv \text{Tr}_B \rho(t) \), can be represented [2, 3] as statistical average,

\[ \rho_D(t) = \langle R(t) \rangle , \]  

of a random density matrix, \( R(t) \), which satisfies the stochastic von Neumann equation

\[ \frac{dR}{dt} = \frac{i}{\hbar} \{ [R, H_d(t)] + \xi_j(t) RD_j - \xi_j(t) D_j R \} , \]  

where \( \xi_j(t) \) are complex random processes which commute one with another and with any other objects, the superscript * means complex conjugation and \( \langle \ldots \rangle \) statistical average with respect to \( \xi_j(t) \). Sometimes it is convenient to write

\[ \xi(t) = x(t) + i y(t)/2 , \] \[ \xi^*(t) = x(t) - i y(t)/2 , \]

with \( x_j(t) \) and \( y_j(t) \) treated as real-valued random processes. Statistics of \( \xi(t) \)’s is completely determined by separate dynamics of the subsystem “B”:

\[ \langle \exp\{ \int [a_j^*(t) \xi_j(t) + a_j(t) \xi_j^*(t)] dt \} \rangle = \langle e^{\int [a_j^*(t) B_j(t) + a_j(t) B_j^*(t)] dt} \rangle \rho_{00} , \]

with \( B_j(t) \equiv \text{exp}[i H_b t/\hbar] B_j \text{exp}[-i H_b t/\hbar] \), left and right arrow denoting chronological and anti-chronological time ordering, respectively, \( a_j(t) \) and \( a_j^*(t) \) being arbitrary test functions, or probe functions (which are not necessarily mutually conjugate), and \( \rho_{00} \equiv \text{exp}[i H_{t_0} t_0/\hbar] \rho_B(t_0) \text{exp}[-i H_{t_0} t_0/\hbar] \).

Clearly, any solution to Eq.(4) can be represented in the form [4], where wave functions (quantum states) \( \Psi_{\alpha}(t) \) satisfy the stochastic Schrödinger equation

\[ \frac{d}{dt} \Psi(t) = -\frac{i}{\hbar} \{ H_d(t) + \xi_j(t) D_j + \epsilon(t) \} \Psi(t) \]

with initial condition \( \Psi_{\alpha}(t_0) P_{\alpha} \Psi_{\alpha}^*(t_0) = \rho_D(t_0) \), and \( \epsilon(t) \) is a suitable (real-valued) gauge function. At that, formula [4] supplies exhaustive statistical information about the noises \( \xi_j(t) \). To avoid a need for \( \epsilon(t) \), of course, it is reasonable to assume

\[ \text{Tr}_D D_j = 0 , \] \[ \text{Tr}_B B_j = 0 , \]
thus excluding from 2 trivial contributions without factual interaction.

III. Because of the complexity of $\xi_j(t)$, the stochastic evolution under Eq.8 is not unitary:

$$\frac{d}{dt} \langle \Psi_\alpha(t) | \Psi_\beta(t) \rangle = y_j(t) \langle \Psi_\alpha(t) | D_j | \Psi_\beta(t) \rangle \neq 0$$ (8)

But this evolution is unitary on average:

$$\frac{d}{dt} \langle \langle \Psi_\alpha(t) | \Psi_\beta(t) \rangle \rangle = \langle y_j(t) \langle \Psi_\alpha(t) | D_j | \Psi_\beta(t) \rangle \rangle = 0 ,$$ (9)

$$\langle \langle \Psi_\alpha(t) | \Psi_\beta(t) \rangle \rangle = \langle \Psi_\alpha(t_0) | \Psi_\beta(t_0) \rangle \propto \delta_{\alpha \beta}$$ (10)

The statement 10 follows from 9 and $\Psi_\alpha(t_0)$'s definition, while the statement 9 follows from remarkably singular statistical properties of $y_j(t)$.

To see the $y_j(t)$'s singularity, it is sufficient to assign in 3 $a(t) = iu(t)/\hbar$ and $a^*(t) = -iu(t)/\hbar$ when $t > \theta$, with real test functions $u(t)$ and $\theta > t_0$. Then

$$\exp \left[ \int a(t) B(t) dt \right] = U \exp \left[ \int a^*(t) B(t) dt \right]$$

and

$$\exp \left[ \int a(t) B(t) dt \right] = \exp \left[ \int a^*(t) B(t) dt \right] U^\dagger ,$$

where

$$U = \exp \left[ -i \int_0^t u(t) B(t) dt / \hbar \right] .$$

Since $U$ is unitary, $UU^\dagger = 1$, in fact it disappears from r.h.s. of 10:

$$\langle \langle \exp \left[ \int_0^t u(t) y(t) (t) \right] \exp \left[ \int a^*(t) \xi(t) + a(t) \xi^*(t) \right] dt \rangle \rangle = \text{Tr}_B \exp \left[ \int a(t) B(t) dt \right] \exp \left[ \int a^*(t) B(t) dt \right] \rho_{00}$$

Here from it follows that any statistical correlation between $y(t)$ and any earlier variables is zero. In particular, the equality 9 is valid because $\Psi(t)$'s undergo the causality principle and depend on earlier $\xi(t)$'s only. The Eq.10 implies also $\langle y(t_1) y(t_2) \rangle = 0 \ , \langle y(t_1) y(t_2) \rangle = 0 , \langle y(t_1) x(t_2) \rangle = 0 , \text{etc.}$

At the same time, generally $\langle x(t) y(t') \rangle \neq 0$ and other $y(t)$'s correlations with later variables also are nonzero.

Let the noise be stationary, that is $[H_0, \rho_{00}] = 0$, and besides has zero mean value, $\langle \xi(t) \rangle = 0$. The latter is ensured by the natural condition $\text{Tr}_B B_j \rho_{00} = 0$. Then 2, according to Eq.3

$$\langle \xi^*_j(\tau) \xi_m(0) \rangle = K_{jm}(\tau) ,

K_{jm}(\tau) \equiv \text{Tr}_B B_j B_m(0) \rho_{00} = K_{mj}^*(\tau) ,

\langle \xi_j(0) \xi_m(0) \rangle = \langle \xi^*_j(0) \xi_m(0) \rangle = K_{jm}(\tau) \theta(\tau) + K_{jm}^*(\tau) \theta(-\tau) ,$$ (12)

where $\theta(\tau)$ is Heaviside step function. Consequently,

$$K_{jm}^{xx}(\tau) \equiv \langle x_j(t) x_m(0) \rangle = \text{Re} K_{jm}(\tau) ,

K_{jm}^{xy}(\tau) \equiv \langle x_j(t) y_m(0) \rangle = (2/\hbar) \theta(\tau) \text{Im} K_{jm}(\tau) \ 	ext{(13)}$$

If $\rho_{00}$ is canonical distribution, $\rho_{00} \propto \exp(-H_0/T)$, then the identity $\rho_{00} B(t) \rho_{00} = 0$ takes place and produces additional symmetry relation

$$K_{jm}(\tau - i\hbar/2T) = K_{mj}(-\tau - i\hbar/2T)$$ (14)

The latter if combined with 12 results in the “fluctuation-dissipation relations” between spectral components of correlators $K_{jm}^{xx}(\tau)$ and $K_{jm}^{xy}(\tau)$ as expressed by their Fourier expansions:

$$K_{jm}^{xx}(\tau) = \int_0^\infty \cos(\omega \tau) \sigma_{jm}(\omega) d\omega ,$$ (15)

$$K_{jm}^{xy}(\tau) = -\frac{2\theta(\tau)}{\hbar} \int_0^\infty \sin(\omega \tau) \tan \left( \frac{\hbar \omega}{2T} \right) \sigma_{jm}(\omega) d\omega ,$$ (16)

with $\sigma_{jm}(\omega)$ being some non-negatively defined spectrum matrix. Unfortunately, in 2 formula 10 was written with wrong plus sign on its r.h.s., and then this mistake migrated to 3 and 4. But, fortunately, it could not influence results of applications of 16 since all that were even functions of $K_{jm}^{xy}(\tau)$. The term “fluctuation-dissipation” reflects that $K_{jm}^{xy}(\tau)$ and other cross correlations between $x(t)$’s and $y(t)$’s describe also response of “B” to its perturbation by “D” and thus possible energy outflow from “D” into “B”. For details and extensions of the stochastic representation 11, see 2 and 3.

IV. For illustration, let “D” be one-dimensional conduction channel with finite energy band, that is formed by discrete sites $s = \ldots -1, 0, 1, \ldots$, and its perturbation by “B” acts as randomly varying potential localized at the only site $s = 0$. Thus $\xi_j(t) D_j \equiv \xi_j(t) D$ where $D_{ss'} = 1$ if $s = s'$ and $D_{ss'} = 0$ otherwise. Definition of the own Hamiltonian of “D” is convenient in the momentum space: $\{H_d(t)\}_{k,k'} = \delta(k - k') E(k), \text{where } -\pi < k < \pi$ and, for instance, $E(k) = \Delta E (1 - \cos k)/2$ with $\Delta E$ being channel’s bandwidth.

In this example, it is natural to treat $\Psi(t)$ in the coordinate space, choose $\epsilon(t) = 0$, and transform Eq.8 into integral equation:

$$\Psi(t, s) = \Psi_0(t, s) + \Psi^S(t, s) ,

\Psi^S(t, s) = -\frac{1}{\hbar} \int_0^t G(t' - t, s) \xi(t') \Psi(t', 0) dt'$$ (17)

where $\Psi_0(t, s)$ and $\Psi^S(t, s)$ are free and scattered parts of the wave function, respectively, and

$$G(\tau, s) = \int_{-\pi}^{\pi} \exp[i ks - i E(k) \tau/\hbar] \frac{dk}{2\pi}$$ (18)

is free Green function.

Consider stochastic scattering of a single particle. Let initially, at time $t_0 = -\tau_0 < 0$, it had wave number $k_0 > 0$ and velocity $v_0 = dE(k_0)/dk_0$, and its wave packet took place $-\Lambda < s < 0$ with $\Lambda \approx v_0 \tau_0 >> 2\pi/k_0$. Then we observe the particle at time $t > 0$. At that, we are interested in the case when duration of the scattering process, $\tau_c$, of the scatterer fluctuations $\xi(t)$. This is possible if $\Lambda$ is sufficiently large while $v_0$ sufficiently small, at least if $L > L_c = \sqrt{\pi \Delta E \tau_c / \hbar}$ (for example, if $\Delta E = 1 \text{ eV}$ and each site occupies $3 \cdot 10^{-8} \text{ cm}$ then $L_c \approx \sqrt{\tau_c}$ where $\tau_c$ is expressed in seconds and $L_c$ in centimeters).

Obviously, now the equality 10 can be written as

$$\langle \sum \langle \Psi(t, s) \rangle^2 \rangle = \sum \langle \Psi(t_0, s) \rangle^2 = \sum \langle \Psi^0(t_0, s) \rangle^2 = \sum \langle \Psi^S(t_0, s) \rangle^2 \ 	ext{(19)}$$
Combining this with the first of Eqs. (17) one easy obtains
\[ \sum \left[ \Psi^0\langle \Psi^S \rangle + \Psi^0\langle \Psi^S \rangle \right] + \langle \sum |\Psi^S|^2 \rangle = 0 \, , \tag{20} \]
where all functions are related to the observation time \( t \).

This formula is nothing but “the averaged optical theorem for inelastic scattering” (clearly, fluctuations \( \xi(t) \) in the course of scattering can make it inelastic).

As it was agreed, at time \( t > 0 \) the scattering event finishes, therefore, we can express final quantum probabilities of the particle’s reflection, \( \mathcal{R} \), and transmission, \( \mathcal{T} \), simply as
\[ \mathcal{R} = \sum_{s<0} |\Psi|^2 = \sum_{s<0} |\Psi|^2 = \frac{1}{2} \sum |\Psi|^2 \, , \tag{21} \]

We took into account also mirror symmetry of the scattering; the Green function \( G(t, s) \) and thus \( \Psi^S(t, s) \) are even functions of \( s \) (at least when \( E(k) \) is an even function). Now, taking average of (21) and applying (10) and (20), we obtain
\[ \langle \mathcal{R} \rangle = -\text{Re} \sum \Psi^0*\langle \Psi^S(t, s) \rangle = 1 - \langle \mathcal{T} \rangle \, . \tag{22} \]

Hence, the optical theorem helps to find the mean reflection probability \( \langle \mathcal{R} \rangle \) directly from mean value of \( \Psi(t, s) \), without knowing its second-order statistics.

Another useful expression for \( \langle \mathcal{R} \rangle \) arises if combine (22) with (17) and then apply the group property \( \sum G(\tau_1, s-s')G(\tau_2, s') = G(\tau_1 + \tau_2, s) \). This yields
\[ \langle \mathcal{R} \rangle = \text{Re} \int_{t_0}^{\infty} \Psi^0*\langle \Psi^S(t', s) \rangle \psi(t') dt' \, , \tag{23} \]

where \( \psi(t) \equiv \Psi(t, 0) \) satisfies closed integral equation
\[ \psi(t) = \Psi^0(0, t) - \frac{i}{\hbar} \int_{t_0}^{t} G_0(t-t')\xi(t')\psi(t') dt' \, \tag{24} \]

with \( G_0(\tau) \equiv G(\tau, 0) \).

Alternatively, at \( t > 0 \) we can consider amplitudes of outgoing waves,
\[ A_k = A_k^0 + A_k^S \, , \quad A_k^0 = \delta(k-k_0) \, , \quad A_k^S = -\frac{i}{\hbar v_L} \int_{t_0}^{t} \exp(iE(k)(t'-t_0)/\hbar) \xi(t')\psi(t') dt' \, \tag{25} \]

In terms of \( A_k^S \), the optical theorem reads
\[ \text{Re} \langle A_{k_0}^S \rangle = \text{Re} \langle A_{-k_0}^S \rangle = -\langle \mathcal{R} \rangle \, , \tag{26} \]
where again the symmetry is taken into account.

Let us divide \( \mathcal{R} \) and \( \mathcal{T} \) into elastic and inelastic parts marked by superscripts “el” and “in”. Obviously,
\[ \langle \mathcal{R}^{el} \rangle \equiv \left( P_{-k_0} \right) , \quad \langle \mathcal{T}^{el} \rangle \equiv \left( P_{k_0} \right) \, \tag{27} \]

These identities together with Eq. (25) and Eq. (24) yield
\[ \langle \mathcal{R}^{in} \rangle = \langle \mathcal{R} \rangle - \langle \mathcal{R}^{el} \rangle \leq \langle \mathcal{R} \rangle - \langle \mathcal{R} \rangle^2 \, , \quad \langle \mathcal{T}^{in} \rangle = \langle \mathcal{T} \rangle - \langle \mathcal{T}^{el} \rangle \leq \langle \mathcal{T} \rangle - \langle \mathcal{T} \rangle^2 \, . \tag{28} \]

In fact, that are one and the same relation, because \( \mathcal{R}^{in} = \mathcal{T}^{in} \) due to the mirror symmetry. Here from we obtain the restriction of total inelastic scattering:
\[ \langle \mathcal{R}^{in} \rangle + \langle \mathcal{T}^{in} \rangle \leq 2 \langle \mathcal{R} \rangle [1 - \langle \mathcal{R} \rangle] \leq 1/2 \, . \tag{29} \]

This is consequence of the “unitarity on average”.

Now consider the stochastic scattering more concretely, basing on the Eq. (24) and assuming that \( \xi(t) \) is a stationary random process, in particular, its mean value is time-independent: \( \langle \xi(t) \rangle = \langle x(t) \rangle = \mathcal{T} = \text{const} \) (of course, \( \mathcal{T} \) must be real).

Let us use the star “\( \ast \) as symbol of causal convolution: \( (a*b)(t) = \int_{t_0}^{t} a(t-t')b(t') dt' \). Due to the stationarity, when averaging Eq. (24) we can write
\[ \langle \xi(t)\psi(t) \rangle = \int_{t_0}^{t} \Xi(t-t')\langle \psi(t') \rangle dt' \equiv \langle \Xi \ast \langle \psi \rangle \rangle(t) \, , \quad \langle \psi(t) \rangle = [1 + (i/\hbar)G_0 \ast \Xi \ast]^{-1} \langle \Psi(0) \rangle \, . \tag{30} \]

The kernel \( \Xi(t) \) of the “mass operator” \( \Xi \ast \) looks as
\[ \Xi(t) = \frac{\mathcal{T}}{\hbar} \delta(t) - \frac{1}{\hbar} G_0(\tau) \langle \xi(t), \xi(0) \rangle + ... \, , \tag{31} \]

where dots substitute higher-order “non-factorable Feynman diagrams”, and
\[ G_0(\tau) = \left( 1 + \langle \mathcal{T} \rangle \right) G_0 \, \tag{32} \]

Correspondingly, Eq. (25) together with (31) yields
\[ \langle \mathcal{R} \rangle = \text{Re} C/(1 + C) \, , \quad \langle \mathcal{T} \rangle = \text{Re} 1/(1 + C) \, , \quad C = (i/\hbar v_0) \int_{t_0}^{t} \Xi(t) \exp(iE_0 t/\hbar) dt \, . \tag{33} \]

We noticed that \( \int_{t_0}^{t} G_0(\tau) \exp(iE\tau/\hbar) d\tau = 1/V(E) \), where \( V(E) = \sqrt{E(D\Delta E - E)/\hbar} \) is particle’s velocity as function of its energy (thus \( v_0 = V(E_0) \)).

Because of the stationarity, both \( \langle \psi(t) \rangle \) and \( \langle \xi(t)\psi(t) \rangle \) oscillate like the source \( \Psi^0(t, 0) \) in (24): \( \langle \psi(t) \rangle \propto \langle \xi(t)\psi(t) \rangle \propto \exp(-iE_0 t/\hbar) \). Hence, any inelastic amplitude of (24) is zero on average:
\[ \langle A_k^S \rangle \propto \delta(|k| - |k_0|) \, . \tag{35} \]

From this point, concentrate on simplest but principal situation characterized by three assumptions as follow.

(i) \( \xi(t) \)’s fluctuations are produced by equilibrium thermal bath, therefore, according to (12-15),
\[ \langle \xi(\tau), \xi(0) \rangle = K(|\tau|) \, , \quad \langle \xi^*(\tau), \xi(0) \rangle = K(\tau) \, . \tag{36} \]
\[ K(\tau) = \int_{0}^{\infty} \frac{e^{i\omega \tau} + \exp(h\omega/T) e^{-i\omega \tau}}{1 + \exp(h\omega/T)} \sigma(\omega) \, d\omega, \quad (37) \]

where \( T \) is bath temperature and \( \sigma(\omega) \geq 0 \). The spectrum \( \sigma(\omega) \) can be naturally introduced through correlation of the random potential \( x(t) = \Re \xi(t) \):

\[ \langle x(\tau), x(0) \rangle = \int_{0}^{\infty} \cos(\omega \tau) \sigma(\omega) \, d\omega. \]

(ii) \( \xi(t) \)'s fluctuations are sufficiently small and short-correlated (wide-band), e.g. in the sense of

\[ \max \sigma(\omega) \ll \hbar \Delta E, \quad (38) \]

so that the scattering can be analyzed in the "Born approximation".

(iii) \( \tau = 0 \), i.e. "there is no potential irregularity and no scattering on average".

Under these conditions, when averaging \( \Re \) and other variables one can manage with the correlation function \( K(\tau) \) only, as if \( \xi(t) \) was Gaussian noise. Due to [3], formula (38) strongly simplifies to

\[ \langle \Re \rangle \approx \Re C \approx \frac{1}{v_{0}^2 h^2} \int_{-E_{0}/\hbar}^{(E_{0} - h\omega)/\hbar} \frac{\sigma(\omega) F(h\omega/T)}{V(E_{0} + h\omega)} \, d\omega, \quad (39) \]

where \( F(X) \equiv 1/[1 + \exp(X)] \) is the Fermi distribution function, and presumably \( \Re C < 1 \). The contributions to \( C \) from \( \omega > 0 \) and \( \omega < 0 \) correspond to scattering with radiation or absorption of energy by the bath, respectively.

When \( \tau = 0 \), then elastic backward scattering must disappear at \( \sigma \to 0 \), that is \( \langle A_{k}^\dagger A_{-k} \rangle \propto 1/\sigma \) at small \( \sigma \). What is for fluctuational contribution, \( \langle A_{-k}^\dagger A_{-k} A_{k}^\dagger A_{-k} \rangle \), to mean probability of this scattering, it is small to the extent of \( \sigma/L \), as well as \( \langle A_{k} A_{-k} \rangle \) at all (see Eq. (41) below). Hence, \( \langle \Re \rangle \ll \langle \Re \rangle \), and the quantity (41) in fact represents the probability of inelastic reflection \( \langle \Re \rangle \).

The latter statement can be confirmed by direct calculation of \( \langle A_{k} A_{k}^\dagger \rangle \) using Eq. (27) and the approximation

\[ \langle \xi(\tau) \psi(\tau) \rangle \approx \langle \xi(\tau) \psi(\tau) \rangle \langle \psi(\tau) \rangle \]

which is valid under above assumptions. The result is

\[ \langle A_{k} A_{k}^\dagger \rangle = \frac{2\pi}{L v_{0}^2 \hbar^2} \sigma(\varepsilon(k)/\hbar) F(\varepsilon(k)/T), \quad (40) \]

where \( \varepsilon(k) \equiv E(k) - E_{0} \). With use of the equality (39), the inelastic reflection probability is

\[ \langle \Re \rangle = \sum_{-k_{0} \neq k < 0} \langle A_{k} A_{k}^\dagger \rangle \quad (41) \]

In fact, of course, for the finite incoming wave packet, this sum contains a finite number \( \approx L \) only of distinguishable outgoing states. The factor \( 2\pi/L \) in (40) is just their separation in the \( k \)-space, and because of \( L \gg 1 \) the sum (41) coincides with r.h.s of (39), that is \( \langle \Re \rangle \approx \langle \Re \rangle \).

VI. We illustrated once again that the general stochastic representation approach to open systems as suggested in [2] and developed in [4] [5] [6] can be useful in concrete considerations replacing complicated dynamical evolution of composite systems by stochastic evolution of a simple partial system. In the above example, if the energy of incoming particle is not fixed but has thermally equilibrium distribution with the same temperature as the scatterer’s temperature, then it is easy to verify that the same distribution will be reproduced after the stochastic inelastic scattering. Hence, we also obtain additional evidences that the stochastic representation ensures automatical agreement with thermodynamics.

To conclude, notice that our approach allows to set the problems about transport processes and their noise (including fluctuations in transport rates, e.g. in electrical conductivity), as well as about dephasing of coherent quantum processes, in a new fashion, with attraction of reach results on linear dynamic systems with randomly varying parameters (in particular, on wave propagation in random media).

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