

Random Schrödinger operators

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Recently considerable attention has been paid to the study of spectral properties of Schrödinger operators with random potentials. Physically this randomization of potentials is considered to describe approximately the motion of quantum mechanical particles in random media. Rigorous results on this field have been accumulated recently, therefore, in this report, the author gives a little survey.

The content of this note consists of three sections. § 1 is devoted to the description of general properties of random ergodic Schrödinger operators. In § 2 the author gives results on asymptotic properties of density of states for this random system. In § 3 spectral properties of one-dimensional systems are discussed.

§ 1. General properties of random Schrödinger operators.

In this section general results on random Schrödinger operators are given briefly. These general characters were first pointed out by Pastur L.A. [5].

Let (Ω, \mathcal{F}, P) be a probability space with a group of P -preserving transformations $\{T_x, x \in \mathbb{R}^n\}$. We assume that $\{T_x\}$ is ergodic*. Let $U(x, \omega)$ be a real valued measurable function on $\mathbb{R}^n \times \Omega$ such that $U(x, T_x \omega) = U(x+y, \omega)$ for every $x, y \in \mathbb{R}^n$ and $\omega \in \Omega$. Then under suitable condition on $U(x, \omega)$ a system of self-adjoint operators $A(\omega)$, which are called random Schrodinger operators, can be defined by

* If $F \in \mathcal{F}$ satisfies $P(T_x F \ominus F) = 0$ for every $x \in \mathbb{R}^n$, then $P(F) = 0$ or 1.

$$A(\omega) = -\Delta + U(\cdot, \omega)$$

in $L^2(\mathbb{R}^n)$, where Δ denotes the Laplacian in \mathbb{R}^n . A remarkable fact of this system of operators is

$$A(T_x \omega) = \tau_x^{-1} A(\omega) \tau_x, \quad ,$$

where $\tau_x f(y) = f(y-x)$ for $f \in L^2(\mathbb{R}^n)$. Therefore for each fixed $\omega \in \Omega$, the spectral structure of the operators $\{A(T_x \omega), x \in \mathbb{R}^n\}$ coincides each other. This together with the ergodicity of $\{T_x\}$ gives

Theorem 1. (Pastur L.A. [15], [17]) For simplicity assume that $U(x, \omega)$ are uniformly bounded. Let $\{E_\lambda(\omega)\}$ be the resolution of identity of $A(\omega)$. Then

(1) for each fixed interval I in \mathbb{R}^1 , $E_I(\omega)$ reduces to zero almost surely or $E_I(\omega)$ has infinite dimension almost surely. The same thing can be said also to each component of the Lebesgue decomposition for $\{E_\lambda(\omega)\}$.

(2) Let $E_I(x, y, \omega)$ be the continuous kernel of the projection $E_I(\omega)$. Then the statement of (1) can be realized according to

$$M(E_I(0, 0, \omega)) = 0 \quad \text{or} \quad M(E_I(0, 0, \omega)) > 0, \quad ,$$

where M denotes the integration with respect to ω by $P(d\omega)$.

The only problem in proving the above theorem is to show that every quantity arising in the statement of the theorem is measurable with respect to $U(\cdot, \omega)$. (for the detail of the proof see [3])

It should be remarked that in the formulation of random Schrödinger operators the cases of periodic potentials, quasi-periodic potentials and even almost periodic potentials are included.

§ 2. Order of singularity of density of states at their edges.

Let V be a smooth bounded domain in \mathbb{R}^n . Consider the Dirichlet problem in V for $-\Delta + U(\cdot, \omega)$. Let $\{\lambda_j^V(\omega)\}$ be the set of the eigenvalues and denote the distribution of the eigenvalues by

$$N_V(\lambda, \omega) = \frac{1}{|V|} \# \{ j, \lambda_j^V(\omega) < \lambda \},$$

where $|V|$ denotes the volume of the domain V . Then we have

Theorem 2. (Pastur L.A. [4]) For simplicity assume that $U(x, \omega)$ are uniformly bounded. Then with probability one

$$N_V(\lambda, \omega) \longrightarrow N(\lambda) \quad \text{as } V \text{ goes to } \mathbb{R}^n \text{ regularly}$$

on each continuous point λ of $N(\lambda)$ and $N(\lambda)$ is a non-random function. Moreover we have an identity $N(\lambda) = M(E_\lambda(0, 0, \omega))$.

The proof can be done without difficulty by using the Feynman-Kac formula. (see for example [3])

The derivative of this non-decreasing function $N(\lambda)$ is called a density of states of $A(\omega)$, which plays an important role in statistical mechanics for $A(\omega)$. Lifshitz I.M. [9] gave a conjecture on asymptotic nature of $N(\lambda)$ at its left edge. This was proved rigorously by Nakao S. [2] for a certain random potential by applying a large deviation theory of Wiener sausage established by Donsker M.D. and Varadhan S.R.S. [2]. Afterwards this result was reconsidered in another potentials by two people. The potentials they considered are

$$U(x, \omega) = \int_{\mathbb{R}^n} \varphi(x-y) \pi(dy, \omega),$$

where $\pi(dx, \omega)$ is a Poisson random measure* with characteristic measure dx and $\varphi(x)$ is a non-negative measurable function.

Theorem 3.

$$(1) \quad \varphi(x) = o(|x|^{-(n+2)}) \quad \text{as } |x| \rightarrow \infty, \quad \text{then}$$

$$\lambda^{n/2} \log N(\lambda) \longrightarrow -\gamma_1^{n/2} \quad \text{as } \lambda \downarrow 0,$$

where γ_1 is the first eigenvalue of $-\Delta$ with the Dirichlet boundary condition on the ball with unit volume in \mathbb{R}^n . (Nakao S. [12])

* random measure taking independent value at each disjoint set and with Poisson distribution of mean dx .

(2) $\varphi(x) \sim K |x|^{-(n+2)}$ as $|x| \rightarrow \infty$ with $K > 0$, then

$$\lambda^{n/2} \log N(\lambda) \longrightarrow -\left(\frac{n}{2}\right)^{n/2} \left(\frac{2C_1}{n+2}\right)^{(n+2)/2} \text{ as } \lambda \downarrow 0,$$

where $C_1 = \inf_{f \in F_0} \{I(f) + \bar{\Phi}(f)\}$, $I(f) = \int_{\mathbb{R}^n} |\nabla \sqrt{f}|^2 dx$,

$$\bar{\Phi}(f) = \int_{\mathbb{R}^n} \left\{ 1 - \exp\left(-K \int_{\mathbb{R}^n} \frac{f(x) dx}{|x-y|^{n+2}}\right) \right\} dy \text{ and } F_0 = \{f \geq 0,$$

$$\int_{\mathbb{R}^n} f(x) dx = 1 \text{ and } I(f) < \infty\}. \text{ (Ôkura H. [3])}$$

(3) $\varphi(x) \sim K |x|^{-(n+\beta)}$ ($0 < \beta < 2, K > 0$) as $|x| \rightarrow \infty$, then

$$\lambda^{n/\beta} \log N(\lambda) \longrightarrow -\left(\frac{n}{\beta}\right)^{n/\beta} \left(\frac{C_2}{n+\beta}\right)^{(n+\beta)/\beta} \text{ as } \lambda \downarrow 0,$$

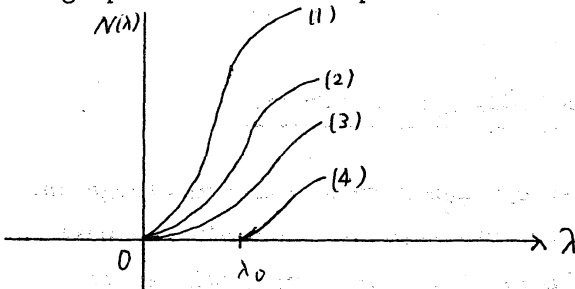
where $C_2 = K^{n/(n+\beta)} \left(\frac{\beta}{n+\beta}\right) \Omega_n$; Ω_n is the volume of the unit ball in \mathbb{R}^n . (Pastur L.A. [6])

It is interesting to compare the above result with deterministic cases.

(4) $U(x, \omega)$ is non-negative, not identically zero and periodic, that is, $U(x, \omega) = U(x + \omega)$ for some periodic function $U(x)$ and $\omega \in \Omega = \mathbb{R}^n / \mathbb{Z}^n$. Then there exists some $\lambda_0 > 0$ such that

$$N(\lambda) = 0 \text{ for any } \lambda \leq \lambda_0.$$

Summing up these four examples we have a graph:



This tells us that the stronger the mixing property of $U(x, \omega)$ is, the more dense the states would be.

If the space dimension $n = 1$, we have a more precise asymptotic formula. Let

$$A(\omega) = - \frac{d^2}{dx^2} + \pi(\cdot, \omega).$$

This corresponds to the $A(\omega)$ with $\varphi(x) = \delta_0(x)$. Then we have

Theorem 4. (Kotani S. [7])

$$N(\lambda) \sim \frac{1}{\pi c^2} e^{-\pi/\sqrt{\lambda}} \quad \text{as } \lambda \downarrow 0,$$

where $c = f(0)$ and $f(x)$ is a unique solution of

$$\begin{cases} f''(x) = \frac{1-e^{-x}}{x} f(x) \\ f(x) \sim x^{1/4} \exp\left\{-\int_0^x \sqrt{\frac{1-e^{-y}}{y}} dy\right\} \quad (x \rightarrow \infty). \end{cases}$$

On the other hand, at the right end point $+\infty$ the following theorem is valid.

Theorem 5. (Nakao S. [2]) Let $U(x, \omega)$ be a general bounded stationary ergodic random field. Then

$$N(\lambda) = \frac{1}{\Gamma(1+n/2)} \left(\frac{\lambda}{4\pi}\right)^{n/2} + o(\lambda^{n/2}) \quad \text{as } \lambda \rightarrow \infty.$$

Therefore at high energy levels at least the mean of spectral resolutions behaves as if there had existed no randomness.

§ 3. One-dimensional random Schrödinger operators.

If the space dimension $n=1$, we can get more precise knowledge on spectral properties. Before stating the results, we explain a well-known eigenfunctions expansion theorem for one-dimensional second order differential operators. Let $q(x)$ be a real valued continuous function and for each $\lambda \in \mathbb{C}$ let $\{\varphi_\lambda(x), \psi_\lambda(x)\}$ be a linearly independent system of solutions :

$$\begin{cases} -\varphi_\lambda''(x) + q(x)\varphi_\lambda(x) = \lambda\varphi_\lambda(x), & \varphi_\lambda(0) = 1, \varphi_\lambda'(0) = 0 \\ -\psi_\lambda''(x) + q(x)\psi_\lambda(x) = \lambda\psi_\lambda(x), & \psi_\lambda(0) = 0, \psi_\lambda'(0) = 1, \end{cases}$$

and define

$$R_1(\lambda) = - \lim_{x \rightarrow -\infty} \frac{\psi_\lambda(x)}{\varphi_\lambda(x)}, \quad R_2(\lambda) = \lim_{x \rightarrow +\infty} \frac{\psi_\lambda(x)}{\varphi_\lambda(x)}.$$

Then these two functions are holomorphic in $C \setminus R$ with positive imaginary on the upper half plane. Another similar functions are defined by

$$m_{11}(\lambda) = \frac{R_1(\lambda)R_2(\lambda)}{R_1(\lambda) + R_2(\lambda)}, \quad m_{22}(\lambda) = - \frac{1}{R_1(\lambda) + R_2(\lambda)}$$

and

$$m_{12}(\lambda) = m_{21}(\lambda) = \frac{R_1(\lambda)}{R_1(\lambda) + R_2(\lambda)}.$$

These four functions define four Radon measures:

$$\sigma_{ij}(I) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\pi} \int_I \operatorname{Im} m_{ij}(\lambda + i\varepsilon) d\lambda.$$

This system of measures satisfies

$$\left\{ \begin{array}{l} \sigma_{12}(I) = \sigma_{21}(I) \\ |\sigma_{12}(I) \sigma_{21}(I)| \leq \sigma_{11}(I) \sigma_{22}(I) \end{array} \right.$$

Using these four measures we can define the kernel of the resolution of identity for the self-adjoint operator $-\Delta + q(\cdot)$ by

$$E_I(x, y) = \int_I \varphi_\lambda(x) \varphi_\lambda(y) \sigma_{11}(d\lambda) + \int_I \psi_\lambda(x) \psi_\lambda(y) \sigma_{12}(d\lambda) \\ + \int_I \varphi_\lambda(x) \psi_\lambda(y) \sigma_{21}(d\lambda) + \int_I \psi_\lambda(x) \varphi_\lambda(y) \sigma_{22}(d\lambda).$$

Therefore spectral properties of our operator are governed by a measure

$$\sigma(I) = \sigma_{11}(I) + \sigma_{22}(I).$$

Now we choose a special random potential. Let M be a smooth compact

Riemannian manifold, Δ be the Laplacian and dx be the normalized volume element. Let F be a smooth real valued function on M satisfying

For any $x \in M$ there exists a multi-index k such that $\partial^k F(x) \neq 0$.

Since dx is a unique invariant measure of the semigroup $e^{t/2\Delta}$, we can define a stationary diffusion process $\{X_x(\omega), x \in \mathbb{R}^1\}$ with generator $1/2\Delta$ and initial distribution dx .

Theorem 6. (Goldseid I.Ya., Molchanov S.A. and Pastur L.A. [5]) If a random potential $U(x, \omega)$ defined by $F(X_x(\omega))$, then with probability one the Schrödinger operator $A(\omega)$ has a purely discontinuous spectrum densely in $[\inf_{x \in M} F(x), \infty)$.

Theorem 7. (Molchanov S.A. [1]) With the same potential as Theorem 6 with probability one each of eigenfunctions of the operator $A(\omega)$ decreases exponentially.

The proofs can be done by using the explicit formula of spectral measures as stated in the beginning of this section. In the proofs an essential role is played by the exponential growth property of $\varphi_\lambda(x)^2 + \varphi'_\lambda(x)^2$. In this connection we give a theorem:

Theorem 8. Let $U(x, \omega)$ be a general stationary ergodic process. Assume that $\varphi_\lambda(x)^2 + \varphi'_\lambda(x)^2$ grows exponentially as $|x| \rightarrow \infty$ almost surely for each $\lambda \in \mathbb{R}$. Then with probability one $A(\omega)$ has no absolutely continuous spectrum.

Proof. Since under the assumption of the theorem the absence of absolutely continuous spectrum of $A(\omega)$ on the half line $[0, \infty)$ or $(-\infty, 0]$ with the Neuman condition at the boundary 0 can be proved by the same method as [8], [5], we have only to show the following

Lemma. If the measures corresponding to $R_1(\lambda)$ and $R_2(\lambda)$ have no absolutely continuous part, then σ_{11} and σ_{22} also have the same property.

Proof. Note

$$\operatorname{Im} (m_{11}(\lambda) + m_{22}(\lambda)) = \frac{\{1 + |R_1(\lambda)|\}^2 \int \operatorname{Im} R_2(\lambda) + \{1 + |R_2(\lambda)|\}^2 \int \operatorname{Im} R_1(\lambda)}{|R_1(\lambda) + R_2(\lambda)|^2}$$

It is known that $\operatorname{Im} R(\lambda)$ tends to absolutely continuous part of the measure corresponding to $R(\lambda)$ as λ approaches to the real line almost everywhere with respect to the Lebesgue measure on \mathbb{R}^1 and $R(\lambda)$ itself has non-zero finite limit almost everywhere as λ tends to \mathbb{R}^1 . Therefore the assertion of the lemma can be proved immediately.

The property of exponential growth of generalized eigenfunctions $\{\psi_\lambda(x), \varphi_\lambda(x)\}$ was first proved by Matsuda H. and Ishii K. [7] in a discrete system by applying the Furstenberg theorem on the exponential growth of the product of independent identically distributed random special linear matrices. The connection of the exponential growth and the absence of absolutely continuous spectrum was first recognized by Casher R.J. and Lebowitz J.L. [1] and proved rigorously by Ishii K. [6]. This property is also essential in proving Theorem 6 and 7.

In one-dimensional case, it is interesting to know how the increase of randomness gives influence to the structure of the spectrum. Up to now precise spectral structures are known in two cases. One is the case of periodic potentials and the other is the above mentioned Markov random potentials. These two cases have quite different features. The problem is to determine bifurcation points of the spectral properties. In this connection it is significant to study a case

$$U(x, \omega) = f(x + \omega_1) + \gamma F(x, \omega_2)$$

where f is a smooth function on \mathbb{R}/\mathbb{Z} , $\omega_1 \in \mathbb{R}/\mathbb{Z}$, the second term is the potential of Theorem 6, $\omega = (\omega_1, \omega_2)$ and ν is a real constant. It is easy to see that this $U(x, \omega)$ is ergodic stationary process. Moreover we can prove the exponential growth of the generalized eigenfunctions of $A(\omega)$ with this potential almost surely for all $\lambda \in \mathbb{R}^1$. Hence applying Theorem 8, we can conclude that with probability one $A(\omega)$ has no absolutely continuous spectrum. In this potential, it is interesting to note that for sufficiently small ν the spectrum of $A(\omega)$ has gaps if the spectrum of $A(\omega)$ with $\nu = 0$ has gaps. So it is probable that there exists a critical constant $\nu_c > 0$ such that for all $\nu \in [0, \nu_c)$ the spectrum of $A(\omega)$ has gaps and for all $\nu \in (\nu_c, \infty)$ there is no gap. Moreover since the exponential growth property is valid also in this case, it is hopeful that there exists only purely discrete spectrum. However these problems remain open.

Among other things it is quite interesting to know the spectral properties for random Schrödinger operators in multi-dimensional case. In this symposium Professor Sinai informed that Molchanov S.A. proved recently that the spectrum of a discrete system with a specially identically distributed independent random potential in $\ell_2(\mathbb{Z}^n)$ consists of only absolutely continuous part if $n \geq 5$.

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