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Mathematical problems of the almost-periodic solids

We put forward a hypothesis that all solids are almost-periodic and discuss the appropriate mathematical problems.

Ми висуваємо гіпотезу, що всі тверді тіла є майже-періодичними, і обговорюємо відповідні математичні проблеми.

1 Introduction

It is well known that all solids are built of light electrons and heavy nuclei. The difference of masses is very large since an electron is about 2000 times lighter than a nucleon and a nucleus consists of tens or hundreds of nucleons. As a result of that we can imagine a solid as a collection of light and fast electrons moving quickly among heavy and slow nuclei. The slow nuclei form a potential for the fast electrons and in the first approximation the electrons follow to slow changes of the potential. It is an essence of the adiabatic hypothesis in the solid state physics.

The nuclei form a carcass of solid and an arrangement of nuclei in the carcass defines a structure of the solid. We classify the solids by a character of this structure.

If the solid is a crystal it leads to important consequences which allow to describe many properties of crystalline solids. First of all since the lattice has a symmetry of some space group the tensors which describe various properties of the crystal (tensor of elastic constants, tensor of dielectric or magnetic susceptibilities, tensor of conductivity etc.) have a symmetry of an appropriate point group. Secondly the nuclei, arranged in a lattice, form a periodic potential for the fast electrons and therefore an electron energy spectrum is a spectrum of the Schrödinger operator with the periodic potential. We can prove that this spectrum is absolutely continuous and has band structure, i.e. it is a union of closed segments of absolutely continuous spectrum. As a result of this fact all crystals are conductors in general.

If the nuclei are arranged randomly the solid has an amorphous structure. In this case electrons move in a random potential and therefore their energy spectrum is a spectrum of the Schrödinger operator with the random potential. If this potential is of the "white noise"type then we can prove that an appropriate spectrum is point. In this case amorphous solids are dielectrics. Electrons are allowed to move in electric field only by means of an electric breakdown.

We have described above two limit cases when nuclei arrangements (and also the corresponding electron potentials) are periodic or random functions. It appears that there exist a set of the almost-periodic functions which include periodic functions as a particular case and satisfy the condition of ergodicity which is the weakest possible exhibition of the randomness property. Therefore it looks reasonable to assume that in general case the nuclei arrangements in solids are almost-periodic. We can express it in other way saying that **all solids are almost-periodic** [1]. It is indeed the case and we shall discuss this idea now in details. Before that we explain what are the almost-periodic functions.

2 Almost-periodic structures

The theory of almost-periodic functions was created mainly by H. Bohr in 1924–1926 years and developed further by A. Besicovitch, S. Bochner, N. Bogoljubov, J. Favard, B. Levitan, J. von Neumann, V. Stepanov, H. Weyl and others. A particular but very important class of the almost-periodic functions (known now as quasi-periodic functions) was studied by P. Bohl and E. Esclangon as early as the end of XIX century.

Now we present essentials of the theory of almost-periodic functions and in order to make our exposition as simple as possible we consider only one-dimensional almost-periodic functions, a generalization of results for many-dimensional case is straightforward. We do not give proofs here, the reader can find them himself in the literature [7, 8, 17, 20, 22, 23].

Among many equivalent definition of the almost-periodic functions we choose the following one.

Definition 1. *Function $f(x)$ is called almost-periodic if it is a uniform limit in a space of trigonometrical polynomials $Trig(\mathbb{R})$, i.e. for any $\epsilon > 0$ there exist such a trigonometrical polynomial $P_\epsilon(x)$ that*

$$\sup_{x\in\mathbb{R}} |f(x) - P_\epsilon(x)| < \epsilon. \tag{1}$$

We denote the set of all continuous almost-periodic functions on $\mathbb{R}$ by $CAP(\mathbb{R})$. Every almost- periodic function $f(x)$ is bounded and therefore we may introduce the norm

$$||f|| = \sup_{x\in\mathbb{R}} |f(x)|. \tag{2}$$

With this norm the set of almost-periodic functions becomes a commutative Banach algebra with the usual definition of addition and multiplication.

Now we enumerate some properties of the almost-periodic functions which we shall use further.

A. For any almost-periodic function there exist a mean value

$$M(f) = \lim_{L\to\infty} \frac{1}{L} \int_0^L f(x)dx. \tag{3}$$

It allows for any almost-periodic function to build a Fourier series

$$f(x) \simeq \sum_n A_n \exp(i\lambda_n x), \quad A_n = M(f(x)\exp(-i\lambda_n x)). \tag{4}$$

We designate the numbers λ_n as the Fourier frequencies and the numbers A_n as the Fourier coefficients of the function $f(x)$. By means of the Fourier series we can build approximative trigonometric polynomials for the almost-periodic function.

We say that a countable set of real numbers $\{\lambda_n\}_1^\infty$ has a rational basis $\{\alpha_n\}_1^\infty$ if the numbers α_n are linear independent and any number λ_n can be presented as their finite linear combination with rational coefficients, i.e.

$$\lambda_n = \sum_{k=1}^{S_n} r_k^n\ \alpha_k, \quad r_k^n \in \mathbb{Q}. \tag{5}$$

We say that the basis is finite if it is finite set, we say that the basis is integer if all numbers r_k^n are integer numbers. If the a Fourier frequencies of the almost-periodic function have a finite and integer basis we designate the appropriate almost-periodic function as a quasi-periodic one. A quasi-periodic function with unique period is pure periodic one.

B.

Theorem 1. *(Kronecker–Weyl) Let $\lambda_k,\ k=1,\dots,n$ be real linearly independent numbers, $\theta_k,\ k=1,\dots,n$ be arbitrary real numbers, $\delta_k,\ k=1,\dots,n$ be arbitrary positive numbers. Let $\chi(x_1,x_2,\dots,x_n)$ be a characteristic function of parallelepiped in $\mathbb{R}^n$ defined by inequalities*

$$\theta_k-\delta_k<x_k<\theta_k+\delta_k,\quad k=1,\dots,n. \tag{6}$$

Continue the function $\chi(x_1,x_2,\dots,x_n)$ to the whole $\mathbb{R}^n$ periodically with periods 2π in all variables $x_k,\ k=1,\dots,n$.

Then uniformly in L we have

$$\lim_{L\to\infty}\frac{1}{2L}\int_{-L}^{L}\chi(\lambda_1x-\theta_1,\dots,\lambda_nx-\theta_n)dx=\pi^{-n}\delta_1\dots\delta_n. \tag{7}$$

C. A number τ is called an $\epsilon-$almost-period of the function $f(x),\ x\in\mathbb{R}$ if

$$\sup_{x\in\mathbb{R}}|f(x+\tau)-f(x)|<\epsilon. \tag{8}$$

It appears that any almost-periodic function has a relatively dense set of $\epsilon-$almost-periods for any $\epsilon>0$, i.e. for any $\epsilon>0$ there is such a number $l(\epsilon)$ that in any interval of the length $l(\epsilon)$ there exist at least one $\epsilon-$almost-period.

For the almost-periodic functions there exist close connection between $\epsilon-$almost-periods and the Fourier frequencies. Namely for any natural number n and any positive number $\delta<\pi$ there exist such a positive number $\epsilon(n,\delta)$ that all $\epsilon-$almost-periods of the almost-periodic function $f(x)$ satisfy the following system of inequalities

$$|\lambda_k\ \tau|<\delta,\ (\mod 2\pi),\quad k=1,2,\dots,n. \tag{9}$$

At the same time for any $\epsilon>0$ we can point out such a natural number n and a positive number $\delta<\pi$ that any real number τ, which satisfy the system of inequalities

$$|\lambda_k\ \tau|<\delta,\ (\mod 2\pi),\quad k=1,2,\dots,n,$$

is an $\epsilon-$almost-period of the almost-periodic function $f(x)$.

D. Function $F(x_1, x_2, \ldots)$ of finite or countable set of variables, each of which admits all real values, is called limiting periodic if it is a uniform limit of periodic ones, i.e. if for any real positive number ϵ we can point out such an integer positive number $n(\epsilon)$ and such a periodic function $F_\epsilon(x_1, x_2, \ldots, x_{n(\epsilon)})$ that

$$\sup_{-\infty < x_k, k=1,2,\ldots < +\infty} |F(x_1, x_2, \ldots) - F_\epsilon(x_1, x_2, \ldots, x_{n(\epsilon)})| < \epsilon. \quad (10)$$

It appears that for any almost-periodic function $f(x)$ there exist such a limiting periodic function $F(x_1, x_2, \ldots)$ of finite or countable set of variables that

$$f(x) = F(x, x, \ldots) = F(x_1, x_2, \ldots)|_{x_1 = x_2 = \ldots = x}. \quad (11)$$

Thus any almost-periodic function is restriction to a diagonal of some limiting periodic function. In other words we can also characterize every almost-periodic function by a sequence of periodic functions.

The properties of the limiting periodic function $F(x_1, x_2, \ldots)$ depends essentially on the basis of the Fourier frequencies of the function $f(x)$. If the basis $\alpha_1, \alpha_2, \ldots$ of the almost-periodic function $f(x)$ is integer then the limiting periodic function $F(x_1, x_2, \ldots)$ is periodic with periods $2\pi/\alpha_1, 2\pi/\alpha_2, \ldots$. If the basis $\alpha_1, \alpha_2, \ldots$ of the almost-periodic function $f(x)$ is finite then the limiting periodic function $F(x_1, x_2, \ldots)$ depends on finite set of variables. If the basis $\alpha_1, \alpha_2, \ldots$ of the almost-periodic function $f(x)$ is finite and integer then the limiting periodic function $F(x_1, x_2, \ldots)$ is periodic function of finite set of variables [21, 22].

E. Let $f(x)$ is a complex almost-periodic function and $\inf_x |f(x)| = k > 0$ then we can define

$$\arg f(x) = cx + \phi(x) \quad (12)$$

where a constant c is called a meam motion, and $\phi(x)$ is some almost-periodic function. The a meam motion c and the Fourier frequencies of the almost-periodic function $\phi(x)$ are linear combinations with integer coefficients of Fourier frequencies of the function $f(x)$ [21].

F. A continuous function $f(x)$ is almost-periodic iff a set of functions $\{f(x+h)\}, -\infty < h < +\infty$ is relatively compact, i.e. if from any infinite sequence $f(x+h_1), f(x+h_2), \ldots$ we can chose a subsequence which converges uniformly for all $x \in \mathbb{R}$ (S. Bochner). In other words any function $u(x)$ from the Banach space $C_b(\mathbb{R})$ of continuous bounded functions is called almost-periodic if the set $\{T_x(\cdot), x \in \mathbb{R}\}$, where $T_x(\cdot) = u(\cdot + x)$, is relatively compact in $C_b(\mathbb{R})$. A closure Ω of this set is known to be a compact in metrizable Abelian group. A normalized Haar measure μ on the set Ω turns out to be T_x-invariant and ergodic. Thus each almost-periodic function generates a probability space (Ω, μ, T_x). The operation of averaging on this space is given by

$$M(f) = \lim_{x\to\infty} \frac{1}{x} \int_0^x f(T_x u) dx = \int_\Omega f(u)\mu(du). \tag{13}$$

H. Bohr formulated also fundamentals of the harmonic and analytic almost-periodic functions. Various generalizations of the almost-periodic functions (e.g. for functional spaces with other metrics, for other groups etc.) were built by A. Besicovitch, B. Levitan, J. von Neumann, V. Stepanov, H. Weyl and others.

Now let us return to the idea that the nuclei arrangements in solids are almost-periodic in general and discuss various consequences.

The first important consequence of the above statement is a classification of solids in terms of nuclei structures and a corresponding partition solids into periodic solids (or crystals), random solids and properly almost-periodic solids. Such a classification of solids was proposed for the first time in [1, 3].

Crystals and amorphous solids are well known for a long time. We can obtain easily the properly almost- periodic nuclei arrangements in crystals by means of displacements of nuclei from equilibrium sites under influence of waves. Indeed the following theorem is valid.

Theorem 2. *(E.D. Belokolos, 1975) [1] Crystal, which is deformed by a finite (countable) set of waves with linearly independent frequencies, creates a quasi (an almost)-periodic potential.*

Proof. At first we consider the one-dimensional case.

Let us assume that nuclei, located in nodes of some lattice, create a periodic potentia $V(x)$. We suppose that the periodic potential $V(x)$ is continuous function and therefore it is uniformly continuous function. It means that for any $\epsilon' > 0$ there exist such $\delta' > 0$ that $|V(x_1) - V(x_2)| < \epsilon'$ as soon as $|x_1 - x_2| < \delta'$. Let us define $\epsilon = \min(\epsilon', \delta')$. Under deformation $u(x)$ a crystal point with a coordinate x is transformed to a coordinate

$x+u(x)$ where $u(x)$ is a trigonometrical sum. If this sum contains infinite set of summands we shall assume that it converges at a whole real axis so that $u(x)$ appears to be an almost-periodic $u(x)$ function.

Let us consider the function $V(x+u(x))$ which describes the potential of a crystal lattice deformed by waves. For the number ϵ, defined above, let us construct a relatively dense set of the $\epsilon-$almost-periods τ common for the functions $V(x)$ and $u(x)$. As it is well known we can do it always [6]. Each of thus constructed number τ is simultaneously $2\epsilon-$almost-period for the function $V(x+u(x))$. Indeed,

$$\begin{aligned} &|V(x+\tau+u(x+\tau))-V(x+u(x))| \leq \\ &|V(x+u(x+\tau))-V(x+u(x))|+\epsilon \leq 2\epsilon. \end{aligned} \tag{14}$$

Here the first inequality follows from the inequality $|V(x+\tau)-V(x)| \leq \epsilon$, and the second inequality follows from the inequality $|u(x+\tau)-u(x)| \leq \epsilon$ and the definition ϵ. Thus for any $\epsilon > 0$ we can construct a relatively dense set of $2\epsilon-$almost-periods for the function $V(x+u(x))$. And therefore as a result of that the function $V(x+u(x))$ is almost-periodic.

Let $u(x)$ is a finite trigonometrical polynomial with frequencies $\omega_s, s = 1, \dots, m$ and the function $V(x)$ has a frequency ω_0. Then joint $\epsilon-$almost-periods of the functions $V(x), u(x)$ satisfy the system of the inequalities $|\omega_s \tau| < \delta(\mod 2\pi), s = 0, 1, \dots, m$ for an appropriate δ. In accordance with the statement above they are simultaneously $2\epsilon-$ almost-periods for the function $V(x+u(x))$. Therefore the function $V(x+u(x))$ is quasi-periodic function.

In conclusion we remark that there is no problems to generalize this proof for the case of $d-$dimensional crystal. □

Thus a vibrating lattice at a fixed moment of time is an almost-periodic arrangements of nuclei. In other words in adiabatic approximation an electron in solid moves in an almost-periodic potential. By means of various reasons (e.g. by the Hume-Rosery phenomenon) these wave distributions of nuclei locations can be stabilized and in such a way these almost-periodic arrangements can be realized in equilibrium also.

We should only remember that in a solid there exist a lot of various of waves: the charge density waves, the magnetic (or spin) density waves, the concentration waves etc., and all these waves may have uncommensurable frequencies. Thus the almost-periodicity in solids can have various physical manifestations.

In 1984 material scientist D. Shechtman discovered in Al-Mn alloys the quasi-periodic structures which were designated later as the quasi-crystals [32]. In 2011 he was awarded the Nobel Prize in Chemistry for discovery “a new principle for packing of atoms and molecules”. In 1992 the International Union of Crystallography acknowledged the possibility for solids to order either periodic or aperiodic. Today physicists know hundreds of quasi-periodic solids, they are ubiquitous in many metallic alloys and compositions [33].

We need varieties of mathematical means to describe quasi-periodic structures. The “cut and project” method [21] represent a quasi-periodic function as a restriction of high-dimensional periodic one to an irrational intersection with one or more hyperplanes. In order to describe a quasi-periodic structure as an aperiodic substitution tiling we use the Delone and Meyer sets [17, 28] and also the Pisot numbers [19] as eigenvalues of the substitution matrices. When we go from crystals to quasi-crystals we must to generalize our notions from lattices and groups to ones of quasi-lattices and groupoids [30].

3 Spectra of the Schrödinger operator with almost-periodic potential

Studies of spectral properties of the Schrödinger operator with quasi-periodic potential in connection with the quantum theory of solids were initiated E.D. Belokolos (1975, 1976) [1, 2], Ya.G. Sinai and E. Dinaburg (1975) [5].

We shall consider the spectral properties of the Schrödinger operator

$$H = -\Delta + u(x), \tag{15}$$

where Δ is the Laplace and $u(x), x \in \mathbb{R}^d$ is a continuous almost-periodic potential. First of all we present basic results about this operator.

Theorem 3. *The Schrödinger operator with almost-periodic potential is self-adjoint essentially.*

For the Schrödinger operator with almost-periodic potential we can prove the existence of the number of states (or an integrated density of states) $N(\lambda)$ and other similar of spectral characteristics.

Theorem 4. *(M.A. Shubin, 1978) [10-13] The Schrödinger operator with almost-periodic potentialt has a number of states*

$$N(\lambda) = \lim_{k\to\infty} |V_k|^{-1} N_{V_k}(\lambda), \tag{16}$$

where V_k is bounded domain in $\mathbb{R}^n$ with the Lebesgue measure $|V_k|$ and $N_{V_k}(\lambda)$ is the standard distribution function of the discrete spectrum in the domain V_k with some self-adjoint boundary conditions.

The number of states $N(\lambda)$ is non-decreasing function of λ and is defined by the above expression everywhere besides the points of discontinuity.

We can prove also the existence of other similar limits, e.g.

$$D(\lambda) = \lim_{k\to\infty} |V_k|^{-1} \sum_{\lambda_j<\lambda} (f\psi_j, g\psi_j), \tag{17}$$

where ψ_j are eigenfunctions and f, g are arbitrary almost-periodic functions.

By considering the inverse functions we can prove the existence of the Fermi energy

$$E^F(\rho) = \lim_{k/|V_k|\to\rho} \frac{1}{p}\sum_{j=1}^{k} \lambda_j, \quad k\to\infty,\ |V_k|\to\infty,\ \rho>0-const, \tag{18}$$

where $\lambda_1 \leq \lambda_2 \leq \ldots$ are the eigenvalues arranged into an increasing sequence with their multiplicity taken in account.

It is known that there exist a single-valued correspondence between any self-adjoint operator A and a projector-valued measure P_λ on a Hilbert space H which is expressed in such way

$$A = \int_{-\infty}^{+\infty} \lambda \, dP_\lambda. \tag{19}$$

A point λ is said to belong to a spectrum $\sigma(A)$ of the operator A, $\lambda \in \sigma(A)$, iff $P_{(\lambda-\epsilon,\lambda+\epsilon)} \neq 0$ for any $\epsilon > 0$. We say that a point λ belongs to an essential spectrum, $\lambda \in \sigma_{ess}(A)$, iff the projector $P_{(\lambda-\epsilon,\lambda+\epsilon)}$ is infinite-dimensional for any $\epsilon > 0$. We say that a point λ belongs to an discrete spectrum, $\lambda \in \sigma_{disc}(A)$, iff the projector $P_{(\lambda-\epsilon,\lambda+\epsilon)}$ is finite-dimensional for any $\epsilon > 0$. It is obvious that

$$\sigma(A) = \sigma_{ess}(A) \cup \sigma_{disc}(A). \tag{20}$$

It appears for the Schrödinger operator with almost-periodic potential that the spectrum is essential.

Theorem 5. *(G. Scharf, 1965) [31] The spectrum of Schrödinger operator with almost-periodic potential is essential, i.e. it does not contain isolated eigenvalues of finite multiplicity.*

Proof. According to H. Weyl the point $\lambda \in \sigma(A)$ iff there exist such a sequence $\{\psi_j\}_{j=1}^{\infty}$ that $\lim_{j\to\infty} ||(A-\lambda I)\psi_j|| = 0$. If this sequence is compact then $\lambda \in \sigma_{disc}(A)$, if this sequence is not compact then $\lambda \in \sigma_{ess}(A)$.

Let us consider any function $\psi \in C_0^{\infty}(\mathbb{R}^d)$ such that $||\psi|| = 1$ and $||(A-\lambda I)\psi|| < \epsilon/2$. Shifting this function by sufficiently large $\delta-$almost periods of the potential $u(x)$ and its derivatives for a sufficiently small $\delta > 0$ we can construct an orthogonal system of functions $\{\psi_j,\ j = 1, 2\ldots\}$ such that $||(A-\lambda I)\psi_j|| < \epsilon$ for all $j = 1, 2, \ldots$. By the above criterion it means that the spectrum of the operator H is essential.

In one-dimensional case no eigenvalue can have infinite multiplicity and that means that the spectrum is a perfect set, i.e. a closed without isolated points. □

Sometimes it is important to have any information on possible gaps in essential spectrum. It appears that there exist a deep connection between a smoothness of potential $u(x)$ and a size of possible spectral gaps Δ. Appropriate studies for a one-dimensional case were initiated by P. Hartman and C.R. Putnam [24].

Theorem 6. *(M.S.P. Eastham, 1976 [23]; V.I. Feigin, 1977 [14]) Let in a self-adjoint operator A in $L^2(\mathbb{R})$, defined by differential expression $-y'' + u(x)y$, a real function $u(x)$ at large $|x|$ has $p > 1$ derivatives. Then in an essential spectrum of the operator A a lacuna of a size Δ with center at a value λ satisfies an asymtotic equality*

$$\Delta = O(\lambda^{-p/2}). \tag{21}$$

Another decomposition of the spectrum $\sigma(A)$ is useful also. According to the spectral theorem any self-adjoint operator A is unitary equivalent to an operator multiplication on λ in $L^2(\mathbb{R}, d\mu)$ for some measure μ. Since any measure μ on $\mathbb{R}$ has unique decomposition in a sum

$$\mu = \mu_{pp} + \mu_{ac} + \mu_{sing}, \tag{22}$$

where μ_{pp} is pure point measure, μ_{ac} is absolutely continuous with respect to Lebesgue measure, μ_{sing} continuous singular with respect to Lebesgue measure, therefore we have the following decomposition of the spectrum:

$$\sigma(A) = \sigma_{pp}(A) \cup \sigma_{cont}(A) = \sigma_{pp}(A) \cup \sigma_{ac}(A) \cup \sigma_{sing}(A). \quad (23)$$

It appears that in one-dimensional case the number of states $N(\lambda)$ determines the spectrum $\sigma(H)$ of the Schrödinger operator H :

Theorem 7. *(L.A. Pastur, 1980) [29]*

$$\sigma(H) = supp(dN). \quad (24)$$

The Lyapunov exponent $\gamma(\lambda)$ of the spectrum is defined as follows,

$$\gamma(\lambda) = \lim_{L \to \infty} |L|^{-1} \ln ||T_L||, \quad (25)$$

where T_L is a linear operator in $\mathbb{R}^2$ mapping $(\psi(0), \psi'(0))$ into $(\psi(L), \psi'(L))$ and ψ being a solution of the equation $H\psi = \lambda\psi$.

In terms of the Lyapunov exponent the absolutely continuous spectrum $\sigma_{ac}(H)$ of the Schrödinger operator H is described in such a way,

Theorem 8. *(S. Kotani, 1982) [26]* $\sigma_{ac}(H) = \overline{\{\lambda \in \mathbb{R} : \gamma(\lambda) = 0\}}$.

The Lyapunov exponent $\gamma(\lambda)$ and the number of states $N(\lambda)$ are real and imaginery parts appropriately of a so called Floquet function which is analytic in the upper half of complex plane $\mathbb{C}_+$ of the spectral parameter λ. This fact leads to a following connection between the number of states and the Lyapunov exponent,

Theorem 9. *(Thouless, 1972) [], (J. Avron and B. Simon, 1983)[] The Lyapunov exponent is*

$$\gamma(\lambda) = \gamma_0(\lambda) + \int_{-\infty}^{+\infty} \ln|\lambda - \lambda'| d|N(\lambda') - N_0(\lambda')|, \quad (26)$$

where values $\gamma_0(\lambda) = [\max(0, -\lambda)]^{1/2}$ *and* $N_0(\lambda) = \pi^{-1}[\max(0, -\lambda)]^{1/2}$ *corresponds to the case* $u(x) = 0$.

We can label the gaps of the spectrum by the elements of the frequency module of the almost-periodic potential similar as it has place for periodic one.

Theorem 10. *(E.D. Belokolos, 1975) [1, 3] Johnson and J. Moser, 1982) [27] For the Schrödinger operator with the potential $u(x) \in CAP(\mathbb{R})$ and $\lambda \in \mathbb{R} \setminus \sigma(H)$ the number of states $N(\lambda) \in \Omega_u$, where Ω_u is the frequencies module of u.*

Now we formulate the main theorem and give a sketch of its proof.

Theorem 11. *(E.D. Belokolos, 1975) [1, 3], (E. Dinaburg and Ya.G. Sinai, 1975) [5] Let us consider the Schrödinger equation*

$$(-\partial^2 + u(x))\psi(x) = \lambda\psi(x) \tag{27}$$

where $u(x)$ is a quasi-periodic potential with rationally independent frequencies $(\omega_1, \dots, \omega_n) = \omega$,

$$u(x) = U(\omega x) = U(\omega_1 x, \dots, \omega_n x). \tag{28}$$

Suppose $U(x_1, \dots, x_n)$ is an analytic function with period 2π in all n variables and ω satisfies the generalized Bragg-Wulff condition

$$|(q, \omega)| \geq \epsilon |q|^{-d}, \quad 0 \neq q \in \mathbb{Z}^n. \tag{29}$$

If $|u(x)|$ is sufficiently small (Belokolos), or λ is sufficiently large (Dinaburg and Sinai), then solutions of the Schrödinger equation admit a Floquet representation, in other words, we possess two linearly independent solutions of the form

$$\psi(x) = e^{ikx} v(x), \quad \bar{\psi}(x) = e^{-ikx} \bar{v}(x), \tag{30}$$

where $v(x)$ is the quasi-periodic function with the same set of frequencies $(\omega_1, \dots, \omega_n)$.

Proof. Let us sketch the idea of the proof. We have the Schrödinger equation

$$(-\partial^2 + u(x))\psi(x) = \lambda\psi(x) \tag{31}$$

with quasi-periodic potential,

$$\begin{aligned} &u(x) = U(\phi) = U(x\omega), \quad x \in \mathbb{R}, \\ &\phi = (\phi_1, \dots, \phi_n), \quad \omega = (\omega_1, \dots, \omega_n). \end{aligned} \tag{32}$$

Here

$$U(\phi) = U(\phi_1, \ldots, \phi_n) \tag{33}$$

is analytic and periodic in any variable $\phi_k,\ k = 1, \ldots, n$ function.

We shall assume also that the potential $u(x)$ is small, i.e.

$$\sup_{-\infty<x<+\infty} |u(x)| = \sup_{\phi\in T^n} |U(\phi)| = \epsilon, \quad 0 < \epsilon \ll 1, \tag{34}$$

where T^n is a $n-$dimensional torus. Evidently we have

$$U(\phi) = \sum_{q\in\mathbb{Z}^n} U_q \exp(i(q,\phi)), \quad (q,\phi) = \sum_{s=1}^{n} q_s\phi_s, \tag{35}$$

and therefore

$$u(x) = \sum_{q\in\mathbb{Z}^n} U_q \exp(i(q,\omega)x). \tag{36}$$

For the Schrödinger equation in the zero approximation of the perturbation theory we have

$$\psi_0(x) = \exp(ikx), \quad \lambda_0 = k^2. \tag{37}$$

In the first approximation of the perturbation theory we have

$$\begin{aligned} \psi_0(x) + \psi_1(x) &= \exp(ikx)\left(1 + \sum_{q\in\mathbb{Z}^n} \frac{U_q \exp(ix((q,\omega)-k))}{k^2 - (k-(q,\omega))^2}\right), \\ \lambda_0 + \lambda_1 &= k^2 + \sum_{q\in\mathbb{Z}^n} \frac{|U_q|^2}{k^2 - (k-(q,\omega))^2}. \end{aligned} \tag{38}$$

We have problems with the perturbation series written above only because of the presence of small denominators

$$k^2 - (k-(q,\omega))^2 = (q,\omega)(2k-(q,\omega)). \tag{39}$$

For example if the wave vector k satisfies the generalized Bragg–Wulff conditions

$$2k = (q,\omega), \quad |U_q| \neq 0, \tag{40}$$

then the standard perturbation series have no sense, we must use the secular perturbation theory which reveals an appearance of gaps in spectrum.

But even if the wave vector k does not satisfy the generalized Bragg–Wulff conditions the convergence of series is not obvious and depends on a rate of vanishing of numerators with growth of $|q|$. A rate of vanishing of denominators depends on the arithmetical properties of the wave vector $2k$ and the vector of frequencies $\omega = (\omega_1, \omega_2, \ldots, \omega_n)$ of the quasi-periodic potential, or, more precisely, on how quickly the linear superpositions of frequencies (ω, q) approximate the wave vector $2k$. It appears that some real numbers $2k$ are approximated by the numbers (ω, q) quite well and some real numbers $2k$ are approximated by the numbers (ω, q) quite bad.

A rate of vanishing of numerators depends on the smoothness of the function $U(\phi)$ which determines how quickly vanish the Fourier amplitudes U_q of the potential $u(x)$. For example, if the potential $U(\phi)$ has p derivatives then $|U_q| \simeq |q|^{-p}$ and if the potential $U(\phi)$ is analytical function in the strip $|Im\phi| = \sup_{1\leq k\leq n} |Im\phi_k| < a$ then $|U_q| \simeq \epsilon \exp(-a|q|)$.

If perturbation series for the wave function $\psi(x)$ and energy λ converge at a some domain of the wave vector k then for the energy λ we obtain absolutely continuous spectrum. If perturbation series for the wave function $\psi(x)$ and energy λ diverge at a some domain of wave vector k then we must use a seculare theory of perturbation and therefore for the energy λ we can obtain at a some domain of wave vector a spectral gap. If these gaps are arranged properly then we obtain for energy the band structure: intervals of absolutely continuous spectrum devided by gaps. If the gaps are distributed chaotically then we can obtain a point spectrum, or even singularly continuous one. Thus depending on properties of quasi-periodic potential we can have various spectra: point, absolutely continuous and singularly continuous. □

In conclusion we remark that even today we do not have complete understanding how the properties of the quasi-periodic potential connect with the properties of its spectrum.

In course these studies we elucidate astonishing fact: many proper quasi-periodic potentials can have a band spectrum similar to for periodic ones [8, 9]. We understand a band spectrum as a union of finite or countable set of intervals of absolutely continuous one. Quasi-periodic solids with such a type of spectrum have many interesting properties and important applications.

In the spectral problem of the Schrödinger operator with an almost-periodic potential we can also use the Kolmogorov–Arnold–Moser technique [4, 15] as it was done E.D. Belokolos (1975), E.I. Dinaburg and Ya.G. Sinai (1975) for quasi-periodic ones.

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