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Yulia E. Karpeshina

Perturbation Theory for the Schrödinger Operator with a Periodic Potential

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Author

Yulia E. Karpeshina
Department of Mathematics
University of Alabama
Birmingham, AL 35294-1170
USA
E-Mail: Karpeshi@vorteb.math.uab.edu

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1. Introduction.

The Schrödinger operator with a periodic potential describes the motion of a particle in bulk matter. Therefore, it is interesting to have a detailed analysis of the spectral properties of this operator. Both physicists and mathematicians have been studying the periodic Schrödinger operator for a long time [1]. The most significant progress has been achieved in the one-dimensional case [2] The two and three dimensional cases are still of great challenge.

Initially, physicists observed that the spectrum of the periodic Schrödinger operator has a band structure and is semibounded below (see f.e.[BS, Ki, Mad, Zi]). Moreover, according to the famous Bethe-Sommerfeld conjecture [BS] there exist only a finite number of gaps in the spectrum. The eigenfunctions of each band can be described as "Bloch functions", which satisfy quasiperiodic conditions in the elementary cell [Bl]. This means that they can be parameterized by the number of the band and the quasimomentum, which is a parameter of the quasiperiodic conditions. The eigenvalues of Bloch eigenfunctions with a fixed quasimomentum form a discrete set.

For physical applications it is important to have a perturbation theory of the Scrödinger operator with a periodic potential. In one-dimensional situation the perturbation theory was constructed by Carvey D. Mc. [C1] – [C3]. However, in many dimensional situations its construction turns out to be rather difficult, because the denseness of Bloch eigenvalues of the free operator increases infinitely with increasing energy. Under perturbation, the eigenvalues influence each other strongly and the regular perturbation theory does not work. The main aim of this book is to construct perturbation formulae for Bloch eigenvalues and their spectral projections in a high energy region on a rich set of quasimomenta. The construction of these formulae is connected with the investigation of a complicated picture of the crystal diffraction.

Another problem, considered here, is a semi-bounded crystal problem, i.e., the Schrödinger operator which has the zero potential in a half space and a periodic potential in the other half space. The interaction of a plane wave with

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[1] see f.e. [A], [Ag], [Ar] – [DavSi], [Di] – [DyPe], [Ea1] – [GiKnTr2], [GorKapp1] – [HøHoMa], [KargKor] – [K17], [Ki] – [Le], [Mad] – [Out], [Pav], [PavSm1] – [Rai], [ReSi4] – [SheShu], [Si2] – [Zi].

[2] see f.e. [Av1], [BelBovChe], [Bent1], [Bu1] – [BuDm3] , [C1] – [C3], [Ea2], [Fir1] – [FirKor], [FroPav2], [GaTr1, GaTr2], [Ha], [KargKor], [Kohn] – [LaPan], [MagWin] – [McKTr2], [Ol], [PavSm1], [PavSm2], [ReSi4], [SheShu], [Ti], [WeKe1], [WeKe2].

a semicrystal will be studied. First, the asymptotic expansion of the reflection coefficients in a high energy region will be obtained, this expansion is valid for a rich set of momenta of the incident plane wave. Second, the connection of the asymptotic coefficients with the potential will be established. Based upon these, the inverse problem will be solved, this problem is to determine the potential from the asymptotics of the reflection coefficients in a high energy region (a crystallography problem).

Let us describe briefly some previous results.

I.M. Gelfand began the rigorous study of the periodic Schrödinger operator [Gelf]. He proved the Parseval relation for Bloch waves in $L_2(R^n)$. The expansion theorem was proved by E.Ch Titchmarsh [Ti] in the one-dimensional situation and by F.Odeh, J.B. Keller [OdKe] in the many-dimensional case. V.L. Lidskiy applied E.Ch Titchmarsh's method to prove the Parseval formula in manydimensional situation [Ea2]. The first rigorous proof of the fact, that the spectrum of the periodic Schrödinger operator is the union of all the Bloch eigenvalues, corresponding to different quasimomenta, was given by F.Odeh, J.B. Keller [OdKe]. M.S.P. Eastam gave another proof of this fact [Ea1, Ea2]. L.E. Thomas showed that the spectrum of the operator is absolutely continuous [Th]. Wilsox C. studied analytical properties of eigenvalues as functions of quasimomenta [Wil].

The detailed investigation of the band structure is still a challenging problem. A first step in this direction was made by M. M. Skriganov [Sk1]–[Sk7]. He gave the proof of the Bethe- Sommerfeld conjecture. He considered the operator

$$H = (-\Delta)^l + V \tag{1.0.1}$$

in $L_2(R^n)$, $n > 1$, where V is the operation of multiplication by a smooth potential. M. M. Skriganov has proved the conjecture for certain n, l, including the physically interesting cases $n = 2, 3, l = 1$ (the Schrödinger operator). He developed the subtle methods of arithmetical and geometrical theory of lattices. This makes proofs sometimes different for rational and non-rational lattices. For example, in the case $4l > n + 1$, only a proof for rational lattices is given.

Another beautiful proof of the Bethe-Sommerfeld conjecture in the dimension two, using an asymptotic of a Bessel function, was found by B.E.J. Dahlberg and E. Trubowitz [DahTr].

However, one can suppose that Bethe and Sommerfeld were guided by the ideas of perturbation theory for the many-dimensional case. The different approaches to the construction of this theory one can find in [FeKnTr1, FeKnTr2], [Fri], [K4] – [K15], [Ve1] – [Ve7]. As it was mentioned before, its mathematical foundation is a complicated matter, because the denseness of Bloch eigenvalues of a free operator ($V = 0$) increases infinitely with increasing energy. The Bloch eigenvalues of the free operator are situated very close to each other in a high energy region. Therefore, when perturbation disturbs them, they strongly influence each other. Thus, to describe the perturbation of one of the eigenvalues, we must study not only that eigenvalue, but also the surrounding ones. This causes analytical difficulties, in particular, "the small denominators problem".

The first asymptotic formula in the high energy region for a stable under perturbation Bloch eigenvalue has been constructed for $l = 1$ by O.A. Veliev

[Vel] – [Ve7]. The stable case corresponds to nonsignificant diffraction inside the crystal. The validity of the Bethe-Sommerfeld conjecture for $n = 2$ and $n = 3$ is a consequence of this formula. The formula in [Vel] – [Ve7] reproduces the first terms of the asymptotic behavior of the eigenvalue in the case of a smooth potential.

The first results about the unstable case, which corresponds to a significant diffraction inside the crystal, were obtained by J. Feldman, H. Knörrer and E. Trubowitz [FeKnTr2] (more precisely about these results see page 16).

In our consideration the perturbation series both for an eigenvalue and a spectral projection are constructed. The method is based on the expansion of the resolvent in a perturbation series. The series converge for a rich set of quasimomenta and have an asymptotic character in the high energy region. They are differentiable with respect to the quasimomentum and preserve their asymptotic character. The particular terms in the series are simple and can be calculated directly. This is the first method which works for a general class of potentials, including potentials with Coulomb and even stronger singularities. This perturbation theory is valid not only for the proof of the Bethe-Sommerfeld conjecture, but, moreover, for the description of the isoenergetic surface. Many other physical values can be determined using these formulae. In the unstable case the perturbation series are constructed with respect to an auxiliary operator, which roughly describes the diffraction inside the crystal.

One of the main difficulties is to construct the nonsingular set, that is, the set of quasimomenta for which the perturbation series converge. This difficulty is certainly of a physical nature. Convergence of the perturbation series for an eigenfunction shows the perturbed eigenfunction to be close to the unperturbed one (the plane wave). This means that this plane wave goes through the crystal almost without diffraction. But it is well known that, in fact, the plane wave $\exp i(\mathbf{k}, x)$ is refracted by the crystal, if $\mathbf{k}$ satisfies the von Laue diffraction condition (see f.e.[BS], [Ki], [Mad]):[3]

$$| \mathbf{k} | = | \mathbf{k} + 2\pi \mathbf{q} |, \tag{1.0.2}$$

for some $\mathbf{q} \in Z^3 \setminus \{0\}$. The refracted wave is known to be $a \exp(i(\mathbf{k} + 2\pi\mathbf{q}, x))$, $a \in C$. This wave interferes with the initial one $\exp(i(\mathbf{k}, x))$ and distorts it strongly. This means that the perturbation series diverges if $\mathbf{k}$ is not far from the planes (1.0.2). Here the question arises: does the series converge when $\mathbf{k}$ is not in the vicinity of (1.0.2)? It turns out that it does, when $2l > n$. However, it is not enough for the control of the convergence of series when $2l \leq n$. There are some additional diffraction conditions arising in this more complicated case. Another problem is that when eliminating the singular set (where the series can diverge), we must take care that this set does not become "too extensive". This means that it must not include the whole set of quasimomenta which correspond to a given energy. We shall show that the nonsingular set is rather rich – it has an asymptotically full measure on the isoenergetic surface of the free operator. Geometric considerations are made in the explicit form for a smooth potential.

[3] In this equation we suppose a cell of periods to be unit.

In the case of a nonsmooth potential the formulae for the nonsingular set are less explicit, but, nevertheless, the set can be determined by a simple computer program.

To construct the nonsingular set in the simplest case $\mathbf{2l > n}$ and $V \in L_\infty$, we delete from the isoenergetic surface S_k of the free operator (S_k is a sphere of radius k centered at the origin of R^n, $0 < \delta \ll 1$) the momenta belonging to the $(k^{-n+1-2\delta})$-neighborhood of the planes $|\mathbf{k}| = |\mathbf{k} + 2\pi\mathbf{q}|$, $\mathbf{q} \in Z^n \setminus \{0\}$. In the rest of S_k the perturbation series converge and the perturbation of the isoenergetic surface is asymptotically small in a high energy region ($k \to \infty$).

The situation becomes more complicated as soon as we lift the restriction $2l > n$. When $2l \leq n$, but $\mathbf{4l > n + 1}$ and V is smooth, we have to delete from S_k some vicinities of the planes

$$|\mathbf{k} + 2\pi\mathbf{m}| = |\mathbf{k} + 2\pi\mathbf{m} + 2\pi\mathbf{q}|, \quad \mathbf{m} \in Z^n, \ \mathbf{q} \in Z^n \setminus \{0\}, \tag{1.0.3}$$

$|\mathbf{k} + 2\pi\mathbf{m}| \approx k$. We call relations (1.0.3) *the Generalized Laue Diffraction Conditions.* The size of the vicinity to delete depends on k and $\mathbf{m}, \mathbf{q}$. Thus, the nonsingular set becomes less extensive than in the case $2l > n$, but nevertheless, it has an asymptotically full measure on S_k. From equation (1.0.3) one can see that the formulae for the nonsingular set depend only on the periods of the potential.

Special considerations are needed for a non-smooth potential. We introduce the concept of the "number" of states and consider its geometrical aspects. The nonsingular set is described in the terms of the number of states.

The situation is most complicated in the case of the **Schrödinger operator**. The singular set has a part which depends essentially on the potential, even when it is smooth. To construct the nonsingular set one has to delete a neighborhood of the surfaces:

$$|\mathbf{k} + 2\pi\mathbf{m}|^2 = |\mathbf{k} + 2\pi(\mathbf{m} + \mathbf{q})|^2 + \Delta\lambda_{\mathbf{mq}}(\mathbf{k}). \tag{1.0.4}$$

Here, as before, $\mathbf{m}, \mathbf{q} \in Z^3$, $|\mathbf{k} + 2\pi\mathbf{m}| \approx k$. The new terms $\Delta\lambda_{\mathbf{m}}(\mathbf{k})$ are smooth functions of $\mathbf{k}$ determined by the potential. For many $\mathbf{m}$, $\Delta\lambda_{\mathbf{mq}}(\mathbf{k}) = 0$, but for a number of $\mathbf{m}$ the functions $\Delta\lambda_{\mathbf{mq}}(\mathbf{k})$ essentially differ from zero; they are the perturbations of Bloch eigenvalues of the free operator in the one-dimensional situation by some periodic potential V_q. We call equations (1.0.4) the *Modified Laue Diffraction Conditions.*

The case of the Schrödinger operator with a nonsmooth potential accumulates all described restrictions on the nonsingular set.

In the case when t is at the diffraction surface (1.0.2), the refracted wave arises in the crystal and there exists a splitting of the degenerated eigenvalue. Suppose that $\mathbf{k}$ satisfies the von Laue condition $|\mathbf{k}| = |\mathbf{k} + 2\pi\mathbf{q}|$ for a unique $\mathbf{q}$: it is generally known that the plane wave $\exp i(\mathbf{k}, x)$ is refracted by the crystal for such k. Physicists consider the refracted wave to be $a \exp i(\mathbf{k} + 2\pi\mathbf{q}, x)$, $a \in C$ (see f.e. [Ki, Mad, Zi]). The resulting wave is a linear combination of the initial and refracted waves. The mathematical study of this problem (Chapter 2) shows that this is a good approximation for the case $2l > n$. Taking a model operator

H_q – which roughly accounts the refraction and splitting – as the initial operator instead of H_0, we construct the perturbation series for t near a diffraction plane. The rigorous study of the diffraction at the Laue diffraction planes (1.0.2), in the case of the Schrödinger operator ($n = 3, l = 1$), shows that such simple approximation is not sufficient any longer. We have to represent a refracted wave as a linear combination of the waves $a_n \exp i(\mathbf{k}+2\pi n\mathbf{q}, x)$, $n \in Z$. This will be an approximate refracted wave. It is constructed by using a model operator, roughly describing the refraction inside the crystal. This operator has a more complicated form than that in the case $2l > n$. Taking the model operator as the initial operator instead of H_0, we construct the perturbation series for t near the diffraction surface.

The perturbation series near the nonsingular set and the planes of diffraction make it possible to describe an essential part of the perturbed isoenergetic surface.

In the case of a semicrystal we consider its interaction with an incident plane wave $\exp(i(\mathbf{k}, x))$. Let $\mathbf{k}$ belong to the nonsingular set for the whole crystal. Therefore, a wave close to $\exp i(\mathbf{k}, x)$ can propagate inside the crystal. For the wave $\exp i(\mathbf{k}, x)$ to "penetrate" actually inside the crystal, we have to eliminate the interaction of the incident wave $\exp i(\mathbf{k}, x)$ with the surface. To do this, we have to impose more restrictions on the nonsingular set. Nevertheless, this new nonsingular set has an asymptotically full measure on S_k. Under some new restrictions on the nonsingular set we construct a high-order asymptotic expansions of the reflected and refracted waves for $\mathbf{k}$ belonging to this nonsingular set. Furthermore, we show that the relations between the asymptotic coefficients and the potential are not very complicated. That is why one can determine the potential from the asymptotic expansion of the reflected wave (only if the potential is known to be a trigonometric polynomial).

Now we want to describe the results more concretely. We study the operator (1.0.1) in three cases, as geometric and analytical difficulties increase:

1. $2l > n$;
2. $4l > n + 1$, $(2l \leq n)$;
3. $n = 3, l = 1$.

The case $2l > n$ is considered in Chapter 2, the case $4l > n+1$ – in the Chapter 3, and the case $n = 3$, $l = 1$ (the Schrödinger operator) is studied in Chapter 4.

Let us write potential $V(x)$ in the form :

$$V(x) = \sum_{m \in Z^n} v_m \exp i(\mathbf{p}_m(0), x), \tag{1.0.5}$$

where $(\cdot, \cdot)$ is the scalar product in R^n and $\mathbf{p}_m(0)$ is a vector of the dual lattice:

$$\mathbf{p}_m(0) = 2\pi(m_1 a_1^{-1}, \ldots, m_n a_n^{-1}).$$

The potential V is real by assumption, so $v_m = \bar{v}_{-m}$. We suppose $v_0 = 0$; this assumption does not restrict the generality of our considerations.

We consider a potential, which satisfies the condition

$$\sum_{m \in Z^n \setminus \{0\}} | v_m |^2 | m |^{-4l+n+\beta} < \infty, \tag{1.0.6}$$

$$| m | = (m_1^2 + ... + m_n^2)^{1/2},$$

for some β obeying the following inequalities:

$$\begin{array}{lll} \beta > 0 & \text{if } 2l \leq n, & n \neq 2 \text{ (in particular, } n = 3, l = 1) \\ \beta \geq 2l - n & \text{if } 2l > n, & n \neq 2 \text{ or } 2l > 3, n = 2; \\ \beta > 1 & \text{if } l < 3\ n = 2. & \end{array}$$

The potential does not need to be smooth to satisfy this condition. For example, in the case $n = 3$, a function, which behaves in a neighborhood of some point x_0 as $| x - x_0 |^{-\zeta}$, $\zeta < 2l$, in particular, a Coulomb potential, satisfies this condition.

For the sake of simplicity we assume that the potential has orthogonal periods $a_1, ..., a_n$, however all the results are valid also for non-orthogonal periods.

It was shown [Gelf, OdKe, Ea1, Ea2, Th] that the spectral analysis of H can be reduced to studying the operators $H(t)$, $t \in K$, where K is the unit cell of the dual lattice,

$$K = [0, 2\pi a_1^{-1}) \times ... \times [0, 2\pi a_n^{-1}).$$

The vector t is called quasimomentum. The operator $H(t)$, $t \in K$, acts in $L_2(Q), Q = [0, a_1) \times ...[0, a_n)$. Its action is described by formula (1.0.1) together with the quasiperiodic conditions:

$$u(x_1, ..., x_{j-1}, a_j, x_{j+1}, ..., x_n) = \exp(it_j a_j) u(x_1, ..., x_{j-1}, 0, x_{j+1}, ..., x_n), \tag{1.0.7}$$

$$j = 1, ..., n.$$

The derivatives with respect to x_j, $j = 1, ..., n,$, must also satisfy the similar conditions.

The operator $H(t)$ has a discrete semi-bounded spectrum $\Lambda(t)$:

$$\Lambda(t) = \cup_{n=1}^{\infty} \lambda_n(t), \ \ \lambda_n(t) \to_{n \to \infty} \infty.$$

The spectrum Λ of operator H is the union of the spectra $\Lambda(t)$,

$$\Lambda = \cup_{t \in K} \Lambda(t) = \cup_{n \in N, t \in K} \lambda_n(t).$$

The functions $\lambda_n(t)$ are continuous, so Λ has a band structure:

$$\Lambda = \cup_{n=1}^{\infty} [q_n, Q_n], \ \ q_n = \min_{t \in K} \lambda_n(t), \ \ Q_n = \max_{t \in K} \lambda_n(t).$$

The eigenfunctions of $H(t)$ and H are simply related. If we extend the eigenfunctions of all the operators $H(t)$ quasiperiodically (see (1.0.7)) to R^n, we obtain a complete system of eigenfunctions of the operator H.

Let $H_0(t)$ be the operator corresponding to the zero potential. Its eigenfunctions are the plane waves:

$$\exp(i(\mathbf{p}_j(t), x)),\ j \in Z^n,\ \mathbf{p}_j(t) = \mathbf{p}_j(0) + t. \tag{1.0.8}$$

The eigenfunction (1.0.8) corresponds to the eigenvalue $p_j^{2l}(t) =| \mathbf{p}_j(t) |^{2l}$. Thus, the spectrum of H_0 is equal to

$$\Lambda_0(t) = \{p_j^{2l}(t)\}_{j \in Z^n}.$$

Using the basis of the eigenfunctions of $H_0(t)$ one can write the matrix $H(t)$ in the form

$$H(t)_{mj} = p_m^{2l}(t)\delta_{mj} + v_{m-j}, \tag{1.0.9}$$

where δ_{mj} is the Kronecker symbol. Of course, the free operator is diagonal in this basis.

Note that any $\mathbf{k} \in R^n$ can be uniquely represented in the form:

$$\mathbf{k} = \mathbf{p}_j(t),\ j \in Z^n,\ t \in K. \tag{1.0.10}$$

Thus, any plane wave $\exp i(\mathbf{k}, x)$ can be written in the form (1.0.8). Naturally, we can rewrite the von Laue diffraction conditions (1.0.2) for (1.0.8) as follows:

$$p_j^{2l}(t) = p_{j+q}^{2l}(t) = k^{2l}, q \neq 0. \tag{1.0.11}$$

Similarly, the Generalized von Laue diffraction conditions and the Modified von Laue diffraction conditions can be represented as follows:

$$p_{j+m}^{2l}(t) = p_{j+m+q}^{2l}(t),\ q \neq 0,\ \ p_j^{2l}(t) = k^{2l} \tag{1.0.12}$$

$$p_{j+m}^{2}(t) = p_{j+m+q}^{2}(t) + \Delta\lambda_{mq}(\mathbf{p}_j(t)),\ q \neq 0,\ \ p_j^{2}(t) = k^{2}. \tag{1.0.13}$$

We will use formula (1.0.8) for plane waves and formulae (1.0.11) – (1.0.13) for the diffractions conditions.

In physical literature, the important concept of the isoenergetic surface of the free operator is used (see f.e. [Ki, Mad, Zi]). It is said that a point t belongs to an isoenergetic surface $S_0(k)$ of the free operator H_0, if and only if, the operator $H_0(t)$ has an eigenvalue equal to k^{2l}, i.e., there exists $m \in Z^n$, such that $p_m^{2l}(t) = k^{2l}$. This surface can be obtained as follows: the sphere of radius k centered at the origin of R^n is divided into pieces by the dual lattice $\{\mathbf{p}_m(t)\}_{m \in Z^n}$, and then all these pieces are transmitted into the cell K of the dual lattice. Thus, we obtain the sphere "packed into the bag" K (Fig.1).
Note that the selfintersections are described by the von Laue diffraction conditions (1.0.11).

Let $S_1(k) \subseteq S_0(k)$. We say that $S_1(k)$ has an asymptotically full measure on $S_0(k)$ if the relation

$$\frac{s(S_1(k))}{s(S_0(k))} \to_{k \to \infty} 1 \tag{1.0.14}$$

holds, where $s(\cdot)$ is the area of a surface.

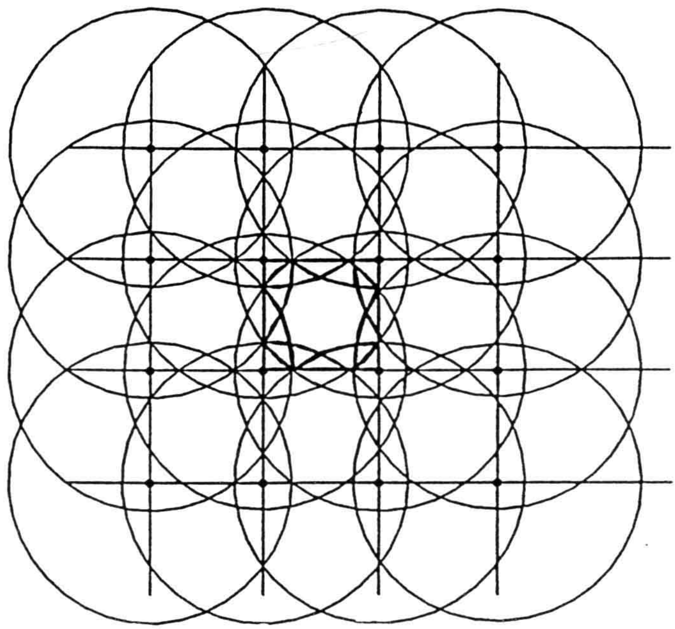

Fig.1 The isoenergetic surface of the

free operator for n=2

In Chapter 2 we consider the case **2l > n**, where V is a trigonometric polynomial. This simplest situation is described in order to clear up the basic method of our considerations – the formal construction of perturbation series and the description of the nonsingular set for which these series converge. In this chapter we introduce the factor α, $-1 \leq \alpha \leq 1$ in front of the potential, and consider the operator:

$$H_\alpha = (-\Delta)^l + \alpha V, \tag{1.0.15}$$

$$V(x) = \sum_{j \in Z^n, |j| < R_0} v_j \exp(i(\mathbf{p}_j(0), x)), \quad R_0 < \infty \tag{1.0.16}$$

We describe the nonsingular set $\chi_0(k, \delta)$ for this case as $S_0(k) \setminus A_0(k, \delta)$, where $A_0(k, \delta)$ is the $(k^{-n+1-\delta})$-neighborhood of the selfintersections of $S_0(k)$. If $t \in \chi_0(k, \delta)$, then (1.0.11) does not hold, i.e., there is a unique j such that $p_j^{2l}(t) = k^{2l}$. Moreover, for all $m \neq j$:

$$\left| p_m^{2l}(t) - p_j^{2l}(t) \right| > 2k^{2l-n-\delta}.$$

This inequality means that the free operator has a unique eigenvalue k^{2l} in the interval $(k^{2l} - 2k^{2l-n-\delta}, k^{2l} + 2k^{2l-n-\delta})$. We will prove that the nonsingular set $\chi_0(k, \delta)$ has an asymptotically full measure on $S_0(k)$.