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Multidimensional Periodic Schrödinger Operator

Perturbation Theory and Applications

Springer

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To the memory of my mother and father and to my family.

Preface

The book is devoted to the spectral theory of the multidimensional Schrödinger operator $L(q)$ generated in $L_2(\mathbb{R}^d)$ by the differential expression

$$-\Delta u(x) + q(x)u(x),$$

where $x \in \mathbb{R}^d,\ d \geq 2$ and q is a real periodic, relative to a lattice Ω, potential. This operator describes the motion of a particle in the bulk matter. To describe the brief synopsis of the book let us introduce some notations and recall some well-known definitions. It is well known that the spectrum of $L(q)$ is the union of the spectra of the operators $L_t(q)$ for $t \in F^*$ generated in $L_2(F)$ by the same differential expression and the conditions

$$u(x+\omega) = e^{i\langle t,\omega\rangle}u(x),\ \forall \omega \in \Omega,$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{R}^d$, t is a crystal momentum (quasimomentum), $F =: \mathbb{R}^d/\Omega$ and $F^* =: \mathbb{R}^d/\Gamma$ are the fundamental domains (primitive cells) of the lattices Ω and Γ respectively, and

$$\Gamma =: \{\delta \in \mathbb{R}^d : \langle \delta, \omega \rangle \in 2\pi\mathbb{Z}, \forall \omega \in \Omega\}$$

is the reciprocal lattice, i.e., is the lattice dual to Ω. The spectrum of $L_t(q)$ consists of the eigenvalues

$$\Lambda_1(t) \leq \Lambda_2(t) \leq \ldots$$

These eigenvalues are called the Bloch eigenvalues. They define functions $\Lambda_n : t \to \Lambda_n(t)$ for $n = 1, 2, \ldots$ of t that are called the band functions of $L(q)$. The n-th band function Λ_n is continuous with respect to t and its range

$$\delta_n =: \{\Lambda_n(t) : t \in F^*\}$$

is the n-th band of the spectrum $\sigma(L(q))$ of $L(q)$:

$$\sigma(L(q)) = \cup_{n=1}^{\infty} \delta_n.$$

The eigenfunctions of $L_t(q)$ are known as the Bloch functions.

The book consists of five chapters. The first chapter presents preliminary definitions and statements to be used in the next chapters. Besides, we give a brief discussion of what is known from the literature and what is presented in the book about the perturbation theory of $L(q)$. In the second chapter, first, we obtain the asymptotic formulas of arbitrary order for the Bloch eigenvalue and Bloch function of the periodic Schrödinger operator $L(q)$ of arbitrary dimension, when the corresponding quasimomentum lies far from the diffraction hyperplanes

$$D_\delta =: \{x \in \mathbb{R}^d : |x|^2 = |x+\delta|^2\}$$

for small values of δ. Then we study the case, when the corresponding quasimomentum lies near a diffraction hyperplane and gets the complete perturbation theory for the multidimensional Schrödinger operator with a periodic potential. Moreover, we construct and estimate the measures of the isoenergetic surfaces in the high energy region which implies the validity of the Bethe-Sommerfeld conjecture for arbitrary dimension and arbitrary lattice. This conjecture was formulated in 1928 and claims that there exist only a finite number of gaps (the spaces between the bands δ_n and δ_{n+1} for $n = 1, 2, \ldots$) in the spectrum $\sigma(L(q))$ of $L(q)$. Note that the construction of the perturbation theory of $L(q)$ is connected with the investigation of the complicated picture of the crystal diffraction. The regular perturbation theory does not work in this case, since the Bloch eigenvalues of the free operator are situated very close to each other in the high energy region.

In the third chapter, using the asymptotic formulas obtained in the second chapter, we determine constructively a family of the spectral invariants of $L(q)$ from the given Bloch eigenvalues. Some of these invariants are explicitly expressed by the Fourier coefficients of the potential which present the possibility of determining the potential constructively by using the Bloch eigenvalues as the input data.

In the fourth chapter, we consider the inverse problems of the three-dimensional Schrödinger operator with a periodic potential q by the spectral invariants obtained in the third chapter. First, we construct a set of trigonometric polynomials which is dense in the Sobolev space $W_2^s(F)$, where $s > 3$, in the $\mathbb{C}^\infty$- topology and every element of this set can be determined constructively and uniquely, modulo inversion $x \to -x$ and translations $x \to x + \tau$ for $\tau \in \mathbb{R}^3$, from the given spectral invariants that were determined constructively from the given Bloch eigenvalues. Then a special class V of the periodic potentials is constructed, which can be easily and constructively determined from the spectral invariants and hence from the given Bloch eigenvalues. Moreover, we consider the stability of the algorithm for the unique determination of the potential $q \in V$ of the three-dimensional Schrödinger operator with respect to the spectral invariants and Bloch eigenvalues.

In the fifth chapter we summarize our results from the point of view of both physicists and mathematicians. I am thankful to Claus Ascheron and Peter Wölfle for their advices that help to improve the readability of the book.

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