The Band Structure of the General Periodic Schrödinger Operator with Point Interactions

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Abstract: The spectrum of Schrödinger operators \( H \) with periodic point potentials in dimensions \( d = 2, 3 \) is studied. In the general case of \( N \) points in the Wigner–Seitz cell it is proven that \( H \) has a band structure with at most a finite number of gaps (Bethe–Sommerfeld conjecture). It is also proven that in the case of a generic local point perturbation no singular continuous components are present; in the non-local case a fractal component like the Cantor set is exhibited, this component can either consist of a singular continuous or a dense point spectrum.

0. Introduction

In the present paper we study the spectrum structure of the Schrödinger operator \( H \) in the space \( L^2(\mathbb{R}^d) \) (\( d = 2 \) or \( 3 \)) with a periodic point potential. Such operators were first investigated by M.L. Goldberger and F. Seitz, who derived an explicit formula for the energy spectrum in the case \( d = 3 \) [1]. A rigorous mathematical derivation of the corresponding dispersion equations, based on the techniques of direct integral decomposition, was given in [2] (see also [5]). In this work it was also proved that the spectrum of \( H \) is purely absolutely continuous and contains at most two bands (see [3a] for \( d = 3 \) and [4] for \( d = 2 \), see moreover [5–7] for other developments, and [3b] for more regular periodic perturbations). In particular, these results confirm the Bethe–Sommerfeld conjecture on the finiteness of bands for the case of periodic point perturbations.

However the mentioned results were obtained under a strong restriction, namely under the assumption that there is only one point interaction in the Wigner–Seitz cell. If the Wigner–Seitz cell contains \( N \) point scatterers, where \( N > 1 \), little is known about the spectrum structure of \( H \). It was proven that there are at most \( N \) bands on the negative part of the energy axis [6,8] but the band structure above \( E = 0 \) is completely

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unknown. Another restriction in the mentioned papers is that they deal only with “diagonal” perturbation matrices (with “local” point perturbations in the terminology of [9]).

In the present paper we consider arbitrary periodic point perturbations of the free particle Hamiltonian $-\Delta$. If the elements in the diagonals of the perturbation matrix exponentially decrease with the diagonal index (in particular, if only the main diagonal of the matrix has non-zero elements), then we prove that $H$ has a band spectrum with a finite number of gaps. Therefore, for “local” periodic point perturbations the Bethe–Sommerfeld conjecture is fulfilled. Moreover, in this case for the “typical” periodic point perturbations the spectrum of $H$ contains no singular continuous components. If the periodic point perturbation is not “local”, the spectrum of $H$ may contain a component which is a Cantor set. This set may be the support of a singular continuous component of the spectrum or may contain a dense set of eigenvalues. It is necessary to stress that the point perturbations that are “nonlocal” in the sense of [9], are local in the ordinary sense: namely, if $\varphi \in D(H)$ and $\varphi(x) = 0$ for all $x$ in some region $G \subset \mathbb{R}^d$, then $H\varphi(x) = 0$ everywhere in $G$ [5].

1. Preliminaries

First we introduce some notations and basic definitions. We denote by $H^0$ the operator $-\Delta$ in the space $L^2(\mathbb{R}^d)$ ($d = 2$ or $3$). Fix a basis $a_1, \ldots, a_d$ in $\mathbb{R}^d$ and denote by $\Lambda$ the lattice generated by this basis

$$\Lambda = \left\{ \sum_{i=1}^{d} n_i a_i : n_i \in \mathbb{Z} \right\}. \quad (1.1)$$

Let $F$ be the elementary cell of $\Lambda$ having the form

$$F = \left\{ \sum_{i=1}^{d} t_i a_i : 0 \leq t_i < 1 \right\}. \quad (1.2)$$

We choose a nonvoid finite subset $K \subset F$ and denote by $A$ the set $A = K + \Lambda = \{ \kappa + \lambda : \kappa \in K, \lambda \in \Lambda \}$; this set is called a crystal. Without loss of generality we shall assume that $0 \in K$.

The main object of our paper is a point perturbation of $H^0$ supported by $A$. To introduce the perturbed operator, we use the so-called “restriction – extension” procedure [5,10].

Namely, let

$$D(S) = \left\{ f \in D(H^0) : f(a) = 0 \forall a \in A \right\}; \quad (1.3)$$

denote by $S$ the restriction of $H^0$ to the domain $D(S)$. Obviously, $S$ is a symmetric operator, and it is not hard to prove that $S$ is closed. The point perturbation of $H^0$ supported by $A$ is, by definition, any selfadjoint extension $H$ of $S$ such that $D(H) \cap D(H^0) = D(S)$. A convenient tool to describe all such extensions is the Krein resolvent formula [11]. Therefore, we recall some necessary facts from the M.G. Krein theory of selfadjoint extensions.

Let $S$ be a closed symmetric operator in a Hilbert space $\mathcal{H}$ having a selfadjoint extension $H^0$, and let $X, z \in \mathcal{H} \setminus \sigma(H^0)$, be the deficiency space of $S : X = \{ x \in \mathcal{H} :$