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Stark Hamiltonians with Periodic Potentials

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1. Introduction

Let $H_0 = -\Delta + Fx_1$ denote the free Stark Hamiltonian on $L^2(\mathbb{R}^n)$. It is essentially selfadjoint on the Schwartz space $\mathcal{S}(\mathbb{R}^n)$. Let V be a realvalued bounded function. Then $H = H_0 + V$ is selfadjoint with domain $\mathcal{D}(H) = \mathcal{D}(H_0)$. The time-dependent Schrödinger equation $i\frac{d\psi}{dt} = H\psi$, $\psi(0) = \psi_0$, has the solution $\psi(t) = e^{-itH}\psi_0$. The questions we want to consider here are the following:

1° Describe the asymptotic behavior of $\psi(t) = e^{-itH}\psi_0$ as $t \to \pm\infty$. This is in a general form the basic question in scattering theory.

2° Describe the spectrum $\sigma(H)$ of H in detail, i.e. classify it according to the usual categories: point spectrum, continuous spectrum, absolutely continouos and singular continuous spectrum.

For the one-dimensional case we obtain fairly complete results, see section 4. For the higher dimensional case we obtain some general results, see section 3, and for the case of a half-crystal we obtain some interesting new results, see section 5.

This presentation is a *preliminary* report on $[J]_3$. Concerning previous papers on Stark effect Hamiltonians with decaying potentials, we refer to the references given in $[J]_2$.

2. Periodic potentials and lattices

A discrete subset of $\mathbb{R}^n$ is called a lattice, if it can be represented in the form

$$T = \{ k_1\mathbf{a}_1 + k_2\mathbf{a}_2 + \ldots + k_n\mathbf{a}_n \mid k_1, \ldots, k_n \in \mathbb{Z} \},$$

where $\mathbf{a}_1, \ldots, \mathbf{a}_n$ are linearly independent vectors in $\mathbb{R}^n$. A function V on $\mathbb{R}^n$ is said to be periodic with the period lattice T, if for all $\mathbf{x} \in \mathbb{R}^n$ and all $\tau \in T$ we have $V(\mathbf{x}+\tau) = V(\mathbf{x})$.

The position of the lattice T relative to the x_1-axis plays an important role in our study. We introduce the following definitions. Let $\mathbf{e}_1 = (1,0,\ldots,0) \in \mathbb{R}^n$. The inner product on $\mathbb{R}^n$ is denoted $< , >$.

Definition 2.1. (i) The lattice T is said to be irrational with respect to $\mathbf{e}_1$, if the set $\{ <\mathbf{e}_1, \tau> \mid \tau \in T \}$ is dense in $\mathbb{R}$.

(ii) The lattice T is said to be rational with respect to $\mathbf{e}_1$, if the set $\{ <\mathbf{e}_1, \tau> \mid \tau \in T \}$ is discrete in $\mathbb{R}$.

This is a classification, since it is easy to see that these are the only possibilities. The translation group associated to the lattice is given by $(U(\tau)f)(\mathbf{x}) = f(\mathbf{x}-\tau)$. Assume that the potential V above is periodic with period lattice T. Then we have the important relation

$$U(\tau)HU(\tau)^{-1} = H - F<\mathbf{e}_1,\tau>. \tag{2.1}$$

3. General spectral results

Throughout this section we assume that the potential V is a realvalued function with period lattice T.

Proposition 3.1. Assume that T is irrational with respect to $\mathbf{e}_1$. Then $\sigma(H) = \mathbb{R}$.

Proof: By (2.1) $\sigma(H) = \sigma(H) - F<\mathbf{e}_1,\tau>$. Since $\sigma(H) \neq \emptyset$ and $\{ F<\mathbf{e}_1,\tau> \mid \tau \in T\}$ is dense in $\mathbb{R}$, the result follows. □

Proposition 3.2. Assume that T is rational with respect to e_1. Assume that $\{\tau \in T \mid \langle e_1,\tau\rangle = 0\}$ is a sublattice of dimension n-1. Assume that $\sigma(-d^2/dx_1^2+Fx_1+V(x_1,\tilde{x})) = \mathbb{R}$ for a dense set of $\tilde{x} \in \mathbb{R}^{n-1}$. Then $\sigma(H) = \mathbb{R}$.

Remark 3.3. A sufficient condition for $\sigma(-d^2/dx_1^2+Fx_1+V(x_1,\tilde{x})) = \mathbb{R}$ is $V(x_1,\tilde{x}) = (\partial/\partial x_1)W(x_1,\tilde{x})$ for some bounded function W with two bounded derivatives, see $[J]_1$.

Proof: We use a direct integral decomposition with respect to the sublattice in the proposition and the the variable $\tilde{x}$. The proof is somewhat long, so the details are omitted. See also section 5.□

Propositions 3.1 and 3.2 cover all cases for n = 2. For n>2 not all cases are covered. We expect to find $\sigma(H) = \mathbb{R}$ in all cases. For a strong electric field it is easy to obtain a result on the type of spectrum.

Theorem 3.4. Assume V, $\partial V/\partial x_1$ and $\partial^2 V/\partial x_1^2$ continuous realvalued bounded functions on $\mathbb{R}^n$ and $\alpha_0 = \inf\{F+(\partial V/\partial x_1)(\mathbf{x}) \mid \mathbf{x} \in \mathbb{R}^n\} > 0$. Assume $\sigma(H) = \mathbb{R}$. Then the spectrum is purely absolutely continuous.

Proof: This result is an immediate consequence of Mourre's commutator method [M]. We use the conjugate operator $A = i\partial/\partial x_1$. The assumption implies that we have the Mourre commutator estimate

$$i[H, A] = F+\partial V/\partial x_1(x) \geq \alpha_0 I.$$

Furthermore, the second commutator $i[i[H, A], A] = \partial^2 V/\partial x_1^2$ is a bounded operator on $L^2(\mathbb{R}^n)$ by our assumption. Thus all the essential conditions for applying Mourre result are verified. The remaining technical conditions are easily verified. □

4. One-dimensional Stark Hamiltonians

In the one-dimensional case there are fairly complete answers to questions 1° and 2° in section 1. We shall briefly recall these results from $[J]_1$. Let us recall that the basic objects in the scattering theory for the pair of operators H and H_0 are the wave operators $W_\pm(H, H_0) = s-\lim_{t\to\pm\infty} e^{itH}e^{-itH_0}$. One asks whether these operators exist and are complete, i.e. $\mathrm{Ran}(W_{\pm}) = \mathcal{H}_p(H)^{\perp}$, the orthogonal complement to the closed subspace $\mathcal{H}_p(H)$ spanned by the L^2-eigenfunctions of H. The point spectrum of H is denoted $\sigma_p(H)$.

Theorem 4.1. ($n = 1$) Assume $V \in C^2(\mathbb{R})$, V periodic with period a, and $\int_0^a V(x)dx = 0$. Then $W_{\pm}(H, H_0)$ exist and are unitary.

Theorem 4.2. ($n = 1$) Assume $V = V_1 + V_2$, where V_1 satisfies the assumptions of the previous theorem and V_2 satisfies $V_2(x) = O(|x|^{1-\varepsilon})$ as $x \to \infty$, $V_2(x) = O(|x|^{-1/2-\varepsilon})$ as $x \to -\infty$ for some $\varepsilon > 0$. Then $W_{\pm}(H, H_0)$ exist and are complete. Furthermore, $\sigma_p(H)$ is discrete in $\mathbb{R}$.

Theorem 4.3. ($n = 1$) Assume $V = W''$, where W is a realvalued bounded function with four bounded derivatives. Then $W_{\pm}(H, H_0)$ exist and are unitary.

Theorem 4.1 is of the expected type. It shows that the crystal becomes "transparent" with respect to the time evolution, if one waits a long time. Theorem 4.2 shows that we can add "impurities" (in the form of V_2) and retain the same result, except the possible occurence of a discrete set of embedded eigenvalues.

Theorem 4.3 shows that the same result holds, even for sums of periodic potentials and for a large class of almost-periodic functions. For example, one can take

$$V(x) = \int_{\mathbb{R}} e^{i\omega x} d\mu(\omega)$$

where μ is a Borel measure satisfying

$$\int_{\mathbb{R}} (\omega^{-2} + \omega^2) d|\mu|(\omega) < \infty.$$

As a special case we can take

$$V(x) = \sum_{k=1}^{\infty} a_k \sin(\omega_k x)$$

with

$$\sum_{k=1}^{\infty} |a_k|(\omega^{-2}+\omega^2) < \infty.$$

5. The half-crystal model

We now consider the case where the crystal fills up half the space. Half-solids have been briefly considered in [S]. Here we add a constant electric field orthogonal to the surface directed into the empty part of space. The results below show that after a long time an electron will eventually move freely, irrespective of the initial position.

Let V_1 be a periodic function on $\mathbb{R}^n$ with period lattice $T = \mathbb{Z}\times\hat{T}$, where $\hat{T}$ is a lattice in $\mathbb{R}^{n-1}$. We assume $V_1 \in C^2(\mathbb{R}^n)$. Let χ be a cutoff function, i.e. $\chi \in C^{\infty}(\mathbb{R})$ realvalued, $0 \leqslant \chi(x_1) \leqslant 1$, $\chi(x_1) = 0$ for $x_1 < -\delta$, and $\chi(x_1) = 1$ for $x_1 > \delta$, where $\delta > 0$ is a fixed parameter. We take as our potential

$$V(\mathbf{x}) = \chi(x_1)V_1(\mathbf{x}).$$

The main result is the following

Theorem 5.1. ($n \geqslant 2$) Let V satisfy the assumptions above. Then $W_{\pm}(H, H_0)$ exist and are unitary. Consequently, $\sigma(H) = \sigma_{ac}(H) = \mathbb{R}$.

The proof of this theorem will only be sketched. Let $F_{\hat{T}}$ denote a fundamental region for the lattice $\hat{T}$, chosen diffeomorphic to the $n-1$-dimensional torus $\mathbb{T}^{n-1}$. The dual lattice is denoted $\hat{T}^*$ and a fundamental region $F_{\hat{T}}^*$, again chosen diffeomorphic to $\mathbb{T}^{n-1}$. We now use the Floquet-Bloch reduction, see for example [Sk] for details. There exists a unitary operator $W_{\hat{T}}$ from $L^2(\mathbb{R}^n)$ to the direct integral space $\mathcal{H}=\int^{\oplus}\mathcal{H}(k)dk$, where k varies over $F_{\hat{T}}^*$. The operator H is transformed into $W_{\hat{T}}HW_{\hat{T}}^{-1} = \int^{\oplus}H(k)dk$. In our case we do not reduce in x_1, so we have $\mathcal{H}(k) = L^2(\mathbb{R})\otimes L^2(F_{\hat{T}})$ and $H(k) = h_0\otimes I_2 + I_1\otimes Q(k) + V(x_1,\tilde{x})$ with $h_0 = -(d^2/dx_1^2)+Fx_1$ on $L^2(\mathbb{R})$ and $Q(k) = (-i\nabla_{\tilde{x}}-k)^2$ on $L^2(F_{\hat{T}})$ with periodic boundary conditions. Here $k \in F_{\hat{T}}^*$. The main step is the following lemma.

Lemma 5.2. The wave operators $\mathcal{W}_{\pm}(H(k), H_0(k))$ exist and are unitary on $\mathcal{H}(k)$, $k \in F_{\hat{T}}^*$.

To prove this lemma, we verify the conditions in the abstract theorems in $[J]_2$. The proof of absence of embedded eigenvalues requires a separate argument Details can be found in $[J]_3$.

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