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Resonance Theory in Atom-Surface Scattering

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Abstract. We study the problem of analytic extension of the resolvent for Hamiltonians arising in scattering of atoms by a quantum surface. We prove that the resolvent extends holomorphically to some regions of the lower half plane with isolated singularities called Landau resonances which are branch points of the resolvent. We study also the effect of impurities on the singularities of the resolvent and show that the presence of impurities adds poles to the Landau resonances.

Introduction

We study in this paper the theory of resonances for Hamiltonians arising in atom-surface scattering. The theory of atomic or molecular collisions with surfaces has been greatly developed by chemists in recent years since the measurement of scattering of atoms by a quantum surface is a way to study the surface structure of materials at atomic scales (see [Ge] for a review).

The typical form of the Hamiltonian is the following: $H = -\Delta + V(x,y)$ on $\mathbf{R}_x^{m-1} \times \mathbf{R}_y$, where y is the direction normal to the surface and $V(x,y)$ is an effective potential describing the interaction between an atom and a crystalline or non-crystalline material. Strictly speaking this Hamiltonian corresponds to a thin slab of material since it is possible for atoms to pass through the crystal. The Hamiltonian corresponding to an impenetrable material is the following: $H' = -\Delta + V(x,y)$ on $\mathbf{R}_x^{m-1} \times \mathbf{R}_y^+$ with Dirichlet boundary condition on $y=0$.

We will concentrate on H but all results proved for H hold for H' under corresponding hypotheses. (The proofs can be adapted almost verbatim.) When the surface is a perfect crystal, $V(x,y)$ tends to zero when y tends to infinity and is periodic in x with respect to some lattice T in $\mathbf{R}^{m-1}$. In this paper we will always assume that V is exponentially decreasing in y in a suitable sense.

For crystalline surfaces, H is usually studied using Bloch's theory to reduce the study of the resolvent $(H-\lambda)^{-1}$ to the study of $(H_p-\lambda)^{-1}$, where the Bloch number p belongs to a fundamental domain of the dual lattice T^* and $H_p = D_y^2 + (D_x+p)^2 + V(x,y)$, $D_{x_i} = (1/i)\partial/\partial x_i$, $D_y = (1/i)\partial/\partial y$ is a reduced