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Time Dependent Approach to Scattering from Impurities in a Crystal

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Abstract. A time dependent scattering theory for a quantum mechanical particle moving in an infinite, three dimensional crystal with impurity is given. It is shown that the Hamiltonian for the particle in the crystal without impurity has only absolutely continuous spectrum. The domain of the resulting wave operators is therefore the entire Hilbert space.

I. Introduction

In the time dependent approach to potential scattering theory, one endeavors to establish the existence and completeness of wave operators $\Omega_{\pm} = \underset{t \to \pm\infty}{\text{s-lim}}\, e^{itH_1} e^{-itH}$ acting in a Hilbert space $\mathscr{H}$, where H is the Hamiltonian operator for the free evolution of the system and H_1 is the perturbed Hamiltonian operator for the system with interactions. Here completeness means that the ranges of $\Omega_{\pm}$ coincide with the absolutely continuous subspace of $\mathscr{H}$ with respect to H_1. The unitary scattering operator S is then given simply by $S = \Omega_+^{\dagger} \Omega_-$ [1, 2].

Mathematically rigorous results asserting the existence and completeness of $\Omega_{\pm}$ have been given in the particular case of single particle potential scattering in which $-H = \Delta$ is the Laplacian acting in $L^2(\mathbb{R}^3)$, and $H_1 = H + W(\boldsymbol{x})$, where $W(\boldsymbol{x})$ is a short range potential, e.g. $W(\boldsymbol{x}) \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ [2–4]. It is a natural question to ask whether these results may be modified to accommodate the situation in which both H and H_1 are altered by the addition of a periodic potential $V(\boldsymbol{x})$, that is, where H and H_1 are given by $H = -\Delta + V(\boldsymbol{x})$, $H_1 = -\Delta + V(\boldsymbol{x}) + W(\boldsymbol{x})$ and $V(\boldsymbol{x}) = V(\boldsymbol{x} + \boldsymbol{a}) = V(\boldsymbol{x} + \boldsymbol{b}) = V(\boldsymbol{x} + \boldsymbol{c})$ for three linearly independent vectors $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}$. The modification would constitute a theory of scattering from an impurity $W(\boldsymbol{x})$ in a crystal, with the role of free Hamiltonian played by $H = -\Delta + V(x)$ [5].

We show that such a modification is indeed possible assuming that $V(\boldsymbol{x})$ is square integrable over a unit cell (Theorem 3, Section III). In fact this modification is almost immediate except for one technical point: since the domain of the resulting wave operators is only the