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Scattering from Impurities in a Crystal

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Abstract. A time independent scattering theory for a particle in a crystal with impurity is given. It is shown that the scattered wave is the solution of a Lippman Schwinger equation, and that the existence of bound states or narrow resonances is related more to the band structure than to the form of the impurity potential.

1. Introduction

This paper is concerned with the scattering of wavelike excitations in solids by localized imperfections: $Q(\boldsymbol{x})$[1]. We extend the treatment of the two body quantum mechanics by Kato and Kuroda [1, 2] and prove the existence of distorded Bloch waves which have the form (Bloch wave) + (outgoing wave)/(incoming wave) and are obtained as solutions of a Lippman-Schwinger integral equation.

We want to emphasize, here, the role played by the critical energies[2]. In ordinary scattering the only critical energy is 0 and this point can be an accumulation point for the eigenvalues for instance if the impurity potential is $Q(x)=|x|^{-1}$. In our case critical energies can be embedded in the bands which form the continuous spectrum of $H_B=-\Delta+V$, and we prove that these points can be also accumulation points for the eigenvalues but now this phenomena originates more from the band structure than from the nature of the potential. As eigenvalues or

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1 Scattering of electrons by foreign atoms, phonons by mass defects or spin waves by magnetic defects can be studied simultaneously with slight modifications (see Callaway [18]).

2 Let V be the periodic potential: $V(\boldsymbol{x}+\boldsymbol{R})=V(\boldsymbol{x})$ if $\boldsymbol{R}\in\mathbb{L}\sim\mathbb{Z}^3$ and suppose $\int_{\mathbb{R}^3/\mathbb{L}} |V(\boldsymbol{x})|^2 d^3x<+\infty$. Call $\mathbb{L}^\perp=\{\boldsymbol{K}\in\mathbb{R}^3 | \boldsymbol{K}\cdot\boldsymbol{R}=2\pi n,\ \forall\boldsymbol{R}\in\mathbb{L}\}$, the reciprocical lattice and $\mathbb{B}=\mathbb{R}^3/\mathbb{L}^\perp$ the Brillouin zone; $H_B=\Delta+V$ can be decomposed in a direct integral $\int_B^\oplus H_B(k)d^3k$; $H_B(k)$ acts on ℓ^2; it is proven in [14] that the spectrum of $H_B(k)$ is discrete and the set of eigenvalues is noted $\{E_1(k), E_2(k), \ldots, E_n(k), \ldots\}$ and the n^{th} eigenvector: $\{c_n^{\boldsymbol{K}}(k)\}\in\ell^2$. The critical points of $E_n(k)$ are the $k\in\mathbb{B}$ such that $\nabla E_n(k)=0$, the values of E_n at these points are the critical energies.