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The one Particle Theory of Periodic Point Interactions

Polymers, Monomolecular Layers, and Crystals

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Abstract. We solve explicitly and without approximation the problem of a quantum-mechanical particle in R^3 subjected to point interactions that are periodic in R^3 with periodicity of the type Z, Z^2, and Z^3. In the first case we get a model of an infinite straight polymer, in the second case we get a model of a monomolecular layer and in the third case we get a model of a crystal. In all three cases the unit cell of the Bravais lattice is allowed to contain any finite number of interaction sites (atomes), placed arbitrarily and with arbitrary interaction strength. In the case: one interaction site per unit cell we find explicit formulas for the resonance bands and energy bands and their corresponding wavefunctions.

Introduction

The one-electron theory of solids is based on the study of a Schrödinger particle in a periodic potential. This theory contains a large body of results that are obtained by perturbation methods or by symmetry arguments. However, it has not been possible up to now to check the perturbation results, which are necessarily only approximate, against an explicitly solvable three-dimensional model.

A class of non-separable two- and three-dimensional generalization of the Kronig-Penney model [1] has been solved in a recent paper by Sutherland [2]. The interactions in [2] are, however carried by lines (in two dimensions) or by planes (in three dimensions) which do not have a direct physical interpretation.

However it has been known for quite a while that there exists a Schrödinger operator with a point interaction in three dimensions. These operators and relatives of them have a history going back several decades. Their study started with Breit, Thomas, Wigner, and others as a model in nuclear physics for potential with short range interactions [3]. They observed that potential scattering converges in the low energy limit to scattering from a point interaction. In the late fifties, Huang, Yang, Lee, Luttinger, and Wu studied multiparticle operators with point interactions in low order perturbation theory [4].

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