Semi-Classical Asymptotics in Solid State Physics

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Abstract. This article studies the Schrödinger equation for an electron in a lattice of ions with an external magnetic field. In a suitable physical scaling the ionic potential becomes rapidly oscillating, and one can build asymptotic solutions for the limit of zero magnetic field by multiple scale methods from "homogenization." For the time-dependent Schrödinger equation this construction yields wave packets which follow the trajectories of the "semi-classical model." For the time-independent equation one gets asymptotic eigenfunctions (or "quasimodes") for the energy levels predicted by Onsager's relation.

This article initiates a study of an approximation widely used in the quantum theory of solids. When one ignores interactions between electrons in a crystal, one is quickly led to consider the one-body Hamiltonian governing the motion of a single electron through a lattice of ions in the presence of external electric and magnetic fields. If the external fields are effectively constant in space and one is interested in wave packets which are large relative to the lattice spacing, a simplified theory for the motion of the packets, known as "the semi-classical model," has been in use since the 1930's. In particular, for the case of an external magnetic field with vector potential A(x), R. Peierls [13] concluded that suitably prepared packets would follow the orbits of the classical Hamiltonian

$$H(x, p) = E_n(p + A(x)),$$

where $E_n(k)$ is an energy band function for the (Bloch) spectrum of the problem without the external field. Through the years there have been a number of efforts to justify this approximation and/or exhibit solutions of the Schrödinger equation with this behavior (Kohn [10], Chambers [3], Zak [14]). However, to the best of our knowledge there has not been a study using multiple-scale techniques as in homogenization. We feel that this approach simplifies the justification of the model considerably. It also makes it possible to refine the model and extend it.

In this paper we only consider problems with external magnetic fields. After discussing the physically relevant scaling of the equations, we begin by constructing