Electrical Effects of Crystal-dislocations in the Presence of High Magnetic Fields

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Abstract

In this paper the scattering rate, S(k, k'), due to lattice dislocation defects is found for carriers moving in a crystal in the presence of a magnetic field. The lattice dislocation is modeled as a 1D line charge and Fermi's Golden Rule (FGR), a basic result of scattering theory, is used to determine the scattering rate. From this rate the associated scattering time and ramifications for carrier mobility are shown.

1 Introduction

Magnetic fields have long since been used as a probing agent to extract information on the electronic properties of metals, semimetals and semiconductors [1][2]. This is due to the consequential change in the Fermi surface of the material and subsequently the density of states (DOS) by the influence of the magnetic field. The presence of the field introduces a force (Lorentz) on the flow of electrons in the material that cannot be described by only the kinetic energy operator in the Hamiltonian of the system. To handle this force another term must be appended to the kinetic energy in the Hamiltonian. This additional term is the magnetic vector potential (A) and despite its functional form must always preserve the real magnetic field the system actually 'sees'. The total Hamiltonian takes the form:

$$H = \frac{1}{2m*}[-i\hbar\nabla + qA(r)]^2$$

Upon choosing an appropriate function for A, the most popular of which is the Landau gauge, the Hamiltonian is applied to the wave equation. It is easily shown that in the presence of a magnetic field the system becomes oscillatory with a frequency given by the classical cyclotron frequency $\omega = eB/m^*$ where m* is the effective mass of the material system. The electrons of the system are thus confined to orbits prescribed by 1/B dependence in the plane perpendicular to the magnetic field direction. This result has paramount consequences and is the reason that the energy in the system deviates from its regular continuity and acquiesces into quantized levels, commonly named Landau levels. These Landau levels are the result of the DOS becoming quasi-periodic under the influence of the magnetic field. Orbital confinement in a magnetic field manifests itself in several measurable phenomena. The de Haas van Alphen effect is the oscillation of magnetic susceptibility of a material and is a direct result of the periodic DOS. Possibly the most popular magneto transport measurement is the Shubnikov-de Haas effect where oscillations in resistivity occur due to the periodic nature of the DOS in a magnetic field and has been a crucial tool in measuring carrier-density in materials. However, this simple picture of the system is incomplete without considering interactions of the orbiting electrons with other disturbing forces. While ionized impurities and phonon scattering in the presence of magnetic fields have been analyzed in detail, it is to our knowledge that dislocation scattering has not [3-8]. In this letter we present theoretical analysis of dislocation scattering in the presence of a magnetic field and its measurable effects using a semi-classical approach.

2 Theory

For the purposes of this calculation the simplest type of 1D defect, a linear lattice dislocation, is used. Modeling the dislocation as an infinite line charge of charge density λ allows for a simple electrostatic approach to be used to determine the scattering potential, U_s, which becomes part of the modified Hamiltonian. From classic electrostatics, the electric field from an infinitely long line charge of charge density is given by:

$$E = \frac{1}{4\pi\varepsilon}\frac{2\lambda}{r}$$

Integrating to obtain the potential and multiplying by the elementary unit charge q gives:

$$U_s = \frac{\lambda}{2\pi\varepsilon} ln(r)$$

This result is called the scattering potential and is added to the existing Hamiltonian.

$$H = \frac{1}{2m*}[-\hbar\nabla + qA(r)]^2 + \frac{\lambda}{2\pi\varepsilon} ln(r)$$

Considering the Schrodinger equation for our system we note that our eigenvector wave function remains the same as in the simpler case of the free electron in a magnetic field with the absence of the dislocation potential, and takes the form[9]:

$$\Psi(x,y,z) = e^{[i(k_y y + k_z z)]}\phi(x)$$

An underlying principle of perturbation theory states that if the perturbing potential is much smaller than the potentials contained in the kinetic terms the change in the wave function is miniscule and can be approximated to the original wave function without any loss in accuracy. This wave function can now be used to calculate our scattering rate through FGR. Once the scattering rate, S(k,k), has been evaluated using FGR, the relaxation time associated with the specific crystal defect under study can be calculated by summing the scattering rate over all unoccupied momentum states. This relaxation time, which can also be thought of as the time a carrier spends between collisions, can be used to calculate the component of mobility associated with this defect.

3 References

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