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

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(Dated: December 14, 2006)

The scattering transition rate, S(k,k'), due to 1D lattice dislocation defects is found for carriers moving in a crystal in the presence of a magnetic field. The 1D lattice dislocation is modeled as an infinite 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.

PACS numbers:

I. INTRODUCTION

Magnetic field have long been used as a probing agent to extract information on the electronic properties of metals, semimetals and semiconductors [1][2]. Magnetic fiels cause a change in the Fermi surface of the material and subsequently the density of states (DOS). In addition, the presence of the field introduces a force (Lorentz) on the flow of electrons in the material that can not be described by the conventional Hamiltonian of the system. To include this force another term must be appended to the kinetic energy term in the Hamiltonian. This additional term is the magnetic vector potential (A) and despite it's 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 ω = eB/m* where m* is the effective mass in the material system. The electrons of the system are thus confined to orbits prescribed by a 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 acquiesces from its regular continuity into quantized levels, commonly named Landau levels. These Landau levels are a 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 directly resulting from the periodic DOS. Possibly the most popular magneto-transport measurement and a crucial tool in measuring carrier-density in materials is the Shubnikov-de Haas effect in which oscillations in resistivity occur due to the periodic nature of the DOS in a magnetic field . 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 semiclassical approach.

II. 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:

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

This potential is added to the existing Hamiltonian.

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

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.

The matrix element of the scattering potential is the mathematical vehicle that must be employed in order to formulate the dislocation scattering rate. Including the wave vector and scattering potential the expanded integral for the matrix element takes the form

$$H_{k,k'} = \frac{A_n A_m}{4\pi\epsilon L_z L_y} \iint_{L_x L_y L_z} e^{i(k_z - k'_z)z} e^{i(k_y - k'_y)y} H_m H_n ln(\frac{x^2 + y^2}{L_D^2}) dz dy dx$$

where the integral is bound by the physical dimensions of the 3D crystal and our scattering potential has been normalized to the Debye length of the specific material system and our magnetic confinement in x has been normalized to the magnetic length [10]. This can first be reduced by performing the z-integration.

$$\int_0^{L_z} e^{i\delta k_z z} dz = \frac{L_z e^{i\pi(n_z - n'_z)}}{\pi(n_z - n'_z)} \sin(\pi(n_z - n'_z))$$

Where we can then make the common argument that in the limit of increasingly small changes in scattering transitions our integral solution in z becomes a kroneker-delta function with strength of our crystal dimension in z

$$L_z \lim_{n \to 0} e^{i\pi(n_z - n'_z)} \frac{\sin(\pi(n_z - n'_z))}{\pi(n_z - n'_z)} = L_z \delta_{k_z k'_z}$$

The natural log couples the x and y integral so that they cannot be done independently but rather the solution of one contributes to the solution of the other. So choosing the y-integral first we find it is merely the Fourier transform of the natural log.

$$\int_0^{L_y} e^{i\Delta_y y} ln(\frac{x^2 + y^2}{L_D^2}) dy = L_D \mathcal{F}\{ln(\frac{x^2 + y^2}{L_D^2})\}$$

$$= \frac{L_y}{2\pi^2 \Delta n_y} e^{-\Delta k_y x}$$

As expected this function is x-dependent and will contribute to the x-integral performed next. By including the solution in y into the x-integral and completing the square inside the power of the exponential, our integral takes on the following form

$$\int_0^{L_x} H_m H_n e^{-(\frac{x}{l_B} + \frac{\Delta k_y l_B}{2})^2} dx$$

However, note the shift in the Gaussian term confuses the simple integration in x. Recalling the property of Hermite polynomials that they are always all even or all odd and the multiplication of Hermite polynomials still retains the purely even/odd nature. For the integration in x, a change of variables is used so that the Gaussian term can more easily be handled. With this change of variables the product of the Hermite polynomials no longer stays purely even or odd but now contains cross terms and so includes all powers of the new variable up to the highest power available. This new integral takes the form

$$\sum_{p=0}^{m+n} a_p \int_0^{L_x} u^p e^{-u^2} du = \frac{1}{2} \sum_{p=0}^{m+n} a_p \Gamma[\frac{p+1}{2}]$$

The sum counts all powers up to the sum of highest powers of the polynomials. The coefficients a_p are the products of corresponding Hermite polynomial coefficients. Putting everything back together and after some algebraic simplification the solution to the matrix element can be given as

$$H_{k'k} = \frac{A_m A_n l_B}{8\pi^2 \epsilon} \delta_{k_z k'_z} \frac{e^{(\frac{\Delta k_y l_B}{2})^2}}{L_y \Delta k_y} \sum_{p=0}^{m+n} a_p \Gamma[\frac{p+1}{2}]$$

The scattering rate is then

$$S(k, k') = \frac{1}{32\pi^3 \hbar} (\frac{A_m A_n l_B}{\epsilon} \delta_{k_z k'_z})^2 \frac{e^{2(\frac{\Delta k_y l_B}{2})^2}}{(L_y \Delta k_y)^2}$$

$$\times \Bigl(\sum_{p=0}^{m+n} a_p \Gamma[\frac{p+1}{2}] \Bigr)^2 \delta(E(k') - E(k))$$

Then considering the integral form of the dislocation scattering time

$$\frac{1}{\tau_{DS}} = \frac{\hbar}{32\pi^3} \Bigl(\frac{A_m A_n l_B}{\epsilon L_y} \delta_{k_z k'_z} \sum_{p=0}^{m+n} a_p \Gamma[\frac{p+1}{2}] \Bigr)^2$$

$$\times (1 - \frac{|p'|}{|p|} \cos\theta \cos\gamma) \int_0^{\infty} (\frac{1}{p - p'})^2 e^{2(\frac{\Delta k_y l_B}{2})^2} \delta(\frac{p'^2}{2m*} - \frac{p^2}{2m*}) dp'$$

Then after performing the integration over all scattered states the closed form solution of the scattering time is given as

$$\frac{1}{\tau_{DS}} = \frac{\hbar}{64\pi^3} \left(\frac{A_m A_n l_B}{\epsilon \hbar L_y} \delta_{k_z k'_z} \sum_{p=0}^{m+n} a_p \Gamma[\frac{p+1}{2}] \right)^2 \frac{m*}{k_y} e^{2(k_y l_B)^2} (1 + \cos\theta \cos\gamma)$$

III. DISCUSSION

The scattering rate is the combination of interactions between the orbiting electrons, the charged dislocation and the magnetic field so it is expected to find three differing parts in the scattering rates final form corresponding to its 3D nature. The kroneker-delta function in k_z space indicates the prohibitive nature of scattering in z. This is not surprising as the uniform magnetic field was chosen to point in the z-direction and parallel to the dislocation. Scattering in the confined x-direction appears as the sum over Γ-functions with weighting coefficients a_p. The confined y-direction shows up in the scattering rate by the gaussian in k_y space. This is indicative of scattering in y with a higher probability in scattering for states closer in energy. The $\cos\theta \cos\gamma$ term accounts for the fact that there is confinement in the x and y directions only. Because of this all scattered states must be projected on the x-y plane. θ is the angle between scattered states and γ is the angle between the plane formed by the incident and scattered wave vectors and the x-y plane. The advantage of having such a closed form solution to dislocation scattering in the presence of a magnetic field is that it is now feasible to calculate and extract such transport characteristics as the magnetic mobility component and subsequently the magneto-resistivity with the presence of dislocations in the crystal sample.

IV. CONCLUSION

The scattering transition rate due to a 1D lattice dislocation was found in the presence of a magnetic field and from this a transition time due to scattering was found. It was seen, in the coordinate system defined here, that scattering to different momentum states was forbidden in z. Scattering involving momentum states follows a gaussian relationship in y and a gamma function relationship in x.

V. REFERENCES

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Acknowledgments

The authors would like to express their gratitude to Dr. Debdeep Jena for necessary and helpful discussion.