Phonon limited mobility in 3D Dirac semimetal Cd$_3$As$_2$

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Abstract. We report the numerical calculations of phonon limited electron mobility, $\mu$ in Cd$_3$As$_2$ three dimensional Dirac semimetal using Boltzmann transport theory over a temperature range 20$<$T$<$300 K. By employing the Ritz iteration technique, we have directly solved the 3D linearized Boltzmann transport equation to obtain the first order perturbation distribution function $\Phi^{-1}(E_k)$ as a function of electron energy $E_k$ and hence the mobility, $\mu$. we have considered electrons scattering by acoustic phonons via deformation potential scattering and polar optical phonons. The $\mu$ due to the latter is dominating the former for T$>$80 K, for electron concentration $n_e = 1\times10^{18}$ cm$^{-3}$. This crossover shifts to lower T, with decreasing $n_e$. The calculations are qualitatively agreeing with the experimental results.

Keywords: Electron-phonon interaction, electron mobility, iteration technique, Cd$_3$As$_2$.

1. Introduction

Recently, an exotic class of quantum materials known as Weyl and 3D Dirac semimetals (3DDS) system has been theoretically predicted. These material exhibits a linear energy dispersion relation, quantum Hall effect, Klein tunneling and various other phenomenon which are analogous to graphene made it a most striking material for next-generation electronic devices.

Following these theoretical predictions, extensive experimental efforts have been put to discover the three-dimensional Dirac phase in the materials like Cd$_3$As$_2$ [1, 2], Na$_3$Bi [3] etc. ARPES experiments were carried out in these materials to observe Dirac nodes [4] and crystal symmetry [5, 6]. Besides these, inherent band gap and linear dispersion, the material found to be interesting from the point of view of vast technological applications particularly those related to high electron mobility [5], optical absorbance [7].

Of the available 3DDS materials, Cd$_3$As$_2$ has received primary attention because of its chemical stability. Lundgren et al [8], Das Sarma et al [9] have studied the electronic transport properties of 3DDS using semi classical Boltzmann transport theory and Kubo formalism to address the transport properties in both temperature gradient and magnetic field. Many experimental mobility results have been reported an ultrahigh mobility of $9 \times 10^{6}$ cm$^2$/Vs at 5 K by Liang et al [10], $1.9 \times 10^{5}$ cm$^2$/Vs at 2.6 K by Cao et al [11] and $1.34 \times 10^{4}$ cm$^2$/Vs by at 3 K by Zhang et al [12], with carrier concentration in the range between $10^{18}$-$10^{19}$ cm$^{-3}$ which is higher than that found in suspended graphene.

In this article, we investigate the acoustic and optical phonon contribution to the mobility in 3DDS by solving the semiclassical BTE by Ritz iterative method. We present the results of the relaxation rates of phonons and intern the calculations of mobility.
2. Theory

We consider the low energy 3D Dirac Fermions with the ground state wave function corresponding to state $k$ is given by $\psi_k = 1/(2V)^{1/2} \exp(i k \cdot r) \chi^*$ with a linear energy relation $E_k = \frac{\hbar v_F}{2} |k|$, where $V$ is the sample volume, $r = (x, y, z)$, $v_F$ is the Fermi velocity, $k$ is the 3D electron wave vector and $s = +1$ or $-1$ for electron or hole system. The density of states is given by $D(E_k) = (g E_k^2)/(2\pi^2 (\hbar v_F)^3)$ with $g = g_s g_d$, as the spin and valley degeneracy.

In the presence of an electric field $E$, the electron distribution function $f(k)$ deviates from its equilibrium value $f_0(E_k)$ and it is given by $f(k) = f_0(E_k) + f_1(E_k)$, where the deviation $f_1(E_k) = v_F k$. $E(-\partial f_0(E_k)/\partial E_k) \Phi(E_k)$, $v_F$ is the electron velocity and $\Phi(E_k)$ is the perturbation function to be found. Following Ziman [13], the equation for charge current density is given by $J = e^2 K_{11} E$ giving the electrical conductivity $\sigma = e^2 K_{11}$, where $K_{11} = (g/8\pi^3)|d^3 k| v_F k (-\partial f_0(E_k)/\partial E_k) \Phi(E_k)$. Mobility, $\mu$ is obtained by $\mu = \sigma n_e \epsilon$, where $n_e$ is the electron density.

In order to study the electron transport in 3DDS, Boltzmann transport equation (BTE) is employed to 3D Dirac fermions to determine $\Phi(E_k)$. Following Nag [14], it is found to be given by

$$1 = \sum_{k'} [1 - f_0(E_{k'}^c)]/[1 - f_0(E_k)] [\Phi(E_{k'}) - \cos \theta \Phi(E_{k'}')] S(k,k')$$

(1)

For the electron scattering by phonons, the 3D differential scattering rate $S(k, k')$ from initial state $k$ to the final state $k'$, is given by

$$S(k,k') = (2\pi \hbar)^2 \sum_q |M(q)|^2 \left[ N_q \delta(E_k - E_{k'} + \hbar \omega_q) + (N_q + 1) \delta(E_k - E_{k'} - \hbar \omega_q) \right] \theta(E_k - \hbar \omega_q)$$

(2)

Here $|M(q)|^2$ is the electron-phonon matrix element, $\hbar \omega_q$ is the phonon energy of wave vector $q$. We consider the electron momentum relaxation process due to acoustic phonons (AP), assumed to be quasi-elastic, and polar optical phonons (OP), assumed to be inelastic, $\theta(E_k - \hbar \omega_q)$ is the step function.

For quasi-elastic scattering (i.e. APs), $\Phi(E_k^{1+}(E_k) = 1/\tau(E_k)$ given by

$$1/\tau(E_k) = \sum_{k'} (1 - \cos \theta) S(k,k') [1 - f_0(E_{k'}^c)]/[1 - f_0(E_k)]$$

(3)

where $\theta$ is the angle between $k$ and $k'$, $S(k,k')$ is the probability of the transition from $k$ to $k'$, for acoustic deformation potential coupling [9].

The electron scattering by OPs is assumed to be due to Fröhlich interaction with a corresponding matrix element, $|M(q)|^2 = (2\pi \hbar \omega_q Vq^2)/(1/\epsilon_0 - 1/\epsilon_0 (1 + \cos \theta))$. Here, $\epsilon_0$ ($\epsilon_\infty$) is the static (optical) dielectric constant of the material with optical phonon energy $\hbar \omega_0$. Since scattering by OPs is inelastic, equation (1) is to be solved for $\Phi(E_k)$, without any approximation, by iteration technique. In order to do this Eq. (1) is expressed in the form of a difference equation coupling $\Phi(E_k)$ with $\Phi(E_k^{1+}\hbar \omega_0)$ [15, 16]

$$1 = S_0(E_k) \Phi(E_k) - S_a(E_k) [\Phi(E_k + \hbar \omega_0) - S_c(E_k) \Phi(E_k - \hbar \omega_0)]$$

(4)

where $S_0(E_k)$, the sum of in and out scattering contributions of quasi-elastic scattering process and out scattering contribution from OPs, and $S_a(E_k)$ and $S_c(E_k)$ denote the in scattering contributions from the inelastic scattering process due to OPs and these are given by
\[ S_0(E_k) = \frac{e^{-\omega_0}}{(h\nu_F)^3} \left( \frac{1}{e_g} - \frac{1}{e_0} \right) \left( 1 - f_0(E_k) \right) \{ (E_k + \hbar\omega_0) \}^{2} (1 - f_0(E_k + \hbar\omega_0))N_0 I_+(E_k) \]

\[ + (E_k - \hbar\omega_0)^2 (1 - f_0(E_k - \hbar\omega_0))(N_0 + 1) I_-(E_k) \theta(E_k - \hbar\omega_0) + \tau_{AP}^{-1}(E_k) \]  

(4a)

\[ S_\pm(E_k) = \frac{e^{\pm\omega_0}}{(h\nu_F)^3} \left( \frac{1}{e_g} - \frac{1}{e_0} \right) \left( 1 - f_0(E_k) \right) \{ (E_k + \hbar\omega_0) \}^{2} (1 - f_0(E_k + \hbar\omega_0))N_0 J_{\pm}(E_k) \]

(4b)

\[ S_\pm(E_k) = \frac{e^{\pm\omega_0}}{(h\nu_F)^3} \left( \frac{1}{e_g} - \frac{1}{e_0} \right) \left( 1 - f_0(E_k) \right) \times [(E_k - \hbar\omega_0)^2 (1 - f_0(E_k - \hbar\omega_0))(N_0 + 1) J_{\pm}(E_k) \theta(E_k - \hbar\omega_0)] \]

(4c)

where \( \tau_{AP}^{-1}(E_k) \) is the relaxation time due to the scattering of APs. \( I_+(E_k) \) and \( J_{\pm}(E_k) \) represent the angular dependence of the electron-phonon interactions and these are given by,

\[ I_\pm(E_k) = \frac{\pi}{\nu} \int (1 + \cos(\theta))/2 \sin(\theta) \{ q_\pm^2(E_k, \theta) \} d\theta \]  

(4d)

\[ J_\pm(E_k) = \frac{\pi}{\nu} \int (1 + \cos(\theta))/2 \sin(\theta) \{ q_\pm^2(E_k, \theta) \} \cos(\theta) d\theta \]  

(4e)

where \( q^2 \) is expressed as, \( q^2_\pm(E_k, \theta) = [(1/\nu_{F})^2(E_k^2 + (E_k \pm \hbar\omega_0)^2 - 2E_k(E_k \pm \hbar\omega_0)\cos(\theta))] \)

\[ \Phi^{m+1}(E_j + n\hbar\omega_0) = S_0^{-1}(E_j + n\hbar\omega_0)[1 + S_\pm(E_j + n\hbar\omega_0)F^{m}(E_j + (n + 1)\hbar\omega_0)] \]

\[ + S_\pm(E_j + n\hbar\omega_0)F^{m}(E_j + (n - 1)\hbar\omega_0) \]

(5)

Eq. (4) is solved for \( \Phi(E_k) \) by Ritz iteration method [16], which in turn is used to find \( \mu \) and \( \sigma \).

3. Results and discussions

Using the following material parameters: \( \rho = 7g/cm^3 \), \( \nu_{ph} = 2.3 \times 10^6 cm/s, \nu_{F} = 10^6 cm/s, D = 20eV, \hbar\omega_0 = 25meV, \varepsilon_0 = 36, \varepsilon_\infty = 12 \), we present the numerical calculation of \( \Phi^{1}(E_k) \) as a function of carrier energy \( E_k \) and electron mobility as a function of temperature limited by APs and OPs.

Fig. 1 Shows the first order perturbation distribution function \( \Phi^{1}(E_k) \) as a function of carrier energy \( E_k \) at 20 and 77 K for a carrier concentration \( n_c = 10^{19} cm^{-3} \) using equation (5). It is seen that the plots of the rates are for inelastic scattering of OPs and in combination with the quasi elastic acoustic phonon. We observe oscillatory bumps at an integral multiple of optical phonon energy \( \hbar\omega_0 \). The oscillatory bumps are well defined at low temperature and kinks disappear with an increase in the temperature which is in contrast to conventional 2DEG [16]. We can also observe a relative change in the position and number of kinks in the considered energy range with the change in carrier concentration which is similar to that observed in conventional 2DEG. Since optical phonon scattering found to dominate the rates at a higher temperature (\( T > 80 \) K). We also observe that the oscillations are found to show the saturation for lower carrier energies as the temperature increases. To see the effect of screening in the inset of fig. (1) we presents relaxation time as a function of electron energy at 20 and 77 K. The effect of screening found to reduce the relaxation time as expected.
Figure 1. Rates as a function of carrier energy.  Figure 2. Mobility as a function of temperature.

In fig. 2 the temperature (20<T<300 K) dependence of electron mobility is shown for electron concentration \(n_e=10^{18}\) cm\(^{-3}\). The curves depict the contribution of APs (dashed) and OPs (short dotted). For the temperature range considered, \(\mu\) due to APs is found to decreases linearly as \(T^{-1}\) in the equi partition regime. The overall mobility (solid line) is found to decrease with temperature and OPs found to dominate the mobility for \(T\) greater than 80 K. We also find that the effect of screening is weak and it enhances the acoustic phonon limited electron mobility by a factor 1.2 in EP regime as shown in the inset of fig. 2.

4. Conclusion
Here, we report theoretical calculations of relaxation time and phonon limited mobility in 3DDS using the semi-classical Boltzmann transport theory for temperature range 20<T<300 K. Mobility due to acoustic phonons is found to be \(\mu\sim T^9\) in BG and \(\mu\sim T^1\) in EP regimes. The Thomas-Fermi screening factor found to enhance the mobility.

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References
[1] Sangjun Jeon, Brian B Zhou, Andras Gyenis, Benjamin E Feldman, Itamar Kimchi, Andrew C Potter, Quinn D Gibson, Robert J Cava, Ashvin Vishwanath, Ali Yazdani, Nat. Mater. 13, 851–856 (2014).
[2] Sergey Borisenko, Quinn Gibson, Danil Evtushinsky, Volodymyr Zabolotnyy, Bernd Büchner, and Robert J. Cava, Phys. Rev. Lett. 113, 027603 (2014).
[3] Liu Z K, Zhou B, Zhang Y, Wang Z J, Weng H M, Prabhakaran D, Mo S K, Shen Z X, Fang Z, Dai X, Hussain Z, Chen Y L, Science 343, 864–867 (2014).
[4] Z K Liu , J Jiang, B Zhou, Z J Wang, Y Zhang, H M Weng, D Prabhakaran, S K Mo, H Peng, P Dudin, T Kim, M Hoesch, Z Fang, X Dai, Z X Shen, D L Feng, Z Hussain, Y L Chen, Nat. Mater. 13, 677–681 (2014).
[5] M Neupane, S Y Xu, R Sankar, N Alidoust, G. Bian, C. Liu, I. Belopolski, T. R. Chang, H. T. Jeng, H. Lin, A. Bansil, F. Chou, and M. Z. Hasan, Nat. Commun. 5, 3786 (2014).
[6] S Jeon, B B Zhou, A Gyenis, B E Feldman, I Kimchi, A C Potter, Q D Gibson, R J Cava,
[7] W Lu, S Ge, X Liu, H Lu, C Li, J Lai, C Zhao, Z Liao, S Jia, and D Sun, Phys. Rev. B 95, 024303 (2017).

[8] R Lundgren, P Laurell, and G A Fiete, Phys. Rev. B 90, 165115 (2014).

[9] S D Sarma, E H Hwang, and H Min, Phys. Rev. B 91, 035201 (2015).

[10] T Liang, Q Gibson, M N Ali, M Liu, R J Cava, and N P Ong, Nat. Mater. 14, 280 (2015).

[11] Cao J, S Liang, C Zhang, Y Liu, J Huang, Z Jin, Z G Chen, Z Wang, Q Wang, J Zhao, Nat. Comm. 6, 7779 (2015).

[12] C Zhang, T Zhou, S Liang, J Cao, X Yuan, Y Liu, Y Shen, Q Wang, J Zhao, Z Yang and F Xiu, Chin. Phys. B 25, 017202 (2015).

[13] J M Ziman, Principles of the Theory of Solids, Cambridge University Press, 2nd Ed.

[14] B R Nag, Electron transport in Compound Semiconductors, Springer, 2008.

[15] Basu P K and Nag B R, Phys. Rev. B 22 4849 (1980).

[16] T Kawamura and S Das Sarma, Phys. Rev. B 45, 3612 (1992).