Effects of Berry Curvature on Thermoelectric Transport of Bilayer Graphene and Other Materials

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I. INTRODUCTION

II. BERRY CURVATURE IN RECIPROCAL SPACE

III. EFFECTS OF BERRY CURVATURE

A. Modification of semiclassical equations

B. Decoupling of the equations of motion and their simplification

$$\dot{\mathbf{r}} = \frac{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{e}{\hbar}(\mathbf{E}\times\boldsymbol{\Omega}) + \frac{e}{\hbar^2}(\Omega\cdot\frac{\partial\varepsilon}{\partial\mathbf{k}})\mathbf{B}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\boldsymbol{\Omega}} \tag{1}$$

$$\dot{\mathbf{k}} = -\frac{\frac{e}{\hbar}\mathbf{E} + \frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\mathbf{k}}\times\mathbf{B} + \frac{e^2}{\hbar^2}(\mathbf{E}\cdot\mathbf{B})\Omega}{1+\frac{e}{\hbar}\mathbf{B}\cdot\boldsymbol{\Omega}} \tag{2}$$

In a 2D sample, Ω is along the z axis, while $\frac{\partial\varepsilon}{\partial\mathbf{k}}$ is in the xy plane, then $\Omega\cdot\frac{\partial\varepsilon}{\partial\mathbf{k}}=0$.
Also, if we take perpendicular electric and magnetic fields, then $\mathbf{E}\cdot\mathbf{B}=0$.
Then the equations simplify to,

$$\dot{\mathbf{r}} = \frac{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{e}{\hbar}(\mathbf{E}\times\boldsymbol{\Omega})}{1+\frac{e}{\hbar}\mathbf{B}\cdot\boldsymbol{\Omega}} \tag{3}$$

$$\dot{\mathbf{k}} = -\frac{\frac{e}{\hbar}\mathbf{E} + \frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\mathbf{k}}\times\mathbf{B}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\boldsymbol{\Omega}} \tag{4}$$

C. Violation of Liouville's theorem and Modification of phase space density

Derivation from the semiclassical equations of Motion

IV. STRATEGY OF CALCULATION OF THERMAL AND HEAT CURRENTS

A. Equilibrium and Non-Equilibrium distribution functions

V. BOLTZMANN TRANSPORT EQUATION AND ITS SOLUTION

Some discussions about the relaxation time approximation....
Under the relaxation time approximation, the Boltzmann Transport Equation (BTE) takes the form

$$\dot{\mathbf{k}}\cdot\frac{\partial}{\partial\mathbf{k}}(f+g) + \dot{\mathbf{r}}\cdot\frac{\partial}{\partial\mathbf{r}}(f+g) = -\frac{g}{\tau} \tag{5}$$

,
which can be cast into the form

$$\frac{g}{\tau} + \dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} g + \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} g = -\dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} f - \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} f \tag{6}$$

.
Here $f = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}+1}$ is the equilibrium Fermi distribution, and g is the non-equilibrium part. Using the decoupled equations of motion, right hand side of Eq. (V) simplifies to (*Need to show the steps*),

$$\frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \left[e\mathbf{E} + \nabla\mu + \nabla T \frac{\varepsilon-\mu}{T} \right]$$

.
When the fields are constant in space and time, we assume that $\frac{\partial g}{\partial \mathbf{r}} = 0$.

Validity of the assumption: When we solve the equation after discarding this term, we would find that (See Eq. (V A)) this term is second order in the applied fields. Then upto linear order, we can discard this term.

Then, the BTE becomes, $\frac{g}{\tau} - \frac{\frac{e}{\hbar}\mathbf{E} + \frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\mathbf{k}}\times\mathbf{B}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g = \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \left[e\mathbf{E} + \nabla\mu + \nabla T \frac{\varepsilon-\mu}{T} \right]$

A. Solution for $\mathbf{B} \neq 0$, $\mathbf{\Omega} \neq 0$, $\mathbf{E} \neq 0$, $\nabla\mu = \nabla T = 0$

In this limit, the equation becomes,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar}\mathbf{E} + \frac{e}{\hbar^2}\frac{\partial\varepsilon}{\partial\mathbf{k}}\times\mathbf{B}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g = \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot e\mathbf{E}$$

If we discard the term $\mathbf{E}\cdot\frac{\partial\varepsilon}{\partial\mathbf{k}}$ in the LHS, we would find that g is a linear function of $\mathbf{E}$. Then, $\mathbf{E}\cdot\frac{\partial\varepsilon}{\partial\mathbf{k}}$ would be quadratic in $\mathbf{E}$. This is why, we can discard this term. (This is not a circular argument. If we do this, everything remains self consistent upto linear order)

Then, the equation takes the form,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar^2}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{\partial\varepsilon}{\partial\mathbf{k}} \times \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{k}} g = \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot e\mathbf{E} \tag{7}$$

We solve this equation, treating the second term in LHS as a perturbation (See Appendix A). We write $g = g_0 + g_1$, such that $\frac{g_0}{\tau} = \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot e\mathbf{E}$, and $\frac{g_1}{\tau} - \frac{\frac{e}{\hbar^2}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{\partial\varepsilon}{\partial\mathbf{k}} \times \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{k}} g_0 = 0$. Then, g_1 is a linear function of $\mathbf{B}$, and it is justified to discard the term $\frac{\frac{e}{\hbar^2}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{\partial\varepsilon}{\partial\mathbf{k}} \times \mathbf{B} \cdot \frac{\partial}{\partial \mathbf{k}} g_1$, as it would be quadratic in $\mathbf{B}$

Then, $g_0 = \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{e\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{E}$. To find g_1, we need to calculate $\frac{\partial g_0}{\partial \mathbf{k}}$, i.e., the quantity $\frac{\partial}{\partial \mathbf{k}} \left[\frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{e\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{E} \right]$.

To calculate it, let us first calculate $\nabla\left[\phi\mathbf{A}\cdot\mathbf{C}\right]$, where ϕ is a scalar function, $\mathbf{A}$ is a vector function, and $\mathbf{C}$ is a constant vector.

$\nabla\left[\phi\mathbf{A}\cdot\mathbf{C}\right] = (\nabla\phi)(\mathbf{A}\cdot\mathbf{C}) + \phi(\mathbf{C}\cdot\nabla)A + \phi(\mathbf{C}\times(\nabla\times\mathbf{A}))$. In our calculation, $\phi \sim \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{e\tau}{\hbar}$, $\mathbf{A} \sim \frac{\partial\varepsilon}{\partial\mathbf{k}}$, and $\mathbf{C} \sim \mathbf{E}$.

Then,

$$\frac{\partial}{\partial \mathbf{k}} \left[\frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{e\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{E} \right] = \frac{\partial}{\partial \mathbf{k}} \left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \right] \frac{e\mathbf{E}}{\hbar} \cdot \frac{\partial\varepsilon}{\partial\mathbf{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \left[(\frac{e}{\hbar}\mathbf{E}\cdot\frac{\partial}{\partial\mathbf{k}})\frac{\partial\varepsilon}{\partial\mathbf{k}} + \frac{e}{\hbar}\mathbf{E}\times(\frac{\partial}{\partial\mathbf{k}}\times\frac{\partial\varepsilon}{\partial\mathbf{k}}) \right]$$

.
The last term is zero because it is the curl of a gradient, $\frac{\partial}{\partial\mathbf{k}}\times\frac{\partial\varepsilon}{\partial\mathbf{k}} = \nabla_{\mathbf{k}}\times(\nabla_{\mathbf{k}}\varepsilon) = 0$.

Finally,

$$g = \frac{\partial f}{\partial \varepsilon} \frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{\tau}{\hbar} \frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot e\mathbf{E} + \frac{\frac{e\tau}{\hbar^2}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \frac{\partial\varepsilon}{\partial\mathbf{k}} \cdot \mathbf{B} \times \left[\frac{\partial}{\partial \mathbf{k}} \left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \right] \frac{e\mathbf{E}}{\hbar} \cdot \frac{\partial\varepsilon}{\partial\mathbf{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \left[(\frac{e}{\hbar}\mathbf{E}\cdot\frac{\partial}{\partial\mathbf{k}})\frac{\partial\varepsilon}{\partial\mathbf{k}} \right] \right] \tag{8}$$

Verification: When $\Omega = 0$, and $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$, this term produces $\sigma_{xy} = -\omega_c\tau\frac{ne^2\tau}{m^*}$. (*Need to show the steps*)

B. Solution for $\mathbf{B} \neq 0$, $\mathbf{\Omega} \neq 0$, $\mathbf{E} \neq 0$, $\nabla\mu \neq 0$, $\nabla T \neq 0$

Here

$$\dot{\mathbf{r}} = \frac{\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}}}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \tag{9}$$

$$\dot{\mathbf{k}} = -\frac{\frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \mathbf{k}} \times \mathbf{B}}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \tag{10}$$

We again take $\frac{\partial g}{\partial \mathbf{k}} \sim 0$.
Under these circumstances, the equation becomes,

$$\frac{g}{\tau} - \frac{\frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \mathbf{k}} \times \mathbf{B}}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \left[\nabla\mu + \nabla T\frac{\varepsilon - \mu}{T}\right]$$

Let $g = g_0 + g_1$, with $g_0 = \frac{\partial f}{\partial \varepsilon}\frac{1}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \left[\nabla\mu + \nabla T\frac{\varepsilon-\mu}{T}\right]$ and $\frac{g_1}{\tau} - \frac{\frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \mathbf{k}}\times\mathbf{B}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g_0 = 0$
Then, *(Need to show the steps)*

$$\frac{\partial g_0}{\partial \mathbf{k}} = \frac{\partial}{\partial \mathbf{k}}\left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\right]\frac{\nabla\mu + \frac{\varepsilon-\mu}{T}}{\hbar} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\left[(\frac{\nabla\mu + \frac{\varepsilon-\mu}{T}}{\hbar} \cdot \frac{\partial}{\partial \mathbf{k}})\frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{1}{\hbar}(\nabla\mu + \frac{\varepsilon - \mu}{T}) \times \underbrace{(\frac{\partial}{\partial \mathbf{k}} \times \frac{\partial \varepsilon}{\partial \mathbf{k}})}_{0}\right]$$

$$+\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\left[\frac{1}{\hbar}(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}})(\frac{\varepsilon\nabla T}{T}) + \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\partial}{\partial \mathbf{k}} \times \left(\frac{\varepsilon\nabla T}{T}\right)\right)\right]$$

The term inside the final third bracket can be further simplified.

$$(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}})(\frac{\varepsilon\nabla T}{T}) + \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\partial}{\partial \mathbf{k}} \times \left(\frac{\varepsilon\nabla T}{T}\right)\right) = (\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}})(\frac{\nabla T}{T}) + \frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \times \left(\frac{\nabla T}{T}\right)\right)$$

$$= (\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}})(\frac{\nabla T}{T}) + \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\nabla T}{T}\right)\frac{\partial \varepsilon}{\partial \mathbf{k}} - (\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}})(\frac{\nabla T}{T})$$

$$= \left(\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \frac{\nabla T}{T}\right)\frac{\partial \varepsilon}{\partial \mathbf{k}}$$

.
When we calculate $g_1 = \tau\frac{\frac{e}{\hbar^2}\frac{\partial \varepsilon}{\partial \mathbf{k}}\times\mathbf{B}}{1+\frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}} \cdot \frac{\partial}{\partial \mathbf{k}} g_0$, this term cancels because $\frac{\partial \varepsilon}{\partial \mathbf{k}} \times \mathbf{B}\frac{\partial \varepsilon}{\partial \mathbf{k}} = 0$.
Finally we get,

$$g = \frac{\partial f}{\partial \varepsilon}\frac{1}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\frac{\tau}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{S} + \frac{\frac{e\tau}{\hbar^2}}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\frac{\partial \varepsilon}{\partial \mathbf{k}} \cdot \mathbf{B} \times \left[\frac{\partial}{\partial \mathbf{k}}\left[\frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\right]\frac{\mathbf{S}}{\hbar} \cdot \frac{\partial \varepsilon}{\partial \mathbf{k}} + \frac{\frac{\partial f}{\partial \varepsilon}\tau}{1 + \frac{e}{\hbar}\mathbf{B}\cdot\mathbf{\Omega}}\left[(\frac{1}{\hbar}\mathbf{S} \cdot \frac{\partial}{\partial \mathbf{k}})\frac{\partial \varepsilon}{\partial \mathbf{k}}\right]\right] \tag{11}$$

with $\mathbf{S} = \nabla\mu + \frac{\varepsilon-\mu}{T}$.
Einstein and Onsager relations are perfectly valid.

VI. EINSTEIN AND ONSAGER RELATIONS

Their apparent violations (when $\Omega \neq 0$) and the resolution with magnetization currents.

VII. CHERN NUMBER IN DIFFERENT MODELS

A. Monolayer and Bilayer Graphene

B. Selective Valley Population

C. Valley Chern Number

D. Calculation of Effective Hamiltonian and its Chern Number

Appendix A: Validity of this perturbation theory

Classically, $\dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} g \sim \dot{\mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{p}} g \sim e(\mathbf{v} \times B) \cdot \frac{\partial}{m \partial \mathbf{v}} g \sim \boldsymbol{\omega} \times \mathbf{v} \cdot \frac{\partial g}{\partial \mathbf{v}} \sim \omega g$.
When $\omega << \frac{1}{\tau}$, it is justified to treat ωg as a perturbation over $\frac{g}{\tau}$, in the LHS of Eq. (V).