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Thermal Coulomb Drag in a Bi-Layer Semiconductor System

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THERMAL COULOMB DRAG IN A BI-LAYER SEMICONDUCTOR SYSTEM

A Thesis
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Master of Science
Physics

by
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Accepted by:
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Abstract

In this work, we investigate the existence of a thermoelectric effect that consists of the appearance of an electric field in one layer when a temperature gradient is applied in the other layer of a double quantum well system. This represents a generalization of the Seebeck effect to the case of two spatially separated electron systems allowed to interact only through the Coulomb repulsion. The induced electric field results from the momentum transfer between the electrons driven out of equilibrium by the temperature gradient and the electrons at rest in the passive layer, a mechanism known in the literature as the Coulomb drag. The rate of momentum transfer is calculated from the Fermi's golden rule applied to a screened Coulomb interaction. The electric field is found to be parallel to and proportional with the temperature gradient. The magnitude of the proportionality constant, an effective Seebeck coefficient, is estimated from the solutions of the Boltzmann transport equation in the two layers. Our result indicates a linear temperature variation, characteristic to degenerate Fermi systems, while the dependence on the distance between the layers introduces the geometric characteristics of the problem.

Dedication

To my mother, with whom everything started.

Acknowledgments

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Chapter 1

Introduction

The experimental evidence that supports the interdependence of electric and thermal transport in solid systems dates back to the first half of the 19th century. First, in 1823, Seebeck observed the existence of an electric current in a closed circuit in a circuit formed from two different metals whose junctions were kept at different temperatures. If T_0 and T_1 are the temperatures of the two junctions, and $\Delta T = T_1 - T_0$, the potential difference measured in the system is given by

$$V = (\alpha_A - \alpha_B)\Delta T, \quad (1.1)$$

where α is a material dependent constant, called the Seebeck coefficient.

Conversely, in the Peltier effect, discovered in 1834, it was observed that heat is released or absorbed at the junction of two different metals when a current flows through it [1]. The Peltier effect is described by the proportionality law

$$\vec{j}_Q = \Pi \vec{j}, \quad (1.2)$$

between the heat current \vec{j}_Q and the electric current \vec{j} in the circuit, Π being the Peltier coefficient. As it can be seen, $\Pi > 0$ means that the junction acts as a heater, while $\Pi < 0$ means that the junction acts as a cooler.

When both an electric current and a temperature gradient are present in an homogeneous

metal, heat exchange was observed in the Thomson effect, reported in 1857 [2]. The rate of heat production was experimentally found to be proportional to the electric current and temperature gradient:

$$\frac{dQ}{dt} = \tau \vec{j} \cdot \nabla T ; \quad (1.3)$$

where τ is the Thomson coefficient.

Finally, the Joule effect is the irreversible heating caused by the passing of an electric current through an element of circuit. The rate of heat dissipation is:

$$\frac{dQ}{dt} = \vec{j} \cdot \vec{E} = \rho j^2 ; \quad (1.4)$$

where ρ is the resistivity of the material.

Thermodynamic considerations can be used to argue that in the presence of an electric field and a temperature gradient, in general, one expects simultaneous electric and energy currents. The Onsager equations for this case can be written as:

$$\begin{aligned} \vec{j} &= L_{EE} \vec{E} + L_{ET} \nabla T \\ \vec{j}_Q &= L_{TE} \vec{E} + L_{TT} \nabla T ; \end{aligned} \quad (1.5)$$

where the coefficients L 's cannot be determined independently from phenomenological considerations.

While a microscopic picture of these elementary thermoelectric phenomena in normal metals emerged at the beginning of the 20th century, when a statistical, quantum mechanical picture of the electron system was developed, the interdependence of electric and energy transport in solid structures has been a continuous subject of interest ever since. In Chapter 2 we discuss the details of the electron transport theory that ultimately explains the phenomenology of the thermoelectric effects and produces quantitative values for the coefficients L 's in Eqs. (1.5).

Efforts to channel the thermoelectric effects into practical applications paralleled the theoretical understanding and have focused on electric cooling/heating or the conversion of thermal energy into electric energy. Increasing the efficiency of this transfer in solid-state devices motivates the effort of finding materials that function as good conductors whose energy loss through heat transport are reduced. Since obtaining such performance in homogeneous systems has serious limi-

tations imposed by the very nature of the crystal structure, lately a lot of attention has been focused on heterogeneous, artificially created structures where the design takes advantage of both material properties and geometric characteristics to enhance the favorable behavior. This type of research involves mostly semiconductor heterostructures because of the extensive possibilities of adjusting the electric properties in the growth process. Moreover, using these materials allow for creative usage of the space dimensionality. Reducing the dimensionality to two directions, as in the case of quantum wells, or to one, as in the case of quantum dots, has been demonstrated to be a very successful way of improving the efficiency of thermoelectric devices [3, 4, 5]. These results are accomplished by increasing the density of states leading to an excellent electric conductivity, while reducing their thermal conductivity through phonon confinement.

As the dimensionality of the electron system involved in thermoelectric transport is reduced, clearly the role of the interaction is enhanced. Since the distance between the electrons decreases, the Coulomb repulsion becomes as important as the kinetic energy of the electrons and interaction induced effects determine more pronounced deviations of the response functions from the free electron model. Additionally, utilizing layered structures in thermoelectric applications puts understanding such effects to a prime position.

In the present work we study an interaction-induced thermoelectric effect that utilizes the Coulomb scattering to connect the presence of a temperature gradient to an electric field. The system of interest is a double quantum well whose layers are spatially separated by a distance d , large enough to inhibit tunneling, but small enough to allow for a strong inter-layer interaction. We demonstrate that an applied temperature gradient in one of the quantum wells is able to induce an electric field in the other well. The microscopic mechanism that underlies this process is quite well known. It is none other than the Coulomb interaction mediated scattering, by which electrons driven out of equilibrium by the temperature gradient impart some of their momentum to the electrons in the passive layer. The net rate of momentum transfer is equivalent, according to the second law of dynamics to a total force being applied, or equivalently to an electric field. The theoretical treatment of this problem follows closely the approach outlined in the case of an electric perturbation. Known as the electric Coulomb drag, the phenomenon by which an electric field in one layer induces an electric field in the other layer was observed experimentally in various set-ups in the early 1980s. In Chapter 3 we review the salient points of the electric Coulomb drag theory and establish the general framework under which we develop the analysis of the thermally induced Coulomb drag in Chapter

4.

In a simple outline, the computational algorithm consists of solving the Boltzmann transport equation (BTE) in both layers. Given that the perturbation is applied in only one layer, the two solutions are matched through the scattering component that is estimated starting from microscopic principles. Our results indicate that the induced electric field is parallel to and proportional with the temperature gradient. The coefficient of proportionality represents essentially a generalization of the Seebeck coefficient and exhibits the same temperature dependence. Its magnitude reflects the spatial separation of the two layers and the effects of the Coulomb screening.

Chapter 2

Thermoelectric Transport in Two-Dimensional Fermi Liquids

The mathematical description of the thermoelectric phenomena is closely related to the fundamental equation that describes the electron transport in degenerate Fermi systems, such as metals and semiconductors. The Boltzmann transport equation (BTE) results from a semi-classical approximation that allows the treatment of electrons as classical objects moving in the phase space under the action of classical perturbations, such as forces and temperature gradients, whose momentum and position are simultaneously determined. At the same time, however, the state and energy of the electrons are calculated quantum mechanically.

In the following considerations, we refer to a two dimensional electron system, in thermodynamic equilibrium at temperature T . The particle density is fixed at n . The electric neutrality is assured by the background of fixed positive ions in the crystalline lattice. The electrons are free quantum particles of momentum \vec{k} and spin σ . The momentum is quantized when periodic boundary conditions are considered. Their mass m is the effective band mass, given by the interactions in the crystal. In a two dimensional system of area A , the state function is:

$$\psi_{\vec{k}} = \frac{1}{\sqrt{A}} e^{i\vec{k}\cdot\vec{r}}. \quad (2.1)$$

At $T = 0$, in the momentum space, the electron states, which are spin degenerate, are ordered by

increasing energy, $\epsilon_k = \frac{\hbar^2 k^2}{2m}$ inside a Fermi sphere whose radius, k_F is related to the particle density:

$$k_F = \sqrt{2\pi n} . \quad (2.2)$$

The corresponding energy is called the Fermi level or chemical potential, μ . At a finite temperature T , the statistical distribution of the electrons in the Fermi sphere is:

$$f_k^0 = \frac{1}{e^{\frac{\epsilon_k - \mu}{k_B T}} + 1} . \quad (2.3)$$

When a perturbation is applied, the distribution function becomes a function of position, momentum and time, $f = f(\vec{r}, \vec{k}, t)$. The Boltzmann transport equation represents the conservation of the number of particles in a volume of phase space:

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = \left. \frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} \right|_{coll} ; \quad (2.4)$$

by expressing the fact that the total change of the distribution function results only from scattering events that take the particles outside the considered volume.

The left-hand side of this equation is obtained by expanding the total derivative of f with respect to time, generating the drift terms:

$$\frac{df(\vec{r}, \vec{k}, t)}{dt} = \frac{\partial f}{\partial t} + \dot{\vec{r}} \nabla_{\vec{r}} f + \dot{\vec{k}} \nabla_{\vec{k}} f . \quad (2.5)$$

We identify $\dot{\vec{r}} = \vec{v}_k$ as the electron velocity, while $\dot{\vec{k}} = \frac{\vec{F}}{\hbar}$ expresses the second law of dynamics, whereby the time variation of the momentum is equal to the applied force, \vec{F} . Here, we consider that the force is produced only by an electric field, $\vec{F} = -e\vec{E}$ ([6], p.95-99). The explicit time dependence, $\frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t}$, is equal to zero in the stationary case.

The collision term in Eq. (2.4) is computed by considering the statistical probability of scattering events that modify the distribution function $f_{\vec{k}}$, associated with a certain momentum \vec{k} , by taking an electron from the state of momentum \vec{k} into a state of momentum \vec{k}' . In general, one can write:

$$\left(\frac{\partial f_{\vec{k}}}{\partial t} \right)_{coll.} = - \sum_{\vec{k}'} \mathcal{P}(\vec{k}, \vec{k}') [f_{\vec{k}}(1 - f_{\vec{k}'}) - f_{\vec{k}'}(1 - f_{\vec{k}})] ; \quad (2.6)$$

where $\mathcal{P}(\vec{k}, \vec{k}')$ represents the quantum mechanical probability of occurrence of the scattering. Eq. (2.6) explicitly considers the statistical probability factor that allows for a certain scattering to happen only if the initial state is occupied and the final state is empty.

The integro-differential transport equation, Eq. (2.4), is impossible to solve exactly. Several important approximations need to be performed in order for a solution to be achieved. First, the perturbation is assumed to be weak, such that second order terms are negligible. In this approximation, the solution can be written as a Taylor expansion in the perturbation, with just one significant term. Thus, the deviation from the equilibrium distribution is proportional to the perturbation. To first order in perturbation, the derivatives that appear in the drift terms are performed on the equilibrium function. Thus,

$$\nabla_{\vec{r}} f(\vec{r}, \vec{k}, t) \approx \nabla_{\vec{r}} f_k^0 = \frac{\partial f^0}{\partial T} \nabla T + \frac{\partial f^0}{\partial \mu} \nabla \mu. \quad (2.7)$$

After the corresponding derivatives of the Fermi function, Eq. (2.3) are introduced, one obtains,

$$\nabla_{\vec{r}} f(\vec{r}, \vec{k}, t) = \left(-\frac{df^0}{d\varepsilon_k} \right) \left(\nabla \mu + \frac{\varepsilon_k - \mu}{T} \nabla T \right). \quad (2.8)$$

The term $\nabla_{\vec{k}} f(\vec{r}, \vec{k}, t)$ can be linearized as well:

$$\nabla_{\vec{k}} f(\vec{r}, \vec{k}, t) \approx \nabla_{\vec{k}} f_k^0 = \nabla_{\vec{k}} \varepsilon_k \frac{df^0}{d\varepsilon_k} = \hbar \vec{v}_k \frac{df^0}{d\varepsilon_k}, \quad (2.9)$$

where we recognized that the drift velocity $\vec{v}_k = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon_k$.

From Eqs. (2.8) and (2.9) we obtain:

$$\frac{df}{dt} = \left(-\frac{df_k^0}{d\varepsilon_k} \right) \left(e\vec{E} + \nabla \mu + \frac{\varepsilon_k - \mu}{T} \nabla T \right). \quad (2.10)$$

A second important approximation is made on the collision term. In general, it can be shown that Eq. (2.6) can be approximated by a single relaxation time, τ that describes the time interval after which, as a result of collisions, the distribution function reaches equilibrium. Thus,

$$\left(\frac{\partial f(\vec{r}, \vec{k}, t)}{\partial t} \right)_{coll.} = -\frac{f(\vec{r}, \vec{k}, t) - f_k^0}{\tau(\vec{k})}. \quad (2.11)$$

In general, for elastic collisions, τ is considered to depend on the momentum \vec{k} only through energy.

Eqs. (2.10) and (2.11) conduce to what is known as the solution of the Boltzmann equation in the relaxation time approximation,

$$f(\vec{r}, \vec{k}, t) = f^0(\epsilon_k) + \tau \vec{v}_k \frac{\partial f^0}{\partial \epsilon_k} \left(e \vec{\tilde{E}} + \frac{\epsilon_k - \mu}{T} \nabla T \right), \quad (2.12)$$

where $\vec{\tilde{E}} = \vec{E} + \frac{1}{e} \nabla \mu$ is the electrochemical potential.

The solution of the BTE is necessary to calculate the electric and energy current that appear in an electron system in the presence of an electric field and a temperature gradient. The electric current is proportional with the sum over all occupied states of the particle velocities, while the energy current sums all available energies (expressed with respect to the Fermi level) multiplied by the particle velocity, weighted by the occupancy function of those states:

$$\begin{aligned} \vec{j} &= -2e \sum_{\vec{k}} \frac{\hbar \vec{k}}{m} f(\vec{r}, \vec{k}, t), \\ \vec{j}_Q &= 2 \sum_{\vec{k}} (\epsilon_k - \mu) \frac{\hbar \vec{k}}{m} f(\vec{r}, \vec{k}, t). \end{aligned} \quad (2.13)$$

A factor of 2 was introduced to account for the spin degeneracy.

When the solution of the Boltzmann equation, Eq. (2.12), is employed, two coupled equations for current and energy transport are obtained:

$$\begin{aligned} \vec{j} &= \hat{\sigma} \vec{\tilde{E}} - \hat{\beta} \frac{\nabla T}{T}, \\ \vec{j}_Q &= \hat{\beta} \vec{\tilde{E}} - \hat{\kappa} \nabla T, \end{aligned} \quad (2.14)$$

where $\hat{\sigma}$ is the conductivity tensor, $\hat{\beta}$ is the thermoelectric tensor, while $\hat{\kappa}$ is the thermal conductivity

tensor. Their components are given by

$$\hat{\sigma}_{ij} = 2e^2 \sum_{\vec{k}} \tau(\varepsilon_k) \frac{\hbar k_i k_j}{m m} \left(-\frac{df_k^0}{d\varepsilon} \right), \quad (2.15)$$

$$\hat{\beta}_{ij} = -2e \sum_{\vec{k}} \tau(\varepsilon_k) \frac{\hbar k_i \hbar k_j}{m m} (\varepsilon_k - \mu) \left(-\frac{df_k^0}{d\varepsilon} \right),$$

$$\hat{\kappa}_{ij} = 2 \sum_{\vec{k}} \tau(\varepsilon_k) \frac{\hbar k_i \hbar k_j}{m m} (\varepsilon_k - \mu)^2 \left(-\frac{df_k^0}{d\varepsilon} \right). \quad (2.16)$$

Eqs. (2.14) give the corresponding values of the phenomenological coefficients L introduced by Eq. (1.5).

In an isotropic, two dimensional system, where $\tau(\varepsilon)$ is constant τ , the thermoelectric tensors are diagonal. Moreover, the sums can be transformed into integrals in polar coordinates in the momentum space,

$$\sum_{\vec{k}} \rightarrow \frac{A}{(2\pi)^2} \int_0^{k_F} dk k \int_0^{2\pi} d\varphi. \quad (2.17)$$

The sharp variation of $\left(-\frac{df_k^0}{d\varepsilon}\right)$ in the vicinity of the Fermi level is successfully exploited when the variable of integration is ε . Therefore, we write:

$$\sigma = \frac{e^2 \tau}{\pi \hbar^2} \int_0^\infty d\varepsilon \varepsilon \left(-\frac{df^0}{d\varepsilon} \right),$$

$$\beta = -\frac{e\tau}{\pi \hbar^2} \int_0^\infty d\varepsilon \varepsilon (\varepsilon - \mu) \left(-\frac{df^0}{d\varepsilon} \right), \quad (2.18)$$

$$\kappa = \frac{\tau}{\pi \hbar^2 T} \int_0^\infty d\varepsilon \varepsilon (\varepsilon - \mu)^2 \left(-\frac{df^0}{d\varepsilon} \right). \quad (2.19)$$

The Sommerfeld expansion ([7], p.760, [8], p.394) allows the analytic computation of the integrals according to

$$\int_0^\infty d\varepsilon f(\varepsilon) \phi(\varepsilon) = - \int_0^\infty d\varepsilon f'(\varepsilon) \psi(\varepsilon) = - \sum_{m=0}^{\infty} \frac{1}{m!} \left. \frac{d^m \psi}{d\varepsilon} \right|_{\mu} (-k_B T)^m I_m. \quad (2.20)$$

$\psi(\varepsilon) = \int_0^\varepsilon d\varepsilon \phi(\varepsilon)$ is the primitive of ϕ , and the integral I_m has the form

$$I_m = \int_{-\infty}^{\infty} dx \frac{e^x}{(e^x + 1)^2} x^m. \quad (2.21)$$

Because of the integrant parity, the integrals I_m of odd order are zero. To second order in $(k_B T/\mu)$,

only $I_0 = 1$ and $I_2 = \frac{\pi^2}{3}$ are considered. With this, the expression of the transport coefficients are:

$$\sigma = \frac{ne^2\tau}{m} , \quad (2.22)$$

$$\beta = -\frac{\pi^2}{3e\epsilon_F} \frac{ne^2\tau}{m} (k_B T)^2 , \quad (2.23)$$

$$\kappa = \frac{\pi^2}{3} \frac{\tau n}{m} k_B^2 T . \quad (2.24)$$

The charge-energy coupling, as observed experimentally in the Seebeck and Peltier effects, is immediately revealed by Eqs. (2.14). If in the expression of the electric current, we set $\vec{j} = 0$, one obtains the mathematical description of the Seebeck effect,

$$\vec{E} = \alpha \nabla T , \quad (2.25)$$

where the Seebeck coefficient is

$$\alpha = \frac{\beta}{\sigma T} = -\frac{\pi^2 k_B^2 T}{3e\epsilon_F} . \quad (2.26)$$

The Peltier coefficient is obtained by setting $\nabla T = 0$ and computing the heat current as a function of the electric current. Thus:

$$\vec{j}_Q = \frac{\beta}{\sigma} \vec{j} , \quad (2.27)$$

leading to

$$\Pi = \frac{\beta}{\sigma} = \alpha T . \quad (2.28)$$

Chapter 3

Electric Coulomb Drag in Bi-Layer Semiconductor Systems

The concept of “drag” was first introduced in 1954 by Conyers Herring [9] to describe the momentum transfer between electrons and phonons in thermal transport whose net effect is to increase the Seebeck coefficient. Physically, the electrons driven out of equilibrium by a temperature gradient, impart some of their momentum to the phonons which become participants in the thermal transport.

The drag mediated by the Coulomb force, or the Coulomb drag, was first discussed by Pogrebinskii in 1977 [10] who calculated the drag in one semiconductor film of a semiconductor-insulator-semiconductor structure which was caused by direct Coulomb interactions with the carriers from the other semiconductor film. The first experimental observation of such a drag effect was done in 1989, by Solomon *et al.*, between a three-dimensional system and a semiconductor-based two-dimensional electron gas system [11].

The frictional drag between isolated two-dimensional electron gas systems was first observed experimentally in 1990, by Gramila *et al.* [12]. In this experiment, schematically described in Fig. 3.1, a current was driven through one layer, while a potential difference was measured in the other one. In 1992, Jauho and Smith [13] proposed a theoretical calculation of the momentum transfer rate between two-dimensional systems as a function of temperature, based on the Boltzmann equation of transport. The model provided a good qualitative agreement with the experimental

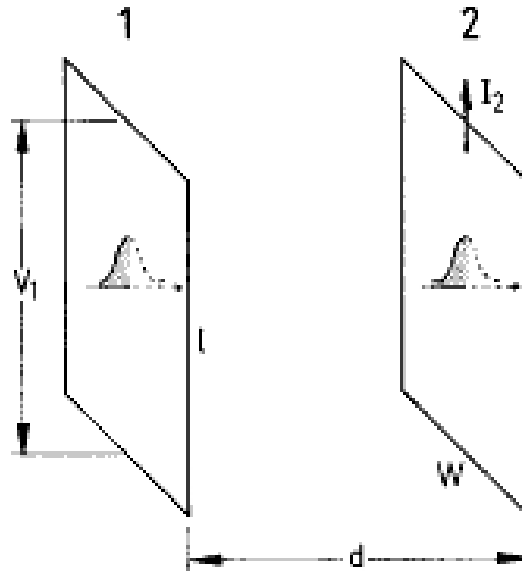


Figure 3.1 In the Coulomb drag experiment, an electric current flows in layer 2, while a potential difference is measured in layer 1.

results for the relaxation time at low temperatures which was found to be proportional to T^2 . The momentum transfer rate was independently calculated using a different formalism [14], yielding the same results (it has been found that disorder enhances the interlayer drag at low temperatures, the drag temperature dependence becoming $-T^2 \ln T$ in this case). Further experimental and theoretical developments in understanding the Coulomb drag effect were made, a relevant review article on this topic being published by Rojo [15] in 1999.

In 2001, D'Amico and Vignale [16] introduced the spin dependent Coulomb drag that acts between spin-polarized electron systems. More recently, in [17] a reproducible giant fluctuation of the drag was reported, depending on electron concentration and on the applied magnetic field, thus having a quantum nature. Random drag sign changes were reported for low temperatures, where fluctuations actually exceed the drag values.

In this chapter we review the fundamental physics that underlies the momentum transfer phenomenon that is responsible for the appearance of an electric field in one layer of a bi-layer system in response to a perturbation applied exclusively in the other layer, by following the salient points discussed in Ref. [13].

For simplicity, the system under consideration is composed of two identical quantum wells, of particle density n . When an electric field \vec{E}_2 is applied to the second layer, the electron distribution function is perturbed from its equilibrium value f_k^0 , described by Eq. (2.3), attaining a value $f_{\vec{k}}$. In the stationary case, this is the solution of a BTE written for the electric field \vec{E}_2 . Assuming that the primary scattering mechanism in layer 2 is provided by isotropic collision with impurities corresponding to a relaxation rate τ_2 , we can immediately write for an electron of momentum \vec{k}_2 and spin σ_2 , from Eq. (2.12),

$$f_{\vec{k}_2, \sigma_2} = f_{k_2}^0 + e\tau_2 \vec{v}_k \cdot \vec{E}_2 \frac{df^0}{d\varepsilon_k}. \quad (3.1)$$

Simultaneously, in layer 1, where there are no applied external perturbations, the only source for the time derivative of the distribution function is the collision term with the electrons in layer 2,

$$\left(\frac{\partial f_{\vec{k}_1}}{\partial t} \right) = \left(\frac{\partial f_{\vec{k}_1}}{\partial t} \right)_{coll}. \quad (3.2)$$

The total momentum of the electrons in layer 1,

$$\vec{P} = \sum_{\vec{k}_1, \sigma_1} \hbar \vec{k}_1 f_{\vec{k}_1}, \quad (3.3)$$

changes accordingly. The net change of momentum in layer 1 is therefore:

$$\frac{d\vec{P}}{dt} = \sum_{\vec{k}_1, \sigma_1} \hbar \vec{k}_1 \left(\frac{\partial f_{\vec{k}_1}}{\partial t} \right)_{12coll}. \quad (3.4)$$

The second law of dynamics equates the total change of momentum with a force, in this case electric acting on the electron system as a whole. If \vec{E}_1 is the corresponding electric field, we have:

$$\vec{F} = -ne\vec{E}_1 = \frac{d\vec{P}}{dt}. \quad (3.5)$$

The rate of momentum transfer between the electrons in the two layers, $\left(\frac{\partial f_{\vec{k}_1}}{\partial t} \right)_{12coll}$, is at the core of the Coulomb drag effect and it needs to be addressed in detail. First, the scattering is considered perfectly elastic and occurs with both momentum and energy conservation. Assuming that the initial momenta of electron 1 in layer 1 and of electron 2 in layer 2 are \vec{k}_1 and \vec{k}_2 , respectively, while

the final values are \vec{k}'_1 and \vec{k}'_2 , the conservation of momentum and energy require,

$$\begin{aligned}\vec{k}_1 + \vec{k}_2 &= \vec{k}'_1 + \vec{k}'_2, \\ \varepsilon_{k_1} + \varepsilon_{k_2} &= \varepsilon_{k'_1} + \varepsilon_{k'_2}.\end{aligned}\tag{3.6}$$

The collision term is calculated by using the Fermi golden rule. Thus, it depends both on the strength of the interaction, represented by its matrix element between the initial and final states and on the statistical probability that counts only occupied initial states and empty final states.

With this,

$$\left(\frac{\partial f_{k_1, \sigma_1}}{\partial t}\right)_{12coll} = - \sum_{\vec{k}_2, \vec{k}'_1, \sigma_2, \sigma'_1, \sigma'_2} w(\vec{k}_1, \vec{k}_2, \vec{k}'_1, \vec{k}'_2) [f_1 f_2 (1 - f'_1) (1 - f'_2) - (1 - f_1) (1 - f_2) f'_1 f'_2],\tag{3.7}$$

where the two-particle collision probability, $w(\vec{k}_1, \vec{k}_2, \vec{k}'_1, \vec{k}'_2)$ is given by:

$$w(\vec{k}_1, \vec{k}_2, \vec{k}'_1, \vec{k}'_2) = \frac{2\pi}{\hbar} \left| \langle \vec{k}_1 \vec{k}_2 | V | \vec{k}'_1 \vec{k}'_2 \rangle \right|^2.\tag{3.8}$$

The interaction potential is considered to be the static screened Coulomb written in Thomas-Fermi approximation [13] whose Fourier transform of momentum $q = |\vec{k}_1 - \vec{k}'_1|$ is

$$V(q) = \frac{2\pi e^2}{\kappa} \frac{q}{2q_{TF}^2 \sinh qd + (2qq_{TF} + q^2)e^{qd}};\tag{3.9}$$

where $q_{TF} = \frac{2me^2}{\kappa\hbar^2}$ is the Thomas-Fermi screening wave vector in a dielectric of constant κ .

In equilibrium, the microscopic reversibility property requires,

$$f_1^0 f_2^0 (1 - f_1^{0'}) (1 - f_2^{0'}) = (1 - f_1^0) (1 - f_2^0) f_1^{0'} f_2^{0'}.\tag{3.10}$$

In the linear approximation for weak perturbations, in the expression of the collision integral, we introduce the solutions of the Boltzmann equation in layer 2, Eq. (3.1), while the electrons in layer 1 are considered to be in equilibrium, i. e., $f_{\vec{k}_1} = f_{\vec{k}_1}^0$. With these simplifications, Eq. (3.7)

becomes:

$$f_1 f_2 (1-f'_1)(1-f'_2) - (1-f_1)(1-f_2) f'_1 f'_2 = \frac{\tau_2}{k_B T} \frac{e\hbar}{m} f_1^0 f_2^0 (1-f_1^{0'}) (1-f_2^{0'}) \vec{q} \cdot \vec{E}_2 \delta(\varepsilon_{k_1} + \varepsilon_{k_2} - \varepsilon'_{k_1} - \varepsilon'_{k_2}). \quad (3.11)$$

where $\vec{q} = \vec{k}_1 - \vec{k}'_1$ is the momentum transferred in collision. With these, the collision integral becomes,

$$\left(\frac{\partial f_{k_1, \sigma_1}}{\partial t} \right)_{12coll} = \frac{\tau_2}{k_B T} \frac{e\hbar}{m} \sum_{\vec{q}, \sigma_2, \sigma'_1, \sigma'_2} w(q) f_1^0 f_2^0 (1-f_1^{0'}) (1-f_2^{0'}) \vec{q} \cdot \vec{E}_2 \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2). \quad (3.12)$$

From Eqs. (3.4) and (3.5) we obtain,

$$\vec{E}_1 = -\frac{\tau_2}{nmk_B T} \sum_{\vec{q}} w(q) \sum_{\vec{k}_1, \sigma_1} \hbar \vec{k}_1 \sum_{\vec{k}_2, \sigma_2} \hbar \vec{q} \cdot \vec{E}_2 f_1^0 f_2^0 (1-f_1^{0'}) (1-f_2^{0'}) \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2). \quad (3.13)$$

The decoupling of the two sums involved in Eq. (3.13) is done by introducing an intermediate variable, $\hbar\omega$, such that

$$\delta(\varepsilon_1 + \varepsilon_2 - \varepsilon'_1 - \varepsilon'_2) = \int_{-\infty}^{\infty} d(\hbar\omega) \delta(\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_1 - \vec{q}} - \hbar\omega) \delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega). \quad (3.14)$$

Consequently, Eq. (3.13) becomes,

$$\begin{aligned} \vec{E}_1 = & -\frac{\tau_2}{nmk_B T} \int_{-\infty}^{\infty} d(\hbar\omega) \sum_q w(q) \sum_{\vec{k}_1, \sigma_1} \hbar \vec{k}_1 f_{\vec{k}_1}^0 (1-f_{\vec{k}_1 - \vec{q}}^0) \delta(\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_1 - \vec{q}} - \hbar\omega) \\ & \times \sum_{\vec{k}_2, \sigma_2} \hbar \vec{q} \cdot \vec{E}_2 f_{\vec{k}_2}^0 (1-f_{\vec{k}_2 + \vec{q}}^0) \delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega). \end{aligned} \quad (3.15)$$

To streamline the calculation, we anticipate some symmetry features of the final result. For an electric field parallel with the \hat{x} -axis, as depicted in Fig. (3.2), in polar coordinates, \vec{q} and \vec{k} make angles α and φ with this direction. Clearly, the result of Eq. (3.15) should be invariant under reflection with respect to the \hat{x} . This condition limits the contributions to the integral from the momentum coupling to

$$\vec{k}(\vec{q} \cdot \vec{E}_2) = \vec{e}_x k q E_2 \cos^2 \alpha \cos \varphi. \quad (3.16)$$

This result establishes that the induced electric field \vec{E}_1 is parallel to \vec{E}_2 . Eq. (3.16) allows the decoupling of the two correlated sums in Eq. (3.15) by introducing, S_1 and S_2 to denote the separate

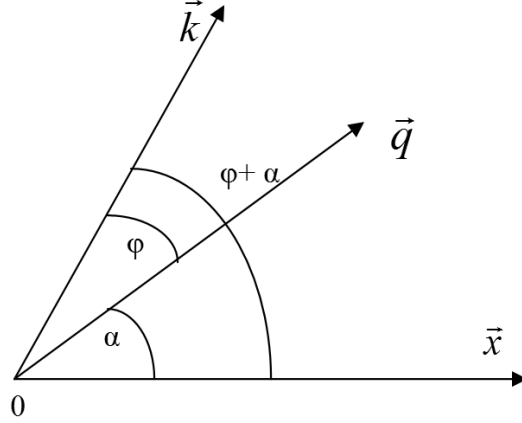


Figure 3.2 The momentum space diagram in polar coordinates

sums,

$$S_1 = \sum_{\vec{k}_1, \sigma_1} \hbar k_{1x} f_{\vec{k}_1}^0 (1 - f_{\vec{k}_1 - \vec{q}}^0) \delta(\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_1 - \vec{q}} - \hbar\omega), \quad (3.17)$$

$$S_2 = \sum_{\vec{k}_2, \sigma_2} \hbar q_x E_2 f_{\vec{k}_2}^0 (1 - f_{\vec{k}_2 + \vec{q}}^0) \delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega), \quad (3.18)$$

and then write Eq. 3.15 as

$$E_1 = -\frac{\tau_2}{nmk_B T} \int_{-\infty}^{\infty} d(\hbar\omega) \sum_q w(q) S_1 S_2. \quad (3.19)$$

By considering the Fermi function identity,

$$f_{\vec{k}_1}^0 (1 - f_{\vec{k}_1 - \vec{q}}^0) = \frac{1}{1 - e^{\frac{\hbar\omega}{k_B T}}} (f_{\vec{k}_1}^0 - f_{\vec{k}_1 - \vec{q}}^0), \quad (3.20)$$

the sum S_1 becomes:

$$S_1 = \frac{\hbar}{1 - e^{\frac{\hbar\omega}{k_B T}}} \sum_{\vec{k}_1, \sigma} k_{1x} (f_{\vec{k}_1}^0 - f_{\vec{k}_1 - \vec{q}}^0) \delta(\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_1 - \vec{q}} - \hbar\omega). \quad (3.21)$$

Standard manipulations that involve the transformation of the sum over momenta into an integral according to Eq. (2.17), are now performed on the expression of S_1 .

The summation over the spin generates an additional a factor of 2, and the expressions of

energies as functions of wave vectors makes use of the angles convention seen in Fig. 3.2, which allows the delta functions of energies to be written in terms of the angle φ . The sum S_1 becomes:

$$S_1 = \frac{\hbar}{1 - e^{\frac{\hbar\omega}{k_B T}}} \frac{1}{2\pi^2} \cos \alpha \left\{ - \int_{k_{min}}^{k_F} dk k^2 \int_0^{2\pi} d\varphi \cos \varphi \left[\delta \left(\frac{\hbar^2 k q}{m} \cos \varphi + \varepsilon_q - \hbar\omega \right) - \delta \left(\frac{\hbar^2 k q}{m} \cos \varphi - \varepsilon_q - \hbar\omega \right) \right] - q \int_{k_{min}}^{k_F} dk k \int_0^{2\pi} d\varphi \delta \left(\frac{\hbar^2 k q}{m} \cos \varphi + \varepsilon_q - \hbar\omega \right) \right\}. \quad (3.22)$$

The angular integrals involved in S_1 are of the form

$$I_{1\pm} = \int_0^{2\pi} d\varphi \cos \varphi \delta \left(\frac{\hbar^2 k q}{m} \cos \varphi \pm \varepsilon_q - \hbar\omega \right); \quad (3.23)$$

and

$$I_{2\pm} = \int_0^{2\pi} d\varphi \delta \left(\frac{\hbar^2 k q}{m} \cos \varphi \pm \varepsilon_q - \hbar\omega \right); \quad (3.24)$$

where we introduced the notation $\varepsilon_q = \frac{\hbar^2 q^2}{2m}$. $I_{1\pm}$ and $I_{2\pm}$ can be calculated analytically by elementary means and since the final results are quite useful for the rest of our calculation, we explicitly write them here,

$$I_{1\pm} = -\frac{2m}{\hbar^2 k q} \frac{\pm \varepsilon_q - \hbar\omega}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\pm \varepsilon_q - \hbar\omega)^2}}; \quad (3.25)$$

$$I_{2\pm} = \frac{2}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\pm \varepsilon_q - \hbar\omega)^2}}. \quad (3.26)$$

It is important to note here that the existence of integrals $I_{1\pm}$ and $I_{2\pm}$ is conditioned by the argument of the square root being real. This means that ω and q are correlated such that

$$|\pm \varepsilon_q - \hbar\omega| \leq \left(\frac{\hbar^2 k q}{m} \right)^2 \quad (3.27)$$

For a given $\hbar\omega$, q is limited to the interval $q \in [q_-, q_+]$, where

$$q_{\pm} = k_F \left(1 \pm \sqrt{1 - \frac{\hbar\omega}{\epsilon_F}} \right), \quad (3.28)$$

while $\hbar\omega \leq \epsilon_F$.

With this, the sum S_1 becomes,

$$S_1 = -\frac{m \cos \alpha}{\hbar q} \frac{1}{1 - e^{\frac{\hbar \omega}{k_B T}}} (\varepsilon_q + \hbar \omega) \left[\int_{k_{min}}^{k_F} dk \frac{k}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\varepsilon_q + \hbar \omega)^2}} - \int_{k_{min}}^{k_F} dk \frac{k}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\varepsilon_q - \hbar \omega)^2}} \right]. \quad (3.29)$$

Next, the integration over the wave vector k yields,

$$S_1 = -\frac{m \cos \alpha}{\hbar \pi^2 q} \frac{1}{1 - e^{\frac{\hbar \omega}{k_B T}}} (\varepsilon_q + \hbar \omega) \left[\sqrt{\left(\frac{\hbar^2 k_F q}{m}\right)^2 - (\varepsilon_q - \hbar \omega)^2} - \sqrt{\left(\frac{\hbar^2 k_F q}{m}\right)^2 - (\varepsilon_q + \hbar \omega)^2} \right]. \quad (3.30)$$

With notations,

$$\begin{aligned} \Omega_-(q, \omega) &= \sqrt{1 - \left(\frac{q}{2k_F} - \frac{m\omega}{\hbar k_F q}\right)^2} - \sqrt{1 - \left(\frac{q}{2k_F} + \frac{m\omega}{\hbar k_F q}\right)^2} \\ \Omega_+(q, \omega) &= \sqrt{1 - \left(\frac{q}{2k_F} - \frac{m\omega}{\hbar k_F q}\right)^2} + \sqrt{1 - \left(\frac{q}{2k_F} + \frac{m\omega}{\hbar k_F q}\right)^2} \end{aligned}. \quad (3.31)$$

we finally write S_1 as

$$S_1 = -N_0 \frac{\hbar k_F \cos \alpha}{2\pi} \frac{1}{1 - e^{\frac{\hbar \omega}{k_B T}}} \left(1 + \frac{\hbar \omega}{\varepsilon_q}\right) \Omega_-(q, \omega); \quad (3.32)$$

where $N(0) = \frac{m}{\pi \hbar^2}$ designates the density of states at the Fermi surface.

The calculation of S_2 , Eq. (3.17), proceeds along similar lines. After using Eq. (3.20), we write,

$$S_2 = \frac{\hbar E_2}{1 - e^{-\frac{\hbar \omega}{k_B T}}} \sum_{\vec{k}_2, \sigma_2} q_x \left(f_{\vec{k}_2}^0 - f_{\vec{k}_2 + \vec{q}}^0\right) \delta\left(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar \omega\right). \quad (3.33)$$

We note that $q_x = q \cos \alpha$ and rewrite S_2 as:

$$S_2 = \frac{\hbar q \cos \alpha E_2}{1 - e^{-\frac{\hbar \omega}{k_B T}}} \frac{1}{2\pi^2} \int_{k_{min}}^{k_F} dk k \left[\int_0^{2\pi} d\varphi \delta\left(\frac{\hbar^2 k q}{m} \cos \alpha - \varepsilon_q - \hbar \omega\right) - \int_0^{2\pi} d\varphi \delta\left(\frac{\hbar^2 k q}{m} \cos \alpha - \varepsilon_q + \hbar \omega\right) \right]. \quad (3.34)$$

The angular integrals involved in this calculation have the same form as the ones in Eq. (3.24), their result being the one shown in Eq. (3.26). After replacing these solutions of integrals $I_{2\pm}$ in the

expression of the sum S_2 , the latter becomes:

$$S_2 = \frac{\hbar q \cos \alpha E_2}{1 - e^{-\frac{\hbar \omega}{k_B T}}} \frac{1}{\pi^2} \int_{k_{min}}^{k_F} dk k \left[\frac{1}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\varepsilon_q - \hbar \omega)^2}} - \frac{1}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\varepsilon_q + \hbar \omega)^2}} \right]. \quad (3.35)$$

After integrating over the k , we finally obtain,

$$S_2 = \frac{\cos \alpha E_2}{1 - e^{-\frac{\hbar \omega}{k_B T}}} \frac{1}{\pi^2} \frac{m^2}{\hbar^3 q} \left[\sqrt{\left(\frac{\hbar^2 k_F q}{m}\right)^2 - (\varepsilon_q - \hbar \omega)^2} - \sqrt{\left(\frac{\hbar^2 k_F q}{m}\right)^2 - (\varepsilon_q + \hbar \omega)^2} \right]. \quad (3.36)$$

Using the simplified notation given by Eq. (3.31), S_2 can be written as:

$$S_2 = E_2 N_0 \frac{\hbar k_F \cos \alpha}{\pi} \frac{1}{1 - e^{-\frac{\hbar \omega}{k_B T}}} \Omega_-(q, \omega). \quad (3.37)$$

With the results of Eqs. (3.19), (3.32) and (3.37), we obtain, after the sum over \vec{q} was transformed into an integral in polar coordinates and the angular part was equated to π ,

$$E_1 = \frac{\tau_2 E_2}{n k_B T} \frac{N_0^2 \varepsilon_F}{4\pi} \int_{-\infty}^{\varepsilon_F} d(\hbar \omega) \int_{q_-}^{q_+} dq q w(q) \frac{\Omega_-^2(q, \omega)}{\sinh^2\left(\frac{\hbar \omega}{2k_B T}\right)}. \quad (3.38)$$

The matrix element of the perturbation is given by the Fermi golden rule, Eq. (3.8), written for the Coulomb interaction potential, Eq. (3.9) by taking into account all the possible final spin orientations of the electrons, leading to,

$$w(q) = \sum_{\sigma'_1, \sigma'_2} w(\vec{k}_1, \vec{k}_2, \vec{k}'_1, \vec{k}'_2) \frac{8\pi}{\hbar} |V(q)|^2. \quad (3.39)$$

We note that the denominator of the integrant in Eq. (3.38), is sharply peaked at small values of ω . Moreover, at small values of q where the matrix element of the Coulomb interaction is important, the integrant is convergent. It is customary, under these circumstances to extend the limits of integration over the whole available interval for both q and ω , regardless of Eqs. (3.28). When the integral over ω extends over the whole real axis, terms odd in $\hbar \omega$ drop out in the integrant since the

integral is done over a symmetric interval. In this approximation, the induced electric field E_1 is

$$E_1 = \frac{\tau_2 E_2}{nk_B T} \frac{mk_F^2}{8\pi^4 \hbar^2} \int_0^\infty dq q |e\phi(q)|^2 \int_{-\infty}^\infty d\omega \frac{\Omega_-^2(q, \omega)}{\sinh^2\left(\frac{\hbar\omega}{2k_B T}\right)}. \quad (3.40)$$

The proportionality between the induced electric field E_1 and the driving field E_2 can be expressed in terms of the ratio of two characteristic relaxation rates,

$$\frac{E_1}{E_2} = \frac{\tau_2}{\tau_D} \quad (3.41)$$

where the Coulomb drag momentum relaxation rate τ_D is defined to be,

$$\frac{1}{\tau_D} = \frac{1}{k_B T} \frac{mk_F^2}{8\pi^4 \hbar^2 n} \int_0^\infty dq q |e\phi(q)|^2 \int_{-\infty}^\infty d\omega \frac{\Omega_-^2(q, \omega)}{\sinh^2\left(\frac{\hbar\omega}{2k_B T}\right)}. \quad (3.42)$$

In Eq. (3.42), the integrals in q and ω can be calculated easily in the low temperature, low frequency regime, when $\hbar\omega \ll \varepsilon_q$ it follows that:

$$\Omega_- = \frac{m\omega}{\hbar k_F^2}. \quad (3.43)$$

Also, we approximate the Coulomb interaction matrix element in the Fermi-Thomas model at small momenta [13], retaining only the small q limit of Eq. (3.9)

$$|V(q)|^2 = \frac{\pi^2 \hbar^4}{4m^2 q_{TF}^2} \frac{q^2}{\sinh^2(qd)}. \quad (3.44)$$

Within these limitations, Eq. (3.42) becomes,

$$\frac{1}{\tau_D} = \frac{1}{k_B T} \frac{m}{16\pi q_{TF}^2 k_F^4} \int_0^\infty \frac{dq q^3}{\sinh^2(qd)} \int_{-\infty}^\infty \frac{d\omega \omega^2}{\sinh^2\left(\frac{\hbar\omega}{2k_B T}\right)}. \quad (3.45)$$

The two integrals can be calculated by using the following identity:

$$\int_0^\infty \frac{dx x^p}{\sinh^2\left(\frac{x}{2}\right)} = 4p! \zeta(p); \quad (3.46)$$

where $\zeta(p)$ is the Riemann zeta function. The integral over ω generates $\zeta(2) = \frac{\pi^2}{6}$. While the

integral over q generates

$$\int_0^\infty \frac{dq q^3}{\sinh^2(qd)} = \frac{3\zeta(3)}{2d^4} \quad (3.47)$$

The expression of $\frac{1}{\tau_D}$ becomes,

$$\frac{1}{\tau_D} = \frac{\pi\zeta(3)}{16\varepsilon_F \hbar} \frac{1}{(q_{TF} d)^2} \frac{1}{(k_F d)^2} (k_B T)^2 \quad (3.48)$$

the result first derived in Ref. [13].

Chapter 4

Thermal Coulomb Drag in Bi-Layer Semiconductor Systems

In this chapter we discuss a generalization of the Seebeck effect from a homogenous system to the bi-layer case, using the momentum transfer mechanism that is involved in the Coulomb drag phenomenon. The treatment of this problem follows closely the algorithm developed in the previous chapter, the difference being the application of a thermal gradient ∇T as the driving perturbation. As before, we consider a bi-layer semiconductor system, formed by two identical quantum wells.

We calculate of the inter-layer momentum transfer via Coulomb interaction between the electrons driven out of equilibrium by the temperature gradient (layer 2) and the electrons in the passive layer (layer 1). The net change of momentum transfer is responsible for the apparition of an induced electric field \vec{E}_1 . We call this effect "thermal Coulomb drag" by analogy with the electric Coulomb drag, previously presented.

As before we point out that the calculation of the rate of momentum transfer depends on the solutions to the transport equation in the two layers. In layer 2, the temperature gradient induces a change in the distribution function given by:

$$f(\vec{r}, \vec{k}, t) = f_{k_2}^0 + \tau_2 \frac{\hbar \vec{k}_2}{m} \cdot \frac{\nabla T}{T} (\varepsilon_{k_2} - \mu) \left(\frac{df_{k_2}^0}{d\varepsilon_{k_2}} \right); \quad (4.1)$$

which represents the thermal part of Eq. (2.12).

The expression of the transport equation in layer 1 is given by Eq. (3.2). Following the same argument as in Ch. 3, we write directly the expression of the induced electric field,

$$\begin{aligned} \vec{E}_1 = & -\frac{\tau_2}{nemk_B T} \int_{-\infty}^{\infty} d(\hbar\omega) \sum_q w(q) \sum_{\vec{k}_1, \sigma_1} \hbar \vec{k}_1 f_{\vec{k}_1}^0 (1 - f_{\vec{k}_1 - \vec{q}}^0) \delta(\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_1 - \vec{q}} - \hbar\omega) \\ & \times \frac{\nabla T}{T} \cdot \sum_{\vec{k}_2, \sigma_2} \left[\hbar \vec{k}_2 (\varepsilon_{\vec{k}_2} - \mu) - \hbar(\vec{k}_2 + \vec{q})(\varepsilon_{\vec{k}_2 + \vec{q}} - \mu) \right] f_{\vec{k}_2}^0 (1 - f_{\vec{k}_2 + \vec{q}}^0) \delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega). \end{aligned} \quad (4.2)$$

As in the case of the electric Coulomb drag, symmetry arguments require that \vec{E}_1 is parallel to the temperature gradient ∇T applied in layer 2, assumed to be along the \hat{x} direction. Then, the decoupling of the two sums proceeds as before. While sum S_1 retains the same expression as in Eqs. (3.17), sum S_2 is:

$$S_2 = \sum_{\vec{k}_2, \sigma_2} f_{\vec{k}_2}^0 (1 - f_{\vec{k}_2 + \vec{q}}^0) \frac{\nabla_x T}{T} [\hbar k_{2x} (\varepsilon_{\vec{k}_2} - \mu) - \hbar(k_{2x} + q_x)(\varepsilon_{\vec{k}_2} + \hbar\omega - \mu)] \delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega); \quad (4.3)$$

With this, the induced electric field becomes:

$$E_1 = -\frac{\tau_2}{nemk_B T} \int_{-\infty}^{\infty} d(\hbar\omega) \sum_q w(q) S_1 S_2. \quad (4.4)$$

The calculation of the sum S_2 takes advantage of Eq. (3.20) leading to:

$$\begin{aligned} S_2 = & -\frac{\hbar}{1 - e^{-\frac{\hbar\omega}{k_B T}}} \frac{\nabla_x T}{T} \\ & \times \left\{ q_x \mu \sum_{\vec{k}_2, \sigma_2} f_k^0 \left[\delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega) - \delta(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega) \right] \right. \\ & - \hbar\omega q_x \sum_{\vec{k}_2, \sigma_2} f_k^0 \left[\delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega) + \delta(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega) \right] \\ & - \hbar\omega \sum_{\vec{k}_2, \sigma_2} f_k^0 k_{2x} \left[\delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega) - \delta(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega) \right] \\ & \left. - q_x \sum_{\vec{k}_2, \sigma_2} f_k^0 \varepsilon_{\vec{k}_2} \left[\delta(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega) - \delta(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega) \right] \right\}. \end{aligned} \quad (4.5)$$

The four terms of S_2 are considered separately below. The first term, after the introduction of Ω_-

from Eq. (3.31), becomes:

$$q_x \mu \sum_{k_2, \sigma_2} f_k^0 \left[\delta \left(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega \right) + \delta \left(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega \right) \right] = \frac{N_0 k_F \cos \alpha}{\pi} \mu \Omega_-(q, \omega) , \quad (4.6)$$

where we incorporated the angular integration results from Eqs. (3.25) and (3.26).

The second term is,

$$-\hbar\omega q_x \sum_{k_2, \sigma_2} f_k^0 \left[\delta \left(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega \right) + \delta \left(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega \right) \right] = -\frac{N_0 k_F \cos \alpha}{\pi} \hbar\omega \Omega_-(q, \omega) . \quad (4.7)$$

The third term is:

$$\begin{aligned} & -\hbar\omega \sum_{k_2, \sigma_2} f_k^0 k_{2x} \left[\delta \left(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega \right) - \delta \left(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega \right) \right] \\ & = -\hbar\omega \frac{1}{2\pi^2} \int_{k_{min}}^{k_F} dk k^2 \int_0^{2\pi} d\varphi \cos(\varphi + \alpha) \left[\delta \left(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega \right) - \delta \left(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega \right) \right] . \end{aligned} \quad (4.8)$$

The angular integral over φ has the same form as the one shown in Eq. (3.23), and after applying its result Eq. (3.25), we obtain for this term the following expression:

$$-\frac{m\omega \cos \alpha}{\hbar q \pi^2} \left[(\varepsilon_q - \hbar\omega) \int_{k_{min}}^{k_F} \frac{dk k}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\varepsilon_q - \hbar\omega)^2}} + (\varepsilon_q + \hbar\omega) \int_{k_{min}}^{k_F} \frac{dk k}{\sqrt{\left(\frac{\hbar^2 k q}{m}\right)^2 - (\varepsilon_q + \hbar\omega)^2}} \right] .$$

After the subsequent integration over the wave number k and the use of abridged notations Eqs. (3.31), we obtain:

$$\frac{N_0 k_F \cos \alpha}{\pi} \left[\frac{\hbar\omega}{2} \Omega_+(q, \omega) - \frac{m\omega^2}{q^2} \Omega_-(q, \omega) \right] . \quad (4.9)$$

The fourth term is:

$$\begin{aligned} & -q_x \sum_{k_2, \sigma_2} f_k^0 \varepsilon_{\vec{k}_2} \left[\delta \left(\varepsilon_{\vec{k}_2 + \vec{q}} - \varepsilon_{\vec{k}_2} - \hbar\omega \right) - \delta \left(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_2 - \vec{q}} - \hbar\omega \right) \right] = \\ & -\frac{\hbar^2 q \cos \alpha}{(2\pi)^2 m} \int_{k_{min}}^{k_F} dk k^3 \int_0^{2\pi} d\varphi \left[\delta \left(\frac{\hbar^2 k q}{m} \cos \varphi + \varepsilon_q - \hbar\omega \right) - \delta \left(\frac{\hbar^2 k q}{m} \cos \varphi - \varepsilon_q - \hbar\omega \right) \right] . \end{aligned} \quad (4.10)$$

As the angular integrals have the same form as Eq. (3.24), by using Eq. (3.26), we obtain,

$$-\frac{N_0 k_F \cos \alpha}{3\pi} \left[\left(\varepsilon_F + \frac{\hbar^2 q^2}{4m} + \frac{m\omega^2}{q^2} \right) \Omega_-(q, \omega) - \hbar\omega \Omega_+(q, \omega) \right]. \quad (4.11)$$

Finally, the end result for S_2 is,

$$S_2 = -\frac{\nabla_x T}{T} \frac{\hbar}{1 - e^{-\frac{\hbar\omega}{k_B T}}} \frac{N_0 k_F \cos \alpha}{\pi} \times \left[\left(\frac{2\varepsilon_F}{3} + \hbar\omega + \frac{2}{3} \frac{m\omega^2}{q^2} - \frac{\hbar^2 q^2}{12m} \right) \Omega_-(q, \omega) - \frac{\hbar\omega}{6} \Omega_+(q, \omega) \right]. \quad (4.12)$$

The further multiplication of S_1 and S_2 will yield terms depending on Ω_-^2 , which is an even function of ω , and on $\Omega_- \Omega_+ = \frac{2m}{\hbar k_F^2} \omega$, which is an odd function of ω . Since only the even terms are relevant for the integration over the ω -real axis, the product $S_1 S_2$ is written as,

$$S_1 S_2 = -m \frac{\nabla_x T}{T} \frac{N_0^2 \varepsilon_F^2 \cos^2 \alpha}{6\pi^2} \frac{1}{\sinh^2 \left(\frac{\hbar\omega}{2k_B T} \right)} \left[\Omega_-^2 \left(1 - \frac{1}{4k_F^2} q^2 - \frac{4m^2}{\hbar^2 k_F^2} \frac{\omega^2}{q^2} \right) + \Omega_- \Omega_+ \frac{m}{2\hbar k_F^2} \omega \right]. \quad (4.13)$$

A factor of π was introduced for the angular integral in q space.

Eq. (4.4) that gives the expression of the induced electric field becomes,

$$E_1 = -\tau_2 \frac{\nabla_x T}{n e k_B T^2} \frac{N_0^2 \varepsilon_F}{12m} \int_{(q)} dq q |V(q)|^2 \times \int_{-\infty}^{\infty} \frac{d\omega}{\sinh^2 \left(\frac{\hbar\omega}{2k_B T} \right)} \left[\Omega_-^2 \left(1 - \frac{1}{4k_F^2} q^2 - \frac{4m^2}{\hbar^2 k_F^2} \frac{\omega^2}{q^2} \right) + \frac{m^2}{\hbar^2 k_F^4} \omega^2 \right]. \quad (4.14)$$

This is the most general expression of the Boltzmann equation for the thermal Coulomb drag effect.

We pursue the analytic calculation in the low frequency limit. In this range, approximations expressed in Eqs. (3.43) and (3.44) apply. Furthermore, we neglect terms that are second order in ω^2 . In these conditions, the induced electric field is

$$E_1 = -\tau_2 \frac{\nabla_x T}{n e k_B T^2} \frac{\pi^2 N_0^2 \varepsilon_F^2}{24 q_T^2 k_F^4} \left[\int_0^{2k_F} \frac{dq q^3}{\sinh^2(qd)} - \frac{1}{4k_F^2} \int_0^{2k_F} \frac{dq q^5}{\sinh^2(qd)} \right] \int_{-\infty}^{\infty} \frac{d\omega \omega^2}{\sinh^2 \left(\frac{\hbar\omega}{2k_B T} \right)}. \quad (4.15)$$

We note that, while the integral over ω is extended to $\pm\infty$ on account of the rapid convergence of the denominator, the integral over q has to be cut off at $2k_F$, the maximum available value. However,

for the values of inter-layer distance d considered, the integrand over q also converges, so the integral can also be extended to $\pm\infty$.

The ω integral can be done by using Eq. (3.46) for $n = 2$, with the particular value of Riemann Zeta function $\zeta(2) = \frac{\pi^2}{6}$. The integrals over q are:

$$\begin{aligned} \int_0^\infty \frac{dq q^3}{\sinh^2(qd)} &= \frac{3\zeta(3)}{2d^4}, \\ \int_0^\infty \frac{dq q^5}{\sinh^2(qd)} &= \frac{15\zeta(5)}{2d^6}. \end{aligned} \quad (4.16)$$

Within these approximations, the expression of the induced electric field is,

$$E_1 = -\tau_2 \frac{\pi^2 k_B^2 T k_F^2}{ne6\hbar} \frac{1}{(k_F d)^2 (q_{TF} d)^2} \left[\zeta(3) - \frac{5}{4} \frac{\zeta(5)}{(k_F d)^2} \right] \nabla_x T. \quad (4.17)$$

We can define the trans-Seebeck coefficient of the bi-layer system as the proportionality coefficient between the induced electric field and the temperature gradient,

$$\vec{E}_1 = \alpha_D \nabla T. \quad (4.18)$$

Thus, α_D is:

$$\alpha_D = -\tau_2 \frac{\pi^2 k_B^2 T k_F^2}{6e\hbar n} \frac{1}{(k_F d)^2 (q_{TF} d)^2} \left[\zeta(3) - \frac{5}{4} \frac{\zeta(5)}{(k_F d)^2} \right]. \quad (4.19)$$

Comparing this value to the single layer Seebeck coefficient, given by Eq. (2.26), we can write:

$$\alpha_D = \alpha_2 \tau_2 \frac{\pi \varepsilon_F}{\hbar} \frac{1}{(k_F d)^2 (q_{TF} d)^2} \left[\zeta(3) - \frac{5}{4} \frac{\zeta(5)}{(k_F d)^2} \right]. \quad (4.20)$$

Chapter 5

Conclusions and Discussion

In this work we develop a theory of a thermoelectric effect, analogous to the Seebeck phenomenon, that is predicted to occur in a bi-layer semiconductor structure on account of the momentum transferred between the layers, mediated by the Coulomb interaction. Phenomenologically, we demonstrate that this mechanism can give rise to an electric field in one layer when a temperature gradient is applied in the other layer. This proof establishes the fact that the Coulomb drag is a robust mechanism of transmission of a non-equilibrium regime from one electron system to another.

By solving the Boltzmann transport equation in the two layers, we are able to derive an analytic expression for the induced electric as a function of the system parameters. We find that, at all temperatures, the electric field is parallel to the direction of the temperature gradient and proportional with its magnitude. The proportionality coefficient is the analogue of the Seebeck thermopower.

At low temperatures, in the low frequency limit, we find that the Coulomb drag thermopower is proportional with the single layer thermopower and inversely proportional to the strength of the Coulomb screening expressed by the Thomas-Fermi screening length and the particle density in the system. The linear temperature dependence, characteristic to Fermi systems, is also preserved.

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