Investigation of superfluidity in ultra-short flows : effect of time-lags in transport phenomena

Peyman Tavallali

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INVESTIGATION OF SUPERFLUIDITY IN ULTRA-SHORT FLOWS; EFFECT OF TIME-LAGS IN TRANSPORT PHENOMENA

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Peyman Tavallali
August 2009

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Summary:

In this thesis, an investigation of the phase-lagged formulation of the high-temperature model of superfluidity is presented. Also, as a consequence of the physical idea behind the latter, a new model for heat transfer at nano-scale is presented. In general, the thesis is about the effect of the time delay in the transport of the energy and momentum in transport phenomena formulations. These time delays depict themselves in the functional form of their corresponding differential equations. As a result, the mathematics behind the modeling is nothing but subclasses of delay differential equations, both partial and ordinary.

In this report, the author has tried to express the idea that the quantum mechanics is not the ultimate player in superfluidity, at least at high temperatures. The main idea is the time lag in the transport of energy (information) in the domain.

Prediction of the superfluidity has not been the unique outcome of the phase-lagged energy propagation formulation. The capabilities of the idea were tested positive on the concept of nano-scale heat transfer. Here, two viewpoints are emphasized. The first is the formulation of the phase lag from the large scale point of view capturing the micro-scale features. The second is the utilization of the idea in the micro-scale world. This resulted into two fundamental conclusions. The new phenomenological nano-scale heat transfer formulation was an early consequence. Later, the implication of the time lag showed great insights about possibilities in the molecular domain: micro-scale justification of high-temperature model of superfluidity.

Summary

Since the model presented in this report is the newest model to describe the superfluidity, and predict it at high temperatures, the author has tried to show the validation of the model by converting it into one of the previous well-known models by using mathematical linear approximation procedure. This approach, clearly, paves the way for the model to suggest that, not only is the model could be correct, both physically and mathematically, but also a more rigorous one among all other models. As mentioned earlier, Delay Differential Equations (DDEs) are a consequence of the idea behind the phase-lagged formulations. As a result, the solutions of these equations become vital to the model. The analytic solution for a subclass of Partial Delay Differential Equations (PDDE) has been proposed. The numerous numerical solutions have also been presented in the text.

The model presented in this report will have the ability of extension into other fields of physics. The model will be useful in areas such as superfluidity, superconductivity, start-up flows, ultra-short phenomena (such as ultra-short laser pulses), supertransport of energy, Quantum Mechanics, etc.

Nomenclature

a	Diffusion coefficient [m^2 / s]
a_i	Acceleration i^{th} component (Chapters 3 & 7) [m / s^2]
b	Body force (Chapter 3) [N / kg]
C	Specific heat per unit volume [$J / (m^3 K)$]
C_p	Specific heat at constant pressure [$J / (kgK)$]
C_v	Specific heat at constant volume [$J / (kgK)$]
c	Generalized body force [N / kg]
c	Specific heat per unit mass (Chapter 3) [$J / (kgK)$]
c	Sound speed (Chapter 2) [m / s]

c	Information propagation speed (Chapter 7) [m / s]
c_p	Phonon speed (Chapter 4) [m / s]
Cte	Constant (units are case dependent)
D	Rate of deformation tensor [$1 / s$]
d	Diameter [m]
E	Energy [J]
e	Internal specific energy [J / K]
e_a	Energy of particle a [J]
F	Force [N]
F_{ij}	Force [N]

Nomenclature

f	Internal parameter (Chapter 2) [$(1 / m^{3/2})$]	K_s	Static compressibility [$1 / Pa$]
f	Distribution function (Chapter 6) [s^3 / m^3]	k	Wave number [$1 / m$]
f	Distribution function (Chapter 7) [$s^3 / kg^3 m^3$]	k	Thermal conductivity [$W / (m.K)$]
g	Body force (Chapter 2) [N / kg]	k_{ab}	a to b conductivity [W / K]
g_i	Temperature gradient (Chapter 3) [K / m]	k_{ph}	Phonon thermal conductivity [$W / (m.K)$]
i	Unit vector (no units)	${}^e k_i^j$	Electron conductivity from j to i [W / K]
i	$i^2 = -1$ (no units)	${}^l k_i^j$	Lattice conductivity from j to i [W / K]
J_1	Bessel function of the 1 st kind (no units)	k_r	Roton thermal conductivity [$W / (m.K)$]
j	Momentum per unit volume [$kg / (m^2 s)$]	k_B	Boltzmann constant [J / K]
K	[$1 / s$]	L	Characteristic length [m]

Nomenclature

I	Energy flux of excitations [J / m^2]	P	Momentum per unit volume [$kg / (m^2 s)$]
l	Length [m]	P	Pressure (Chapter 2) [Pa]
M	Moment vector [mN]	p	Pressure (Chapter 3 & 5) [Pa]
m	Mass [kg]	p	Coefficient (Chapter 6) (no units)
m	Number of excitations per unit mass (Chapter 2) [$1 / kg$]	p_0	Pressure at infinity [Pa]
m_0	Rest mass of the particle [kg]	p_n	Normal auxiliary pressure [Pa]
m_{He}	Mass of helium (atomic mass) [kg]	p_s	Superfluid auxiliary pressure [Pa]
N	Total number of particles (no units)	p_E	Equilibrium pressure [Pa]
n	Number of lattice points in the box (Chapter 6) (no units)	p_v	Non-equilibrium pressure [Pa]
P	Auxiliary function (Chapter 5) [m / s]	$p_{<ij>}$	Stress deviator [Pa]
		Q	Energy current density [W / m^2]

Nomenclature

$\mathbf{q}$	Heat flux per unit area (Chapter 2 sections 2.3.2.1 & 2.3.2.2 & 2.3.2.3, Chapter 3) [W / m^2]	r	Rate of body energy support per unit volume (Chapter 2) [W / m^3]
$\mathbf{q}$	Unit vector (Chapter 2 section 2.3.1.2) (no units)	r	Position in the radial direction (Chapter 5) [m]
q	Numerical coefficient (Chapter 4) (no units)	S	Entropy per unit volume [$J / m^3 K$]
q	Numerical coefficient (Chapter 6) [s]	S	Slip (Chapter 6) (no units)
q_{atob}	Energy flow per unit of time [W]	$S(\mathbf{k})$	Structure factor (no units)
R	Dissipative energy term [W / m^3]	s	Flux of excitations [$J / (Ns)$]
R_1, R_2	Radius [m]	s	Specific entropy [$J / kg.K$]
$\mathbf{r}$	Position vector [m]	T	Temperature [K]
$\mathbf{r}_p$	Particle position [m]	T_c	BEC temperature [K]
		T_0	Lambda temperature [K]
		$\bar{T}_{IJK}$	Cell average temperature [K]

Nomenclature

t	time $[s]$	$\mathbf{v}_n$	Normal velocity $[m / s]$
t_{ij}	Stress tensor $[Pa]$	v_{cr}	Critical speed $[m / s]$
t_{new}	Non-dimensional time (Chapter 4) (no units)	$\mathbf{w}$	Relative velocity $[m / s]$
U	Specific internal energy per unit of mass (Chapter 2) $[J / kg]$	$\mathbf{x}$	Position vector $[m]$
U	Unit step function (Chapter 4) (units depend on the case)	x_{new}	Non-dimensional position (no units)
u_1	First sound speed $[m / s]$	Y_1	Bessel function of the 2 nd kind (no units)
$\mathbf{u}$	Velocity vector (Chapter 5) $[m / s]$	z	Position $[m]$
u_2	Second sound speed $[m / s]$	α	Thermal diffusivity $[m^2 / s]$
u_4	Forth sound speed $[m / s]$	β, β'	Phenomenological constants $[J.K / m^3]$
V	Volume $[m^3]$	δ	Identity tensor (no units)
$\mathbf{v}$	Velocity $[m / s]$	ε	Energy (Chapter 2) $[J]$
$\mathbf{v}_s$	Superfluid velocity $[m / s]$	ε	Specific internal energy (Chapter 3) $[J / kg]$

Nomenclature

ε	Specific Lennard-Jones energy (Chapter 7) [J / mol]	$\lambda_0, \lambda_1,$ λ_2	Bulk viscosities [$Pa.s$]
$\Phi(r)$	Lennard-Jones potential (Chapter 7) [J / mol]	λ	Viscosity [$Pa.s$]
ϕ	Phase of wave packet (no units)	μ	Effective mass of roton (Chapter 2 Section 2.3.1.1) [kg]
φ	Stress tensor [Pa]	μ	Chemical potential (Chapter 2 section 2.3.1.1 equations 2.27 & 2.30) [m^2 / s^2]
η	Viscosity (Chapter 2) [$Pa.s$]	μ	Dynamic viscosity (Chapter 2 section 2.3.2.3) [$Pa.s$]
η	Specific entropy (Chapter 3) [J / kgK]	ν	The creation rate of excitations per unit mass (Chapter 2, section 2.3.2.1) [$1 / (kg.s)$]
θ	Absolute temperature (Chapter 3) [K]	ν	Kinematic viscosity (Chapter 2, section 2.3.2.3 & Chapter 3) [m^2 / s]
θ	Angle (no units)	Π	Stress tensor [Pa]
θ	Non-dimensional temperature (Chapter 6) (no units)		
κ	Thermal conduction coefficient [$W / (m.K)$]

Nomenclature

Π_r	Number of rotons per unit volume [$1 / m^3$]	τ_0, τ_1, τ_2	Relaxation times [s]
ρ	Density [kg / m^3]	τ_T, τ_q	Phase lags (time lags) [s]
ρ_n	Normal density [kg / m^3]	τ_{new}	Non-dimensional time lag (no units)
ρ_s	Superfluid density [kg / m^3]	χ_a	Energy-Temperature equivalence coefficient [J / K]
ρ_{ij}^{no}	Normal density tensor [kg / m^3]	ψ	Order parameter (Chapter 2) [$(1 / m^{3/2})$]
ρ_{ij}^s	Superfluid density tensor [kg / m^3]	ψ	Helmholtz free energy (Chapter 3) [J / kg]
σ	Stress tensor [Pa]	$\zeta_1, \zeta_2, \zeta_3, \zeta_4$	Coefficient of second viscosity [$Pa.s$]
σ	Entropy (Chapter 2) [J / K]	$\frac{D}{Dt}$	Material time derivative (unit depends on the operated)
σ	Specific Lennard-Jones distance (Chapter 7) [m]	$\hbar$	Planck's constant divided by 2π [$J.s$]
${}^0\tau_0^0$	Time-lag [s]		
τ	Dissipative term of stress tensor, stress tensor [Pa]

Nomenclature

$()_{,i}$	$= \frac{\partial}{\partial x_i}$
div	Divergence

Chapter 1 : Introduction

Since the discovery of superfluidity in 1938, there have been plenty of attempts to justify the peculiar behaviors seen in superfluids. From those early days up to the present, all prominent physicists (and even mathematicians) have tried to model the superfluid state using various methods ranging from quantum mechanics to continuum mechanics.

It has to be stated that many of these models are capable of predicting the phenomenon. However, there is one big problem in all of the models. That problem is the unawareness of the true microscopic cause for the superfluidity. Some physicists believe that there is a quantum mechanics explanation behind the phenomena. Their justifications are, somehow, acceptable as long as the low-temperature physics is under scrutiny.

In this report, after a vast and thorough literature survey, the author has tried to express the idea that the quantum mechanics is not the ultimate player in superfluidity, at least at high-temperature. The main idea is the time lag in the transport of energy (information) in the domain. It is a simple physical idea, which shows that the phase lag (time delay or time lag) predicts superfluidity. By superfluidity, it is meant that the transport of energy and momentum can occur by waves experiencing very little resistance.

Prediction of the superfluidity has not been the unique outcome of the phase-lagged energy propagation formulation. In fact, in Chapter 5, it is shown that the time lag in information transport will lead to more insights about the previous models of physical phenomena. At first, the capabilities of the idea were confirmed in Chapter 6, on the concept of nano-scale heat transfer. It was observed that the idea can be expanded to more fields in physics. At this point, one could clearly observe that the simple idea, which was originally and systematically proposed by Einstein, has not been employed in

related physical formulations. The formulations spanning from equations like heat and mass transfer up to the fundamental ones, such as quantum mechanics. In this work, two viewpoints are emphasized. The first is the formulation of the phase lag from the large scale point of view, capturing the micro-scale features (Chapters 3, 4 and 5). The results are partial differential equations (large scale point of view) capturing superfluidity and wave transport of energy (micro-scale feature). The second is the utilization of the idea in the micro-scale. The latter resulted into two fundamental conclusions. The new nano-scale heat transfer formulation was an early consequence (Chapter 6). Later, the implication of the time lag showed great insights about possibilities in the molecular domain (Chapter 7).

Since the model presented in this report is the newest model to describe the superfluidity, and predict it at high temperatures, the author has tried to show the validation of the model by converting it into one of the previous well-known models by using mathematical linear approximation procedure. This approach suggests that not only could the model be correct, both physically and mathematically, but also a more rigorous one among all other models. On the other hand, it was possible to discuss some other properties of the superfluidity by using the new model, e.g. the fountain effect.

The equations arising in the new model of superfluidity and transport phenomena are a new class of Differential Equations, which are denoted Delay Differential Equations (DDEs). There have been some attempts to solve DDEs, both partial and ordinary ones, but only a few ones can solve the equations encountered in this report. Here, it was shown that there is the possibility to solve some subclasses of the Partial DDEs, occurring in the model, in a general and systematic way. These solutions are completely new and they seem to provide a hint gate into the solution spaces of PDDEs. The main

characteristic of these solutions is the damped wave behavior, which has been shown using the numerical tools for solving the Phase-Lagged Heat Equation (PLHE).

It is to the point, to mention that, the model presented in this report will, probably, have the ability of extension into other fields of physics. The reason is the pure simple idea behind the modeling. The model will be of great use in areas such as superfluidity, superconductivity, start-up flows, ultra-short phenomena (such as ultra-short laser pulses), supertransport of energy, etc.

The roadmap of the thesis is as follows. In Chapter 2, a thorough literature review is done. Almost all known superfluid models have been gathered as a unique collection in that chapter. In Chapter 3, the high-temperature model of superfluidity is extended. The extension has been over the original Kulish and Chan model of high-temperature superfluidity. In Chapter 4, the solutions of the phase-lagged heat equation are found for special cases, both analytically and numerically. In Chapter 5, solutions for the approximated model, of the extended model of Chapter 3, are presented. This chapter was motivated by one of Professor Leggett's pioneering papers on the superfluid topic. In Chapter 6, a new phenomenological heat transfer model is considered. This model is in accord with observations of the nano-scale heat transfer; e.g. slip boundary condition and heat wave. Finally, in Chapter 7, new results, with respect to time lag in information transport at molecular level, are presented and used as a justification for the high-temperature model of superfluidity.

An important fact has to be mentioned about the report. This work started with a simple idea. The author expected that the idea could possibly be implemented in few areas of physics, such as heat and mass transfer to justify the wavy transport of energy at small-scales. However, the consequences were beyond a dissertation! Upon Chapters 6 and 7,

Chapter 1

it was understood that some equations, in physics, need partial reformulation. As an example one can mention the relationship between the time delay and quantum mechanics. The latter can be a challenging topic in itself for an in-depth research in the future.

Chapter 2 : Literature Review

2.1- Superfluidity at Low Temperatures

Although there were some notations about the peculiar behavior of liquid 4-He [1], it is believed that superfluidity was found simultaneously by Kapitza [2], in Moscow, and Allen and Misener [3], in Cambridge, in 1938. The superfluidity becomes apparent at a characteristic temperature known as “Lambda point” ($T_\lambda = 2.177\text{ K}$) and below, in 4-He, that flows through narrow capillaries (with the radius of the order of $10^{-5} - 10^{-6}\text{ m}$). The fluid flows with very little resistance against its motion. The first time the term *superfluid* was used, was in a paper by Kapitza [2], in which, according to the analogy with superconductors, the name was adopted. As a reminder, superconductors are materials, in which the flow of electricity does not experience any resistance. In that paper, the viscosity of He-II was estimated to be 1500 times smaller than that of He-I at normal pressure (He-I is the helium-4 above T_λ and He-II is below it; see Figure 1). An upper limit of the order 10^{-9} C.G.S. to the real value was mentioned ($\text{C.G.S} = 0.001\text{ Pa.s}$).

Another property of the observed phenomenon at that time was the high thermal conductivity. The high thermal conductivity was considered a consequence of what Kapitza [2] believed to be a turbulent flow. Although the high Reynolds number might be an indication of turbulent flow in liquid He, Allen and Misener [3] addressed the point that as the velocity of the superfluid is almost independent of pressure, any known formula could not give a value of the viscosity that would have much meaning in defining the Reynolds number. As a result of this debate, one can propose that the high

thermal conductivity is not a necessarily consequence of what might be a turbulent flow.

The strange thermal conductivity behavior of liquid helium made Mendelson [4] state that “the concept of heat conductivity in the accepted sense as a constant ratio of heat current density to the temperature gradient has thus lost its usefulness when dealing with liquid helium II”. In Chapter 6, it will be mentioned that the concept of heat conductivity is questionable. Also, it will be shown that the boundary slip is a consequence of nano-scale heat transfer.

Figure 1- Phase diagram of Helium 4 ([5])

Thermodynamically, the phase transition to superfluid state is accompanied by a specific heat anomaly (see Figure 2) [6]. Since entropy is released as the temperature is lowered through T_λ the superfluid state has less entropy than the extrapolated normal state at the same temperature. Roughly speaking, the superfluid state is more ordered than the normal phase.

Albeit no evidence of superfluidity was found up to 1.05 K, in 3-He [7], an evidence of a new phase in 3-He was discovered by Osheroff *et al* [8]; but to mention the true historical event, one should reference the fact that at that time it was believed a new solid phase was found! However, the new phase was originally a superfluid state. A suggestive justification for the observed pressure-temperature diagram was presented using the

Clausius-Clapeyron equation. The observed phase change was at $T=2.65 \text{ mK}$ and $P=33.9053 \text{ atm}$ [8]. A phase diagram of Helium-3 can be seen in Figure 3.

Figure 2- Specific heat of liquid helium (4-He) [9]

Figure 3- Phase diagram of Helium-3 in the absence of magnetic field [10]

One of the best explanations about the experimental physics of superfluidity in definition (which inherently shows the idea of two-fluid model presented in the coming sections), has been proposed by Leggett [11]. The corresponding paragraphs from his work is quoted here:” *...In fact, from a modern point of view, superfluidity is not a single phenomenon but a complex of phenomena, and the picture becomes clearer if one considers not a channel between two bulk reservoirs, as in the experiments of Kapitza and Allen and Misener, but rather an annular geometry. Let us then consider a hollow*

cylinder of height h , inner radius $R - d/2$ and outer radius $R + d/2$, where $d \ll R$; for the moment we assume that deviations from exact cylindrical symmetry are small (but nonzero). Then, if the cylinder is filled with 4-He, we can observe two conceptually distinct (though related) phenomena. The first is sometimes called the Hess-Fairbank effect: the system appears to come out of equilibrium with its rotating container. To amplify this definition, we all know that if we take our annulus filled with water and set it on an old-fashioned gramophone turntable which we then set into rotation, the water will come (after a delay of maybe 1 min) into rotation with the annulus and will thereafter rotate with it as long as the turntable continues to rotate. When we stop the rotation, the water also gradually comes to rest. Imagine now that we do the same experiment with He, starting above the lambda point and rotating **very slowly** (for a 1-cm-radius annulus, the angular velocity would have to be $\leq 10^{-4}$ rad/sec to see the specific behavior to be described; in practice smaller radii are used and the criterion is not quite so stringent). The helium behaves in exactly the same way as the water, coming into rotation with the container. Now suppose that, while still rotating with this low angular velocity, we cool the system through the lambda temperature. The helium then appears to gradually come out of equilibrium with the container, i.e., to cease to rotate even though the container is still rotating! In fact, as T falls to zero, the He appears at first sight to come to rest in the laboratory frame (or, to be more precise, rather in the frame of the fixed stars). It is clear that this behavior cannot simply reflect very long relaxation times, since the liquid has come out of equilibrium with the container: **the “non-rotating” state must be the true thermodynamic state**. This Hess-Fairbank effect is the exact analog of the Meissner effect in a superconductor. It is conventional to define the **superfluid density** $\rho_s(T)$ [or superfluid fraction $\rho_s(T)/\rho$, where ρ is the total density] in terms of the experimentally observed value of the temperature-dependent

moment of inertia $I(T) \equiv L/v$ relative to its classical value $I_{cl} \equiv NmR^2$: $\rho_s(T)/\rho \equiv 1 - I(T)/I_{cl}$. The second phenomenon is the following: Again put the He, above T_λ , in the annulus and set the latter into rotation, but this time much faster. This time, as we cool through T_λ , we see very little change: to all intents and purposes the liquid continues to rotate with the container. Now stop the container. The He continues to rotate, apparently indefinitely. One can show rigorously that for the container stationary the rotating state cannot be the thermodynamic equilibrium one, so what we are seeing here is an example of an extremely long-lived metastable state. I shall refer to this phenomenon as **metastability of superflow**...”

Physical consequences of superfluidity are numerous. Concepts such as non-existence of boundary layer, creeping flow and thermomechanical occurrence of superfluid helium II are important as they oppose to the known ordinary fluids behaviors. As a superfluid does not have any apparent viscosity, the boundary layer concept looks irrelevant for superfluids. Experiments, showing the nonexistence of boundary layer, have been conducted in some cases; e.g. Venturi tube experiment [12] and superfluid wind tunnel [13].

The thermomechanical effect (when helium flows out of a vessel through a thin capillary a heating is observed in the vessel [14]) is shown to be the reason for the Fountain effect. The Fountain effect is observable when a temperature difference is imposed between the ends of a capillary filled with liquid 4-He below λ -point. A gradient of the density in excited atoms (non-superfluid atoms) will force them to diffuse towards the colder end and the superfluid to the opposite direction. As the temperature decreases, this effect intensifies [3] (Terms like excited atoms and non-superfluid atoms will be discussed in next section in more detail.)

Rollin and Simon [15] observed that the liquid helium below the lambda transition temperature would place itself as a film along the solid surfaces of the containers. This creeping effect of helium is known as *Rollin Film*. Daunt and Mendelssohn [16] expanded these observations by confirming that liquid helium II collects always at the lowest available level. More interestingly they showed that the rate of transfer (balancing the heights) is independent of the differences in height between the levels and of the underlying material. It was also shown that the rate of the phenomena is exactly proportional to the width of the connecting surfaces. The Rollin film characteristics are affected by temperature rather than gravity [16]. They concluded their observations that the heat transfer was believed to be caused by the transport of matter, subsequently they stated that the heat conductivity was very small.

There are other observations about the existence of superfluidity. Before talking about those issues, it is better to present some more unfamiliar physical concepts and states such as BEC. In the next section, those matters are defined and then one can proceed with the survey based on their interpretations.

2.2- Low-Temperature Superfluidity, Bose-Einstein Condensation, Bardeen-Cooper-Schrieffer and Quantized Vortices

London [17] for the first time mentioned that the peculiar behaviors of the Helium-4 at lambda point might be considered as a consequence of BEC (Bose-Einstein Condensation); a state of matter which were believed to be just imaginary. It was hoped that the concept would shed light on the peculiar behavior of He-II and it really did in many cases. The helium atom is composed of an even number of elementary particles (2 protons, 2 neutrons, 2 electrons) and according to general concepts of quantum field

theory, the many-body wave function of the system should obey a kind of statistics known as “Bose statistics” [18]. It is possible to show that the thermodynamic behavior of a gas obeying Bose statistics (and excluding any interaction between atoms), would show below certain temperature (which depends on the mass and density) that a finite fraction of atoms occupy a single one-particle state [19]. London [20] could show that helium with the assumption of a non-interacting gas with the known density of 4-He the BEC would occur at 3.13 K which is close to lambda temperature (2.177 K). He could also explain the quantitative behavior of specific heat of helium using the BEC idea. In the same paper it was shown that there has to be a jump of slope in C_v at that transition temperature. What London [20] showed was not simply accepted by all as long as the Helium-II is neither dilute nor non-interacting.

With respect to the BEC model, a very rough qualitative description about superfluidity is that as long as all atoms are in the lowest energy state, they cannot lose any more energy, not even by friction. As a result, the fluid cannot have any energy loss (or apparent viscosity). Tisza [21] could also justify the experimental results for thermomechanical and Fountain effects by the idea from BEC. He mentioned that the viscosity was entirely due to atoms in the excited states (non-superfluid); the atoms which are not condensed into BEC.

One of the first quantitative attempts to show that the interatomic potential does not alter the existence of a Bose-Einstein condensation in 4-He was conducted by Feynman[22]. It was the idea which saved London’s perceptions [20]. He could show that, in spite of large interatomic forces, liquid 4-He should exhibit a transition analogous to the transition in an ideal Bose-Einstein gas. It was shown that the motion of atoms is somehow like free particles and the potential barriers do not affect the motion as the

other atoms might move out of the way. Although it was an adequate attempt to show BEC-like behaviors in helium, rough estimates in that paper showed the transition to be of third order not second [23]. In fact, it is believed that second order transition is responsible for superfluidity.

The idea of BEC was a good motivation to perform experiments to reach it [24]. Those experiments finally led to temperatures of around $200nK$. The extremely low density (hundred thousandth the density of the normal air) is the key to reach BEC to avoid conventional condensation into liquid and solid. Under such conditions, the formation time of molecules or clusters by collisions is stretched to seconds or minutes. As a result of such temperatures and densities, the BEC in dilute gas was shown to really exist in Sodium-23 [25], Rubidium-87 at $170nK$ [26], Rubidium-85 [27], lithium-7 at $200\mu K$ [28], atomic hydrogen at $50\mu K$ [29] dilute gases. Also, the evidence of BEC in potassium was found by Modugno [30] by the method of sympathetic cooling with evaporatively cooled rubidium at around $160nK$. The BEC in *molecules* was also reported [31, 32] in 6-Li. As a reminder, one has to mention that all are alkali elements. Although Bose–Einstein condensation and superfluidity are intimately connected, they do not necessarily occur together [33]. In the same paper, it was mentioned that, in lower dimensions, superfluidity occurs in the absence of Bose–Einstein condensation, an ideal Bose gas or disordered three-dimensional system can have a condensate, but shows no superfluidity [34]. Leggett [19] previously pointed out such problem and in his words: “...in the sixty years since London’s original proposal, while there has been almost universal belief that the key to superfluidity is indeed the onset of BEC at the lambda temperature it has proved very difficult, if not impossible, to verify the existence of the latter phenomenon directly”. Leggett [35] brought up the question that whether BEC is a

necessary condition for *NCRI* (nonclassical rotational inertia) in a bulk three-dimensional system or not. NCRI (the explanations of Professor Leggett presented in the previous section) is an indication for the superfluid part of a system.

A close area to superfluidity is superconductivity. Superconductivity by some scientists is believed to be nothing but superfluidity occurring in a charged system [19]. London [36] explicitly emphasized the relation between these two phenomena. He mentioned that the “super-transport” phenomena must be caused by some elementary mechanics in which quantum mechanics plays an essential role.

Remarkable progress in the phenomenological description of superconductivity was made in the early 1950s; in particular, by introducing the concept of a “macroscopic wave function” or order parameter. The possibility of some relation between superconductivity and superfluidity was also reflected in some of Feynman’s works [37], however the milestone of this relationship was founded by a theory for superconductivity.

Theory of superconductivity (BCS (Bardeen-Cooper-Schrieffer) theory) opened new doors to superfluidity [38]. The theory was based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy. They postulated that in the superconducting state the electrons within a “shell” of width $k_B T_c$ around the Fermi energy (where T_c is the temperature of the superconducting transition and k_B is the Boltzmann constant) tend to form Cooper pairs, a sort of giant “dielectronic molecule,” whose radius is huge compared to the average distance between electrons (so that, between any two electrons forming a Cooper pair there are billions of other

electrons, each forming their own pairs). An essential feature of the BCS theory of superconductivity is that the Cooper pairs, once formed, must all behave in exactly the same way, that is, they must have exactly the same wave function, as regards to both the center of mass and the relative coordinate. In summary and simple words, the Fermi particles form Bose ones by pairing in Cooper pairs.

The main difference between 3-He and 4-He is due to nuclear spin for which they are half (obeying Fermi statistics) and zero (obeying Bose statistics), respectively. It is known that below $T=2.65 \text{ mK}$ not only one, but also three anomalous phases of liquid showing superfluidity exist; see Figure 4 [19].

The Fermi statistics of 3-He is annoying, but one can find the resemblance with superconductors. It might be possible that the fermions pair up to form “Cooper pairs”- a sort of giant diatomic quasi molecules, whose characteristic “radius” is very much larger than the typical interatomic distance- which are now able to obey Bose statistics and finally undergo BEC [19]. Imagining a noninteracting gas of such particles in thermal equilibrium at a temperature $T \ll T_F = \varepsilon_F / k_B$ (where ε_F is the “Fermi energy,” determined by the mass and density), then all states lying well below ε_F in energy are occupied by a single particle, and all those well above ε_F are empty [39].

Landau [40] showed that under appropriate conditions, even at the presence of strong interparticle interactions, the qualitative picture remains valid and the system is called “degenerate Fermi liquid”. For the case of 3-helium experiments showed that it is really a degenerate Fermi liquid below $\sim 100 \text{ mK}$ to around 3mK [39]. In contrast to the thermally disoriented molecules in ordinary gases, all the Cooper pairs in 3-He-A have

the same direction of angular momentum, hence the system behaves exactly as a ferromagnet [41]; an expectation to pure anisotropic fluid.

Figure 4- Phase diagram of Helium-3 in the presence of magnetic field [10]

Anderson [42] mentioned that the most important equations of the dynamics of the superfluid helium-II and superconductors follow directly from the simple assumption that the quantum field of the particles has a mean value which may be treated as a macroscopic variable. The concept of superfluid velocity

$$\mathbf{v}_s = (\hbar / m) \nabla \phi \quad (2.1)$$

was explained to be an important concept in supertransport phenomena, although immaturely. The particle field operator ψ ¹ was introduced and mentioned that it has a macroscopic mean value

¹ Order parameter: the macroscopic state of superfluids can be described by a complex number known as the order parameter, which is defined for every point in space. The order parameter, ψ , represents a macroscopic variable similar to temperature or pressure. ψ only has meaning when considered on length scales larger than the atomic scale and can vary over macroscopic distances. In the lowest energy state of a superfluid, the magnitude and phase of the order parameter are uniform throughout space. Spatial variation

$$\langle \psi(r, t) \rangle = f(r, t) \exp[i\phi(r, t)]. \quad (2.2)$$

The ϕ is coupled to external forces while f is just an internal parameter. In a multiply connected region, it is

$$\oint \nabla \phi \cdot ds = 2\pi n \quad (2.3)$$

in which the integration is performed around a nonsuperfluid obstacle. At absolute zero the quasi-particle model pictures the superfluid as forming a continuous fluid. The above statements become clearer as only a single wavefunction describes the fluid. The stated velocity $\mathbf{v}_s$ is important in the theory of superfluidity. One reason is that unlike the analogy with single particle quantum mechanics, $\mathbf{v}_s$ characterizes the behavior of a macroscopic number of particles and, as a result, it can be regarded as a classical quantity[11]. One assumption behind $\mathbf{v}_s$ is that it is only based on the simple Bose condensation.

The BEC was not the only goal for the experimentalists; they even tried to reach BCS states in some cases. Kinast [43] observed the evidence for superfluidity in Fermi gas of 6-Li. In fact, the author mentioned that without invoking the superfluidity it could be difficult to explain the observations of the experiments. It has been observed that fermionic atom pairs in the BCS-BEC crossover occur in potassium-40 [44]. Even more, in 40-K found the ultracold molecules from a Fermi gas of atoms [45]. The emergence of Bose-Einstein Condensate from a Fermi gas was reported by Greiner *et al.* [46]. Other Fermionic superfluidity was also reported [47, 48].

in the order parameter causes energy excitations in the superfluid. The superfluid is completely defined by defining ψ .

As it is believed by some physicists, a possible consequence of BEC might be superfluidity, as a result the latter elements would be able to show the superfluid state such as quantized vortices. When superfluid is set into rotational motion, there have been some cases in which the circulation imposed on the superfluid is just observable at some topological defects in the fluid, Figure 5. The diameter of the dark circle is corresponding to the 2-*mm* bucket.

Figure 5- Photographs of stable vortex arrays [49]. The angular velocities are (a) 0.3 sec^{-1} (b) 0.3 sec^{-1} (c) 0.4 sec^{-1} (d) 0.37 sec^{-1} (e) 0.45 sec^{-1} (f) 0.47 sec^{-1} (g) 0.47 sec^{-1} (h) 0.45 sec^{-1} (i) 0.86 sec^{-1} (j) 0.55 sec^{-1} (k) 0.58 sec^{-1} (l) 0.59 sec^{-1} [49]

Quantized vortices in a rotating gas provide conclusive evidence for superfluidity for some scientists, because they are a direct consequence of the existence of a macroscopic wavefunction that describes the superfluid. The velocity field of the superfluid is proportional to the gradient of the wave function's phase, as mentioned in previous paragraphs. In such a case, flow must be irrotational and angular momentum can enter the system only in the form of discrete line defects (vortices) [33]. As indicated by

Pitaevskii and Stringari [50], the superfluidity in a Fermi gas should be investigated through rotational phenomena such as quantized vortices. From a quantum mechanics view point, it is obvious when a quantum-mechanical particle moves in circle the circumference of the orbit has to be an integer multiple of the de Broglie wave length. For a rotating superfluid, it leads to quantized vortices. Unlike a normal fluid that rotates like a rigid body, a superfluid BEC would show quantized vortices scattered in the medium under the influence of rotation. This corresponds to an array of vortices. It is known that when an atom goes around the vortex core, its quantum mechanical phase changes by exactly 2π . Many of these kinds of vortices have been observed, in superfluids [49, 51-53].

When a quantum fluid is rotated, it attempts to distribute the vorticity as uniformly as possible. For a superfluid the circulation of the velocity field is quantized in units of $k = h / M$, where M is the atomic mass and the h is Planck's constant. The quantized vortex lines are distributed in the fluid with a uniform area density [51]. There exists $2\omega / k$ circulation quanta per unit area when the angular velocity is ω [6].

Metastable vortex patterns have been observed in classical inviscid fluids. However, the final number and charge of the vortices depends chaotically on the initial conditions, in contrast to the regular vortex lattices that one might have reproducibly observed in superfluids. Furthermore, vortex patterns in classical fluids are only stable at extremely low viscosity (that is, for Reynolds numbers $> 10^5$) [33].

It is appropriate to name some of the applications of low-temperature superfluidity, at the end of this section. It can be used in many space explorations; such as in superfluid clock and superfluid gyroscope [54]. An area in which the uniquely rich structure of the order

parameter (pair wave function) of superfluid 3-He has had fruitful consequences in studies of chaos and turbulence, and particularly of the way in which topological defects in the order parameter are generated in quenching through a phase transition (a process that is in fact frequently regarded as a model for processes believed to occur in the early universe) [39]. Another area is metrology (the determination of the fundamental constants) in which the “superfluid amplification” property might be useful.

2.3- Review of Theories of Superfluid State

In 1940, Darrow [55] gathered all the peculiar characteristics of the superfluid Helium known to scientists, up to that time, but it was a long way ahead to reach a good understanding of the superfluidity and also an in-depth theory about the phenomenon. In the subsequent subsections, some of the most important models are presented. These are the most prominent models that have been developed so far. The starting point is the oldest “Two fluid theories”.

2.3.1- Two Fluid Theories

2.3.1.1- Helium-4

The first robust quantitative model for helium superfluidity was first introduced by Landau [56, 57], although Tisza [21] qualitatively and explicitly stated the fact that the helium-4 can be regarded as a two-fluid system. Truly, it is not necessarily an adequate theorem. In fact, it is not that one encounters two distinct fluids under investigation, but it is merely a model (quantum model) to be described in classical terms. It has to be emphasized that Landau never introduced the facts of BEC.

As mentioned in the previous section, if the fluid (Helium II) is rotated in an axial-symmetric vessel with constant angular velocity, one part of the fluid would rotate like normal fluids and the other would remain stationary. Again, for emphasis, one has to mention that this model does not imply that there can be a true distinction between real fluid particles. The rest is the *phenomenological* model presented by Landau [57] with some minor corrections he made later [58], in accordance to measurements done by Peshkov [59].

The following theory is sometimes referred to as Landau-Khalatnikov two-fluid model, because of the great contributions of Khalatnikov in the formulation of this model [60].

One can start the discussion about this model by considering its microscopic properties. This way of presenting it is due to Landau's point of view.

Denoting ε the energy of an elementary excitation² [61], in liquid helium, as a function of its momentum p , the form of energy spectrum for small values of the momentum p is easily determined. Small momenta correspond to long-wavelength excitations, which in a liquid are obviously just longitudinal sound waves. The corresponding elementary excitations are therefore sound quanta or *phonons*, whose energy is a linear function of the momentum,

$$\varepsilon = cp \quad (2.4)$$

where c is the speed of sound. As the momentum increases, the curve $\varepsilon(p)$ departs from a straight line. This part corresponds to the potential part of the flow.

² From quantum mechanics, it is known that for every slightly excited macroscopic system a conception can be introduced as "elementary excitation", which describe the collective motion of the particles and which have certain energies and momenta.

Landau observed it is not possible to justify the thermodynamic (temperature dependence) behaviors by just considering phonons. Consequently, another kind of excitations named as *rotons* was also introduced. Rotons are vortex part of the flow. The lowest level of the vortex spectrum is situated above the lowest level of the potential spectrum. The corresponding energy near the minimum is

$$\varepsilon = \Delta + \frac{(p - p_0)^2}{2\mu} \quad (2.5)$$

in which p_0 is the value of the momentum at which the function ε has a minimum equal to Δ . μ is the effective mass of the roton. The latter quantity along Δ , p_0 are found experimentally ($\Delta / k_B = 8.6K$, $p_0 / \hbar = 1.91\text{\AA}^{-1}$ and $\mu = 0.16m_{He}$) [60]; see Figure 6.

Figure 6- Elementary excitations energy distribution [9]

In order to define the energy distribution of the elementary excitations, it is necessary to conduct experiments on liquid helium. One of the examples of these ilk of experiments is neutron scattering. The energy excitation spectrum is connected to the structure factor S (of the liquid for neutron scattering) by the relation

$$E(k) = \frac{\hbar^2 \mathbf{k}^2}{2mS(\mathbf{k})} \quad (2.6)$$

[62]. It was shown that for small k (the wave number) the energy raises linearly (phonons) and larger values shows the Landau proposed rotons.

Qualitatively, Feynman [63] argued that the lowest energy states are phonons. These statements about phonons and equation (2.6) truly credited Landau's two-fluid model [62]. The thermodynamic and hydrodynamic behaviors of liquid helium were reviewed by Feynman [62], who mentioned that separating the fluid into two parts is a mathematical artifact and not a true concept. Qualitatively, the proposed wave function by Feynman and his coworker would suggest that the roton is a kind of quantum-mechanical analog of macroscopic vortex ring, of diameter about equal to the atomic spacing. An important concept of the vortex rings is that their location is not definable.

For rotons, the energy distribution is determined according to Boltzmann distribution, and Bose distribution for phonons. In this manner the model of an ideal gas of excitations is appropriate at temperatures which are not near the lambda point.

With respect to this theory, superfluidity occurs at a velocity which is smaller than a critical value as

$$v_{cr} = \min \frac{\varepsilon(p)}{p}. \quad (2.7)$$

There can be two independent motions simultaneously in a superfluid according to discussions presented so far. One part is carried along by excitations, acting like normal liquid (with the velocity $\mathbf{v}_n$) and the rest is the superfluid (superfluid velocity defined as $\mathbf{v}_s$) as long as its velocity is less than some critical value stated by (2.7). The two motions are independent of each other and one can write the momentum per unit volume $\mathbf{j}$ of Helium II as

$$\mathbf{j} = \rho_s \mathbf{v}_s + \rho_n \mathbf{v}_n. \quad (2.8)$$

The ρ_s and ρ_n are superfluid and normal density, respectively. The total density of the fluid is

$$\rho = \rho_s + \rho_n. \quad (2.9)$$

The ratio ρ_n / ρ is unity at lambda point and zero at $T = 0$. Despite all other mixtures, in which the amount of components can have a range of density values, the superfluid and normal density cannot obtain values other than that appropriate to the thermodynamic state specified. As a result of this discussion, it is impossible to obtain a pure sample of superfluid. To some extent, what has been stated here implies that it might be possible to imagine the whole fluid as one component and describe it with other constitutive laws. In the next subsection, some models based on this idea are presented.

All thermodynamic relations regarding the superfluid helium-II can be considered according to the two-fluid model, in which the phonons and rotons are the corresponding parts in every relation. As the densities of both parts are small, the gases of excitations are assumed to be ideal gases. The relative velocity in deriving thermodynamic relations is ignored, and the issue is just considered in the case of a sound propagation problem.

Finding the Helmholtz energy from the phonon and roton distributions, one can derive its negative value with respect to temperature to find the entropy. It is also possible to derive the specific heat from the entropy by the relation

$$C = T \frac{\partial S}{\partial T}. \quad (2.10)$$

One has to take the phonon and roton parts separately and add them up at the end to find the thermodynamic relations

$$S = k_B \Pi_r \left(\frac{\Delta}{T} + 1.5 \right) + \frac{16\pi^5 k_B}{45} \left(\frac{k_B T}{2\pi\hbar c} \right)^3 \quad (2.11)$$

and

$$C = k_B \Pi_r \left(\frac{\Delta^2}{T^2} + \frac{\Delta}{T} + 0.75 \right) + \frac{16\pi^5 k_B}{15} \left(\frac{k_B T}{2\pi\hbar c} \right)^3 \quad (2.12)$$

in which

$$\Pi_r = \frac{2p_0^2 \sqrt{\mu k_B T} e^{-\frac{\Delta}{T}}}{(2\pi)^{3/2} \hbar^3} \quad (2.13)$$

is the number of rotons per unit volume of helium. Taking into account the relative velocity, the formulas would be much more complicated and the reader is referred to the book by Khalatnikov [60]. The last terms in both equations correspond to phonons and the first ones to rotons.

Now, according to the discussions stated previously one qualitative reason for the thermomechanical effect is that as the superfluid creeps out, and it is not able to carry heat with itself (because it does not contain any phonon or roton, it is superfluid), the heat in the vessel is distributed over a smaller amount of helium. When the helium flows in the reverse phenomena would happen. The superfluid part is not able to carry heat, being then the reversible part of the fluid [57].

In the temperature range from 0.8 to 1K, it is the rotons that contribute most to the thermodynamic functions, although the contribution decreases rapidly with decreasing temperature.

Landau formulated the governing equations of the liquid into operators, or in other words into the language of quantum mechanics, which really attracted serious criticism (like London [5]) to his model. In quantization of the motion of the liquid into quantum mechanics operator forms, the continuity equation would become

$$\dot{\rho} + \text{div} \frac{\rho \mathbf{v} + \mathbf{v} \rho}{2} = 0 \quad (2.14)$$

and

$$\dot{v}_i + \left(v_k \frac{\partial v_i}{\partial x_k} + \frac{\partial v_i}{\partial x_k} v_k \right) + \frac{1}{\rho} (\nabla P)_i = 0 \quad (2.15)$$

in which the pressure P is equal to $\rho^2 \left(\partial / \partial \rho \right) (E / \rho)$ as in a classical liquid. The latter equation, equation (2.15), is similar to Euler's equation [56, 57]. There is no intension to examine this quantum mechanics language, for the time being, because of its extensive prerequisites in quantum mechanics.

In a phonon gas one can assume that the gas is in energy equilibrium. This is the way Landau considered his derivations. However, it is possibly a problem for these kinds of formulations that the system is assumed to be in energy equilibrium. In fact, some new ideas are in direct contradiction to such assumptions. In the coming subsections, this problem will be mentioned in details, in the realm of extended thermodynamics.

The assumption, on which the hydrodynamics of superfluid is built on, is that the ordered motion of the excitations carries along only “normal” density ρ_n . The remaining part is the superfluid with density

$$\rho_s = \rho - \rho_n \quad (2.16)$$

which performs an independent motion. The latter motion is irrotational. Hence, there are two independent motions in a superfluid with velocities $\mathbf{v}_n$ and $\mathbf{v}_s$ in which

$$\nabla \times \mathbf{v}_s = 0. \quad (2.17)$$

The last equality is not violated until the flow velocities have reached certain critical values where the normal and superfluid parts of the liquid begin to interact. One has to be careful that this concept is not a very rigorous one. No experimental validity of such a thing seems to exist [64]. However, Feynman [62] solved this problem by supposing that the superfluid component is curl free at the microscopic level and on the macroscopic level creates quantized vortices. This picture seems to be faulted and it will be considered at the coming subsections, where recent mathematical tools in mechanics imply that equation (2.17) is just a special class of some motions in super fluid dynamics. This issue will be under study later.

Before proceeding further, the convention is accepted that any subscript (or superscript) n refers to the normal part and any s refers to the superfluid part. The other subscripts, such as k , represents the coordinate direction number; in this text, the Einstein summation convention is obeyed, except when stated otherwise. One thing about the densities is that although they are functions of temperature and pressure, they do not depend on the history of the flow in any discernible way [65].

If the dissipation is ignored, the equations governing the superfluid, that is the conservation of mass, momentum and entropy, are, respectively

$$\frac{\partial \rho}{\partial t} + j_{i,i} = 0 \quad (2.18)$$

$$\frac{\partial j_i}{\partial t} + \Pi_{ik,k} = 0 \quad (2.19)$$

$$\frac{\partial(\rho s)}{\partial t} + (\rho s v_{ni})_{,i} = 0. \quad (2.20)$$

The last equation, in fact, shows that the entropy is merely conveyed by means of normal component ($\rho s v_{ni}$ is *entropy current*). However, the superfluid has its own entropy. The equation of evolution of the superfluid velocity is

$$\frac{\partial v_{si}}{\partial t} + \left(\mu + \frac{v_{sk} v_{sk}}{2} \right)_{,i} = 0. \quad (2.21)$$

For the case of steady flow on a streamline, two Bernoulli-like equations evolve

$$\frac{\mathbf{v}_s^2}{2} + \mu = \text{const.} \quad (2.22)$$

$$p + \rho_s \frac{\mathbf{v}_s^2}{2} + \rho_n \frac{\mathbf{v}_n^2}{2} = \text{const.} \quad (2.23)$$

These formulations are called ***phenomenological*** as they are not constructed on any apparent system of axioms. The latter is like the formulations in “***rational continuum mechanics***” where the axioms reduce to equations of motion.

To completely define the fluid motion one needs to find the mass current (momentum per unit volume) j , the stress tensor Π_{ik} and the scalar quantity μ . Considering the conservation of energy

$$\frac{\partial E}{\partial t} + Q_{i,i} = 0 \quad (2.24)$$

and also using the Galilean invariance principle, one can obtain the mass current as

$$j_i = \rho_n v_{ni} + \rho_s v_{si} \quad (2.25)$$

the stress tensor as

$$\Pi_{ik} = \rho_n v_{ni} v_{nk} + \rho_s v_{si} v_{sk} + p \delta_{ik} \quad (2.26)$$

and the energy current density as

$$Q_i = \left(\mu + \frac{v_{sk} v_{sk}}{2} \right) j_i + T \rho_s v_{ni} + \rho_n v_{ni} (v_{nk} v_{nk} - v_{np} v_{sp}). \quad (2.27)$$

The scalar μ can be shown to be the chemical potential. The above simplified equations are for the case of small velocities. In cases, of the propagation of sound, the nonlinear character of the fluid plays a role and the region of application of the general equations becomes apparent.

Again, under non-equilibrium conditions the usual definitions of thermodynamic quantities lose their meaning and must be made more precise. In fact, Landau's superfluid formulations are all based on the assumption of quasi-equilibrium. Khalatnikov [60] stated that s will not be the true entropy. However, for situations close to equilibrium, when the gradients of all quantities are small, the entropy defined in this manner $s(\rho, E, |\mathbf{v}_n - \mathbf{v}_s|)$ will be almost identical to the true entropy.

If the system is close to thermodynamic equilibrium, the *thermomechanical* force that causes superfluid and normal fluid to move differently, can be expressed as $\mathbf{F} = \rho_s s \nabla T$. This force sets up a counter-flow in which superfluid flows up the

temperature gradient from the heat sink to source and the normal fluid would do vice-versa. This is a direct consequence of the two-fluid formulation.

All of the formulas, presented so far for the equations of motion, were for the non-dissipative cases. On the other side, if one considers the dissipative terms in the hydrodynamic equations, the above equations would change to similar ones. The continuity equation surely remains the same as equation (2.18). After some investigation the mass current relation will be

$$\frac{\partial j_i}{\partial t} + \Pi_{ip,p} + \tau_{ik,k} = 0 \quad (2.28)$$

in which the dissipative term is

$$\tau_{ik} = -\eta \left(v_{ni,k} + v_{nk,i} - \frac{2}{3} \delta_{ik} v_{nl,l} \right) - \delta_{ik} \left(\zeta_1 (j_{m,m} - \rho v_{np,p}) + \zeta_2 v_{na,a} \right). \quad (2.29)$$

The equation of evolution of the superfluid velocity is

$$\frac{\partial v_{si}}{\partial t} + \left(\mu + \frac{v_{sk} v_{sk}}{2} \right)_i = \left(\zeta_3 (j_{p,p} - \rho v_{nm,m}) + \zeta_4 v_{na,a} \right)_i \quad (2.30)$$

and of course, as previously stated, it is assumed that $\text{curl}(\mathbf{v}_s) = 0$. The entropy balance equation will be of the form

$$\frac{\partial(\rho s)}{\partial t} + \rho s v_{np,p} + \frac{q_{i,i}}{T} = \frac{R}{T} \quad (2.31)$$

in which the dissipative term R is

$$R = \zeta_2 (\text{div}(\mathbf{v}_n))^2 + \zeta_3 (\text{div}(\mathbf{j} - \rho \mathbf{v}_n))^2 + 2\zeta_1 \text{div}(\mathbf{v}_n) \text{div}(\mathbf{j} - \rho \mathbf{v}_n) + \frac{1}{2} \eta \left(v_{ni,k} + v_{nk,i} - \frac{2}{3} \delta_{ik} v_{nl,l} \right)^2 + \kappa \frac{(\nabla T)^2}{T} \quad (2.32)$$

One has to remember that

$$q_i = -\kappa T_{,i}, \quad (2.33)$$

κ is the thermal conduction coefficient. The coefficients $\zeta_1, \zeta_2, \zeta_3, \zeta_4$ are the coefficients of second viscosity and, as Khalatnikov [60] mentioned, according to Onsager symmetry principle $\zeta_1 = \zeta_4$. In order for the function R to be positive, the coefficients η, ζ_2, ζ_3 and κ must be positive and $\zeta_1^2 \leq \zeta_2 \zeta_3$.

There are some points about the boundary conditions in superfluid and normal flow that must be stated for a better understanding of the model. The perpendicular component of the mass flux must vanish at any stationary wall. The condition for $\mathbf{v}_n$ is a little bit strange but resulted from the theorem; the tangential velocity of $\mathbf{v}_n$ on any stationary solid surface is equal to zero. The perpendicular component of $\mathbf{v}_n$ on the solid surface is not zero in the case of heat transfer between the fluid and the surface. The heat flux has to be continuous on the perpendicular direction of the boundary. The temperature itself might have a discontinuity on the boundary, proportional to the fluid and solid properties. The latter is shown, in details, in Chapter 6. An interesting property, of the latter, is that the heat exchange between the solid surface and the moving fluid results in a tangential force. If the heat transfer is absent on the solid boundary $\mathbf{v}_n$ is also zero in the perpendicular direction to the surface [14].

In case of incompressible flow, and also in the absence of heat transfer on the boundaries, the equations of motion can be explicitly decoupled from each other and written as

$$\frac{\partial \mathbf{v}_n}{\partial t} + (\mathbf{v}_n \cdot \nabla) \mathbf{v}_n = -\frac{1}{\rho_n} \nabla p_n + \frac{\eta}{\rho_n} \nabla^2 \mathbf{v}_n \quad (2.34)$$

$$\mathbf{v}_s = \nabla \varphi_s \quad (2.35)$$

$$0 = \nabla^2 \varphi_s. \quad (2.36)$$

Equation (2.34) is explicitly identical to the Navier-Stokes equation for a fluid of density ρ_n and viscosity η (Normal flow). The superfluid flow is defined by (2.36) with the boundary problem of an ideal potential flow. The pressure distribution is defined by

$$p = p_0 + p_n + p_s \quad (2.37)$$

$$p_s = -\rho_s \frac{\partial \varphi_s}{\partial t} - \frac{\rho_s}{2} v_s^2 \quad (2.38)$$

in which p_0 is the pressure at infinity, p_s , and p_n are superfluid and normal auxiliary pressures, respectively [14].

In any case, whether the presence of dissipation is considered or not, one has to be aware that the Reynolds number for the superfluid part is infinite.

One important point regarding the dissipations in liquid helium II is that in many derivations leading to the equations of motion, the relative speed between the normal and superfluid components should be small. If not, then the constancy of the superfluid circulation required for strict superfluidity would break down. One critical relative velocity for this phenomenon was found by Landau [65] to be about 60 m/s .

In propagation of sound waves in super fluid helium, it is assumed that the normal and superfluid components of superfluid are small compared to the sound speed and all the thermodynamic quantities almost equal to their equilibrium values. By linearizing the hydrodynamic equations, one can obtain two velocities for the sound waves.

$$u_1 = c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_\sigma} \quad (2.39)$$

$$u_2 = \sqrt{\frac{\sigma^2 \rho_s}{\rho_n (\partial \sigma / \partial T)}} \quad (2.40)$$

in which σ is the entropy. At 1.4 K the first sound speed is 236 m/s and the second is 20 m/s. Some measurements show that in the propagation of heat pulses at temperatures below 1 K and above 0.1 K, the speed of propagation was found to be 230 m/s [66]. However, this value is not accurate, see Figure 7.

Figure 7- Velocity of the second sound [67]

The further assumptions, in deriving these two formulas, were that the coefficient of thermal expansion $\left(\frac{\partial \rho}{\partial T}\right)_p$ is very small. The first velocity corresponds to the oscillation of pressure (density) and is the velocity of ordinary sound. The second sound corresponds to the oscillation of temperature (entropy). It is interesting to mention that in a review article Dingle [67] declared that the second sound might exist in other materials under some conditions. This concept is known to be true [68]. For sufficiently low temperatures (below 0.5K) u_2 tends to $c/\sqrt{3}$, in which the motion of the fluid corresponds mostly to the phonons. In waves of the first sound, the helium moves as a

whole. On the other hand, in second sound, the normal and superfluid parts move with respect to each other, in such a way, that the total current is zero. The possibility of sustaining an undamped temperature wave is stated as a specific property of a low-temperature superfluid [57].

One has to mention that if the thermal expansion is taken into account, the two sounds would become coupled.

In cases, where dissipative terms are considered in the general equations, it is possible to show that the absorption of the first sound is due to the first and second viscosity. Also, the absorption of the second sound comes from the thermal conductivity.

Shockwaves, with surfaces of discontinuity, are sound waves with large amplitude propagating in a liquid. Discontinuities in the first sound correspond to usual shock waves, while the second sound discontinuities (discontinuity in temperature) are just a characteristic of superfluids. Some quantities are constant, in the discontinuity, and they are the current density, the momentum density, the force acting on a unit mass of the superfluid part of the system and the energy density. Thermodynamically, if one considers discontinuities of small intensity and just expands the thermodynamic variables $\tilde{\mu}$, $\tilde{\sigma}$ and $\tilde{\rho}$ (the $\sim$ shows the dependence of the variables on p, T, w) to the second order of the relative velocity

$$\mathbf{w} = \mathbf{v}_n - \mathbf{v}_s, \quad (2.41)$$

it will be obvious that the weak discontinuities, in the pressure or temperature, propagate at the velocities of the corresponding sounds. Further inspection shows that different points on the second sound front move with different velocities which lead to the deformation of the wave front in time.

In narrow capillaries, when the wavelength of the excitations becomes comparable or greater than the diameter of the pipe, the normal part becomes stationary and it is possible to have sound propagation in the superfluid part only; these oscillations are called forth sound [69]. A linearized system of hydrodynamic equations with $\mathbf{v}_n = 0$ lead to the velocity of the forth sound as

$$u_4^2 = \frac{\rho_s}{\rho} u_1^2 + \frac{\rho_n}{\rho} u_2^2 \quad (2.42)$$

in which u_1, u_2 are the velocities of the first and second sounds respectively. If the oscillations of a thin layer superfluid are under scrutiny, the propagation of the superfluid component is called third sound [69].

As it is stated before, the onset of temperature gradient would cause the macroscopic motion of the normal fluid. The equation of motion can describe such a thing. To be more accurate regarding the heat flow in the fluid, one should take care of the coefficient of thermal conduction. The thermal conduction k consists of two parts, the roton part k_r and the phonon part k_{ph} :

$$k = k_{ph} + k_r. \quad (2.43)$$

It is implied from the equations governing k_{ph} and k_r , that the roton part of the coefficient of thermal conductivity increases slowly with decreasing temperature. It can be found that k_{ph} is mainly contributed to the heat transfer phenomena, at low temperatures.

The same discussion about the thermal coefficient can be explained for the first viscosity. That is, one will come to the point that the roton part of the viscosity is always

constant while the phonon part increases exponentially with decreasing temperature.

However, for temperatures below $0.7K$, the temperature dependence is changed to T^{-5} .

It has to be mentioned that, for temperatures below $1.4K$, the constant contribution of the roton viscosity is negligible, with respect to the phonon part. The unusual properties of the liquid helium II lead to the appearance of second viscosity coefficients. The second viscosity is due to changes in total number of phonons and rotons. Verifying those coefficients is possible by some simplifying assumptions and experimental data. The reader is encouraged to read Khalatnikov [60], for more detail procedures dealing with the derivations of viscosities and thermal conduction coefficients. Khalatnikov [70] followed his approach with a microscopic theory based on Boltzmann equation for elementary excitations. However, some believe that his theory does not take into account the effect of some interactions of excitations, which could restrict the ranges of velocity and temperature where the theory can be trusted.

As the Landau's model is almost presented here, it is to the point to remind three particular predictions of his model:

1- The critical velocity $v_{cr} = \min \frac{\varepsilon(p)}{p}$

2- The normal density fraction [71]

3- Second sound [59].

The above formulations were all based on 4-He liquid. This theory mostly concerns about the hydrodynamic aspects of superfluid 4-He.

London [36] criticized some concepts of Landau's theory. He mentioned the velocity operator in Landau's theory as a contradiction to basic principles of quantum mechanics

[67]. He mainly tried to construct an idea for a new general theory of quantum hydrodynamics. His early proposal was based on ideal non-interacting Bose gas having a Bose-Einstein condensation temperature of

$$T_c = \frac{2\pi\hbar^2}{mk_B} \left(\frac{N}{2.6V} \right)^{2/3}. \quad (2.44)$$

In which N is the total number of particles and V is the volume.

Tisza [72], based on his early notations about two-fluid flow, constructed a quasi-thermodynamic theory. The main point of his theory was a hybrid system, in which he tried to unite some properties of a liquid with some of the Bose-Einstein gas. In his theory, it was mentioned that excited states are “compressional” and “shear” modes. The latter was said to be a consequence of phonons and the former as a characteristic of a gas-like system. Despite Landau’s theorem, Tisza [72] debates that phonon is also a part of superfluid. The two-fluid model of Tisza [72] is based on four postulates:

- 1- The lowest energy function has a minimum for some value of the confining volume.
- 2- The lowest energy is characterized by a vanishing microscopic rigidity.
- 3- The shear modes of motion of liquid helium have a gaseous character. The elementary excitations correspond to translations of atoms with definite values of mass momentum and energy.
- 4- There exists a temperature such as T_0 (lambda temperature) for which

$$\rho_n / \rho \begin{cases} = 0 & \text{if } T = 0 \\ < 1 & \text{if } 0 < T < T_0 \\ = 1 & \text{if } T \geq T_0 \end{cases} \quad (2.45)$$

and $\rho_n + \rho_s = \rho$ with ρ_n / ρ monotonically increasing between zero and lambda temperature. The experimental relation is

$$\rho_n / \rho = (T / T_0)^{5.5} \quad (2.46)$$

(All subscripts have the same meaning as in Landau's theorem.); see Figure 8.

Figure 8- Densities distribution for liquid He-II [9]

Tisza's model [72] has the assumption that for reversible processes the densities obey separate conservation laws, and no transition between mixture components occur.

The first two assumptions, state that the system at zero temperature without any external pressure, condensates into liquid; a quantum liquid³ [6]. The molecular model compatible with the third postulate is a Bose-Einstein liquid. One weak point, in his early theory, was the presence of adiabatic conditions. On the other hand, the hydrodynamic equations derived by him are just for the range of temperature in which the phonons have no participation in entropy (above 1 K). The Lagrangian mechanics was used to derive such equations. The strong aspect of his theory, with respect to Landau's theory, is its

³ A system composed of particles, whose quantum mechanical zero point energy is large compared to their interaction energy, does not solidify even at absolute zero temperature and remains a so-called quantum liquid.

ability to show the temperature dependence of the second sound velocity. He could show that by using some experimental results [73], side by side with his theory; in this case the velocity of second sound would be

$$c_2 = 26 \left[(T / T_0) (1 - (T / T_0)^{5.5}) \right]^{0.5}. \quad (2.47)$$

However, Tisza emphasized that the quantum-mechanical justifications were not derived from first principles.

It is important that in the derivations of the 3rd and 4th sound speed, by Atkins [69], the Landau's theory of superfluid Helium-4 was used not Tisza's.

Despite criticisms about the two-fluid model, there have been some theoretical supports about the subject using other methods. For example, many aspects of the Landau's model were supported by using linear irreversible thermodynamics [74]; even more, they rejected the single continuum model by Lebon and Jou [75]. Interestingly, Hawaii and Tilley [74] equations had small differences to those offered by Landau. Another example is the two-fluid model proposed by Zilsel [76]. The model is for the equations of motion for reversible processes in a two-fluid model based on variational principles. Again, the model seems similar to Landau's model [57] and its extension by Khalatnikov [60]. The difference between the models is just due to transition between the two components of the fluid.

Most of the models use the hypothesis of local equilibrium. The models, presented so far, are not satisfactory to some extent. The reason is not only local equilibrium but also the inseparability of the two fluids.

All theories were based on 4-He superfluidity; a liquid which obeys the Bose-Einstein statistics. It was not obvious whether these theories might answer the nature of new kind of superfluids or not.

2.3.1.2- Helium-3

The First attempt, to tackle 3-helium, was by Anderson and Morel [77]. But their attempt was particular and not general. They generalized the BCS and, before any experimental result about the superfluid 3-He, showed that the generalization would, in some cases, result in an anisotropic superfluid; although their approach was primitive, they were mature in conclusion. Their proposed transition temperature was 0.02 K for the 3-He to become a BCS condensate showing superfluid behavior. Cooper pairs form from two fermions which in the next step are correspondent to BCS condensation. Qualitatively, it was mentioned that the liquid helium can be assumed as a Fermi liquid. The pairing intends to minimize the free energy of the system.

After the publication of Osheroff and his collaborators [8], about a new phase in helium-3, a paper to interpret those results was published [78]. In that paper, Leggett [78] tried to show that the NMR (nuclear magnetic resonance) results indicate that at 2.65 mK , the liquid makes a second-order transition to a phase in which the “spin-orbit” symmetry is spontaneously broken. It was assumed that it could be a BCS-type phase. The concept of spontaneously broken spin-orbit symmetry (SBSOS) was deeply considered in a subsequent paper [79]. In fact, the ordering of a system implies that the system undergoes a transition to a state with less symmetry, that is, invariance under some transformations has been lost. The symmetry breaking associated with superfluid transitions is gauge symmetry breaking. It should be noted here that if a system has an

internal structure, such as the superfluid 3-He, the rotational symmetry is broken simultaneously. The superfluid seems to be more ordered than the normal phase. Consequently, it is expected that Helium-3 in at least one of the phases must be anisotropic.

Below the “A” transition, an anisotropic state does exist, see Figure 3 and Figure 4. The superfluid state changes the various susceptibilities and that these changes react back very strongly on the exchange enhancement effects [80]. Leggett [81] proposed a microscopic theory of the NMR in an anisotropic superfluid 3-He in which equations for the motion of the magnetization spin axes of the Cooper pairs showed two resonances. In more simplistic language, Leggett showed that the fact is that 3-He-A is an anisotropic BCS-type superfluid. One reason for such a phenomenon is that despite electrons ion superconductivity, the Cooper pairing in 3-He seems to have a finite quantum angular momentum. As a result the anisotropic behavior in the material is obviously possible.

Static-nuclear-magnetization measurements showed that magnetization in the “A” phase is temperature-independent while “B” phase is not [82]. The transition between the A and the B phase is of the first order, which suggests that these are ordered phases with different symmetries [6].

Now, one can proceed with the fundamentals that leads to the anisotropic two-fluid model of liquid 3-He. As one can discover again from these formulations, this approach is completely phenomenological. Maybe in future works an axiomatic approach might be to the point and might bring more rigors in deriving mathematical formulations governing this kind of fluid.

Imagine the system of superfluid 3-He is placed in an annulus then moved with the velocity $\mathbf{v}$ and the system is allowed to come to equilibrium. The normal density ρ_n is defined as the ratio of the equilibrium momentum of the system to the velocity $\mathbf{v}$. In other words it can be written

$$\mathbf{P} = \rho_n \mathbf{v}. \quad (2.48)$$

The assumption behind this formula is that the Cooper pairs do not change their wave function, i.e., remain at rest. The superfluid density as in 4-He is defined as $\rho_s = \rho - \rho_n$, where ρ is the total mass density of the liquid. If one generalizes these results, it is obvious that

$$\mathbf{P} = \rho_n \mathbf{v}_n + \rho_s \mathbf{v}_s. \quad (2.49)$$

The latter however need to be modified. Leggett [83] proposed that for a liquid in which the Fermi liquid effects are not taken into account, the momentum velocity relationship is

$$P_i = \rho_{ij}^{no} v_j \quad (2.50)$$

(v_j is the wall velocity) where ρ_{ij}^{no} is the normal fluid density tensor. Probably this concept is a direct representation of experimental observations and the proposed formula is to show the anisotropic behavior of the superfluid. The symmetry-breaking effects orienting, which is a reason for anisotropic behavior, usually consider those associated with the magnetic fields, dipole forces, walls, currents and electric fields (five continuous symmetries are simultaneously broken in 3-He-A: one gauge symmetry, two rotational symmetry in real space and two in spin space [84]).

The concept of sound propagation is fascinating in liquid helium-3; as some of the sound speeds, in the anisotropic phases, depend on the directions. As a result, the anisotropic characteristic of the fluid flourishes in the sound speeds. First sound velocity is stated to be explained by

$$c_1^2 = N / mK_s \quad (2.51)$$

where K_s is the static compressibility. The similar definitions about the fourth sound⁴, in 4-He, are applicable here. Consequently the velocity of the forth sound is

$$c_4^2 = c_1^2 (\rho_{\alpha\beta}^s / \rho) q_\alpha q_\beta \quad (2.52)$$

where $\rho_{\alpha\beta}^s$ is the superfluid density tensor, the c_4 and c_1 are the velocities of the forth and first sound, respectively, and the unit vector $\mathbf{q}$ is the direction of the propagating wave. In the B phase the density is believed to be isotropic and the velocity of the fourth sound is

$$c_4^2 = c_1^2 (\rho_s / \rho). \quad (2.53)$$

The second sound is another concept in which no density and pressure variations are involved but only the temperature variation plays a role. The corresponding velocity is

$$c_2^2 = (\rho_s / \rho_n)_{\alpha\beta} (TS^2 / \rho C_v) q_\alpha q_\beta \quad (2.54)$$

where S is the specific entropy per unit volume and C_v is the specific heat. The concept of third sound is encountered in the case of wave propagation on the surface of the superfluid.

⁴ If one puts the liquid in a narrow tube then the normal component is clamped and the oscillations, in pressure and density of the superfluid part, are still possible.

A controversial concept, in superfluid helium-3, especially in 'A' phase, was the concept of intrinsic angular momentum. Some authors totally specified that such a concept might not even exist according to BCS models [85]. On the other hand, some fruitful hydrodynamic theories were built on the fact [86] that such a phenomenon does exist. Pleiner [87] emphasized that even in the case that the intrinsic angular momentum exists, the stress tensor can be symmetrized by a proper redefinition of the linear momentum density. His approach to the hydrodynamics is completely linear, despite nonlinear ones⁵ [88]. In the hydrodynamic equations presented by him, not only the two-fluid model is used, but also the density tensors are present to show the anisotropic behavior of the superfluid. It is believed that the concept of anisotropic fluid should not be reflected in the density. In fact, this kind of representation is misleading due to the classical (and obvious) definition of the density as it should be a scalar, not any kind of tensorial quantity of order two. There are books and literature about fluids with microstructure. In most of them, the anisotropic behavior of the material is NOT represented in the density, but in stress tensors and couple stress tensors (for example [89] explained explicitly fluids with microstructure.). Again, this shortcoming in these models of 3-He is a potential future work. Models presented by Stokes [89] in his book are very deep and acceptable for 3-He.

Generally speaking, disregarding spin motion, beside five conservation laws for a simple fluid (conservation of mass, momentum and energy) two other equations seem to be at use by scientists to specify the behavior of superfluid 3-He-A; one for broken symmetries and the other for the net orbital momentum [90]. The results for the latter are

⁵ A nonlinear approach was performed by Saslow and Hu, by substituting material time derivative with the partial time derivative. They also considered the effect of a finite magnetic field on the hydrodynamics of the A phase.

complicated, which for example consists of two heat conductivities and five ordinary viscosities! Fortunately, the ‘B’ phase is more regular than its neighboring A phase [10]. The mass hydrodynamics of this phase are believed to be similar to superfluid He-II; the two-fluid theory of Landau. The two-fluid model is *still* at use for 3-He. On the basis of two-fluid theory many quantum hydrodynamic models have been proposed which are out of the scope of this literature survey (see for example [91-93] and nonlinear case [94]).

In order to finish this subsection, the reader should be aware about one interesting aspect arising from this kind of superfluid. Helium 3 brought the idea of a new principle which might be the third law of thermodynamics. Simply talking, this law is: *“there can be a state that any interacting system approaching zero temperature condenses into a single or a succession of ordered states”* [10].

2.3.2 Single Continuum Models

One of the first attempts to demonstrate the helium II behavior as a single continuum was done by Atkin and Fox [95, 96], Lebon and Jou [75], to overcome the problem of inseparability, in the two-fluid model. Also, there have been other attempts to show that the two-fluid theory is a property of the classical hydrodynamics of a one-component fluid [97]. At this moment, it is possible to present some of the models created to represent helium liquid as a single-component liquid. As a shortcoming to these models, it is necessary to emphasize that all of them are about liquid helium-II. No single continuum model exists for 3-He, to the author’s knowledge, specifically the anisotropic A-phase.

2.3.2.1- Generalized Continuum mechanics

Atkin and Fox's [95] first approach to superfluid helium-II was brilliant. They based their approach on a multipolar point of view to liquid helium. They tried to suggest a kind of vortex line according to generalized angular momentum equation. Also, they added some new terms to deal with phonons and rotons; an approach which can compensate the new degree of freedom in liquid helium-II. Although they could find solutions for the representation of the second sound, they were not able to show other phenomena in superfluid such as fountain effect and narrow channels effects. This approach is to some extent suspicious; an introduction of a term into the angular momentum might be interpreted as a kind of anisotropic behavior in a liquid [89] which is not the case for at least superfluid helium-II.

To parish the inconsistency observed in the first model, Atkin and Fox [98] again performed another approach to helium-II. In fact, it is an unusual use of continuum mechanics approach to superfluid helium, as to consider the description of motion of a material in which there exists a flow of excitations (envisaged by Landau [57]) but without the notional separation of the total density in to two parts [98]. It is assumed that the motion of the liquid helium atoms may be represented by a single-ingredient continuum. The flow of excitations is represented by an additional vector field $\mathbf{w}$ relative to the fluid. Atkin and Fox [98] claimed that their approach models the superfluidity in 4-He more physically than two-fluid theories. This time, despite their earlier models, they did not generalize the angular momentum equation. The only generalization they did was the introduction of the flow of the excitations. The system of partial differential equations (PDE) in their model consisted of

$$\frac{D\rho}{Dt} + \rho v_{i,i} = 0 \quad (2.55)$$

$$\sigma_{ji,j} + \rho b_i = \rho \frac{Dv_i}{Dt} \quad (2.56)$$

$$\sigma_{ji} = \sigma_{ij} \quad (2.57)$$

$$\sigma_{ij} = -p\delta_{ij} + 2\mu D_{ij} + \alpha w_i w_j \quad (2.58)$$

$$\rho \frac{Dm}{Dt} + (\rho m w_i)_{,i} = \rho \nu \quad (2.59)$$

$$\rho f_i = -\beta T_{,i} + \bar{\alpha} D_{ij} w_j \quad (2.60)$$

$$m \frac{Dw_i}{Dt} + \rho m w_j w_{i,j} = c_i + f_i \quad (2.61)$$

$$\rho \frac{DU}{Dt} - \sigma_{ij} D_{ij} + q_{i,i} + \rho w_i f_i = \rho r \quad (2.62)$$

$$q_i = \bar{\beta} w_i \quad (2.63)$$

in which ρ is the density, v_i the velocity of particle, $\frac{D}{Dt}$ the material time derivative, σ the stress tensor, b the body force, m the number of excitations per unit mass, w the relative velocity of excitations to the fluid, p an arbitrary hydrostatic pressure, α a negative coefficient, μ also a positive coefficient, c a generalized body force due to external agencies, q the heat flux, U the specific internal energy per unit of mass, r the rate of heat supply from the external world, f a possible intrinsic body force due to internal mechanisms in the fluid, ν the creation rate of excitations per unit mass and D the rate of deformation tensor. $\bar{\alpha}$, β and $\bar{\beta}$ depend only on m and T ; and they obey the relations $\bar{\alpha} = \alpha$ and $\beta = \bar{\beta}/T$. It has to be noted that, in their formulations, no one

discovers two densities at the first glance, but there is still a relative motion of excitations and, as a result, the idea of two-fluid theory is implicitly used (or in other words the excitation flow and the background fluid). Equations (2.59) and (2.61) are balances of amount and momentum of the excitations. They verified the thermodynamic admissibility of their formulations based on the Clausius-Duhem inequality [99]. An explicit implication of (2.63) is that all the heat transfer phenomena is due to excitations and tacitly, with respect to these formulations, the fountain effect is explainable. This time, they could not justify a continuum version of the quantized vortices in He-II.

The same authors [100] claimed that experimental verification of Landau's theory of superfluid helium is not unequivocal. They published another paper simultaneously considering a non-dissipative equations of motion [101]. Their approach is more direct and with fewer assumptions compared to the Landau and Khalatnikov procedures. The equations obtained are admissible according to thermodynamics and also the principle of material frame indifference [99]. The latter is one of the most debatable axioms in *rational continuum mechanics*. They considered the flux of excitations relative to material by s (and its energy flux by l_i which is motivated by the Landau momentum-energy curve) and a generalized body force c . The l_i is not involved in entropy inequality (to ensure a zero entropy concept), but only in their *postulated* energy balance

$$\rho \frac{DU}{Dt} + l_{i,i} + q_{i,i} - T_{ij} v_{j,i} = \rho c_i s_i + \rho r. \quad (2.64)$$

The acceptable comment, about $curl v^s = 0$, is to the point. They point out that such condition in Khalatnikov and Landau approaches is a defining class of possible motions rather than a constraint that must be satisfied by all motions (this condition is not frame indifference.). This time, they did not consider the creation and elimination of

elementary excitations, as they did in their previous papers. The authors were able to derive a two-fluid theory just by change of variables $s = v - v^s$ and defining an appropriate change for densities. What is palpable is that their approach is more general than that of the Landau-Khalatnikov two-fluid theory.

According to the theories presented in this chapter there is a potential future work for liquid superfluid *helium-3A*: to consider it as an anisotropic liquid with an additional degree of freedom for the flow of excitations. Finally, one has to bear in mind that all these single continuum models cannot gather all the properties of the superfluid helium in one systematic approach.

2.3.2.2- Extended Thermodynamics (ET)

Extended thermodynamics is a macroscopic theory of non-equilibrium processes using fluxes, beside the traditional variables, as independent fields. As a good consequence, the assumption of local equilibrium is not present any more. The fundamental fields, in ET, are density, velocity, absolute temperature, non-equilibrium part of stress and heat flux. The physical motivation to adopt fluxes as independent variables is to take into account their nonvanishing relaxation times and to eliminate the *paradox of infinite velocities of propagation*. In the study of non-equilibrium thermodynamic processes, an extended approach is obligatory when one is concerning about ultra fast phenomena or when the relaxation times of the process is large compared to those involved in the process [102]. With respect to previous discussions, the anomalous characteristics of liquid helium-II are believed to have some connections to quantum mechanics, in which the introduction of the hypothesis of local equilibrium is not allowed.

One of the best elaborations of ET, in superfluid mechanics, was done by Mongiovi and Peruzza [103]. They assumed thermodynamic processes near equilibrium. As a result, linearized equations for the fundamental fields $\rho, T, v_i, p_V, p_{<ij>}$ and q_i were used. One imminent idea, about the derivation, is to consider nonlinear approaches as a potential future work. The equations are

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial x_i} = 0 \quad (2.65)$$

$$\rho \frac{\partial v_i}{\partial t} + \frac{\partial}{\partial x_j} [(p_E + p_V) \delta_{ij} + p_{<ij>}] = 0 \quad (2.66)$$

$$\rho \frac{\partial e}{\partial t} + \frac{\partial q_j}{\partial x_j} + [(p_E + p_V) \delta_{ij} + p_{<ij>}] \frac{\partial v_i}{\partial x_j} = 0 \quad (2.67)$$

$$\tau_0 \frac{\partial p_V}{\partial t} + \lambda_0 \frac{\partial v_i}{\partial x_i} - \beta' T \lambda_0 \frac{\partial q_j}{\partial x_j} = -p_V \quad (2.68)$$

$$\tau_2 \frac{\partial p_{<ij>}}{\partial t} + 2\lambda_2 \frac{\partial v_{<i}}{\partial x_{j>}} - 2\beta T \lambda_2 \frac{\partial q_{<i}}{\partial x_{j>}} = -p_{<ij>} \quad (2.69)$$

$$\tau_1 \frac{\partial q_i}{\partial t} + \lambda_1 \frac{\partial T}{\partial x_i} - \beta' T^2 \lambda_1 \frac{\partial p_V}{\partial x_i} - \beta T^2 \lambda_1 \frac{\partial p_{<ij>}}{\partial x_j} = -q_i \quad (2.70)$$

In these equations, $e = e(p, T)$ is the internal specific energy, $p_E = p_E(\rho, T)$ is the equilibrium pressure, τ_0 , τ_2 and τ_1 are the relaxation times of the non-equilibrium pressure p_V , of the stress deviator $p_{<ij>}$ and of the heat flux q_i , respectively. λ_0, λ_2 and λ_1 are bulk viscosity, shear viscosity and the thermal conductivity respectively. The entropy principle imposes that all these six coefficients must be greater than zero. β, β' are phenomenological coefficient linked to the thermal dissipation. Angular brackets denote the symmetric traceless part with respect to indices included in them. It is seen

that convective terms are not present due to linearization. The authors were able to show that by change of variables

$$\mathbf{u}^{(n)} = \mathbf{v} - \beta T \mathbf{q} \quad (2.71)$$

$$\mathbf{u}^{(s)} = \mathbf{v} - \frac{\tau_1}{\rho \beta T^2 \lambda_1} \mathbf{q} \quad (2.72)$$

it is possible to restore a kind of two fluid theory showing the properties of liquid helium-4. To name some, one can allege the first and second sound.

Other people [104] also tried to emphasize on ET and justify the properties of superfluid according to one fluid model. However, their approach is similar to what was presented above.

2.3.2.3- Phase-Lagged Models of Energy Transport

At short transient time and micro-scale heat transfer phenomenon, it is likely that Fourier's law is not accurate. Onsager [105] noted that the mentioned law can be in contradiction to the principle of the microscopic irreversibility. There are references about the micro-scale and wave theory of heat conduction in which the main stream of the works were to eliminate the paradox of instantaneous propagation of heat transfer phenomenon [68].

The assumption, hidden behind the classical constitutive equations, such as Fick's or Fourier's laws, is the one of the energy transport speed being infinite. The application of the classical constitutive equations to diffusion problems leads to the appearance of the Poisson kernels in the solutions of these problems in infinite or semi-infinite domains, that is,

$$u(r, t) = \frac{1}{(2\sqrt{\pi Dt})^m} \int_{\Omega} u(r, 0) e^{-r^2/4Dt} dr \quad (2.73)$$

where m is the dimension of the domain Ω , and D is the diffusion coefficients of the domain in question. It is evident, from (2.73), that even if the initial distribution $u(r, 0)$ is such that $u(r, 0) \neq 0$ as $r \leq R$ and $u(r, 0) = 0$ as $r > R$, $u(r, 0) > 0$ for any values of r and t . In other words, however short the duration of the energy transport process is, the influence of the initial disturbance is sensed everywhere within the domain. Hence, the speed of energy transport has to be infinite, in order for the solution given by (2.73) to apply.

In practice, however, this paradox rarely causes a problem, because for a very small value of t , the value of the exponential function in (2.73) becomes practically indistinguishable from zero, so that even the most advanced means of measurement are not able to detect the difference. Yet, there are cases, in which the paradox of an infinite speed of energy transport cannot be ignored. Thus, for instance, if $r \leq 2Dt$, the classical assumptions become no longer valid and cannot be applied, even in principle. Consequently, one may expect that when the characteristic size of the domain becomes small enough, the classical solutions can no longer be used and are to be substituted by other models [106].

As an example, in case of heat transfer phenomenon in rigid conductors, the time required (relaxation time) for the heat transfer to occur in phonon-electron or phonon scattering processes, is of the order of picoseconds to nanoseconds. As a result, the mean free path for the heat conduction is of the order of nanometers, and in case of liquid helium is of the order of millimeters at approximately 4 K [68]. In fact, the relaxation time depends on the diffusion coefficient value. And, as another example, the penetration

length for heat conduction, in case of solid medium at room temperature, is of the order of submicrons ($10^{-8} m$ to $10^{-7} m$).

An important issue, to consider here, is that although in micro-scales the concept of continuous temperature field seems to break down, the quantities of heat flux and temperature gradient are still at use in those scales. These are challenges to be faced in future. Rigorous proofs are needed to answer such challenges.

The first constitutive equation, concerning about the thermal waves, were proposed by Cattaneo [107] and Vernotte [108] (known as CV model). It is an attempt to eliminate the infinite speed of heat propagation in a medium. The proposed formula, by Cattaneo, was a relation between the heat flux and the history of temperature gradient and after some modification led to

$$\mathbf{q} + \tau \frac{\partial \mathbf{q}}{\partial t} = -k \nabla T . \quad (2.74)$$

This is the constitutive equation in the CV model. Here τ is the mean free time (relaxation time) found by dividing the mean free path to the phonon speed in heat transfer. The time derivative in (2.74) is the *thermal inertia*. Obviously, if the time lag (relaxation time) is equal to zero one would obtain the Fourier law of heat conduction.

The resulting heat equation in solid media is

$$\nabla^2 T = \frac{1}{\alpha} \frac{\partial T}{\partial t} + \frac{1}{C} \frac{\partial^2 T}{\partial t^2} \quad (2.75)$$

The above formula is known as the *telegraph* equation. The telegraph equation has been solved by various methods, such as Laplace transforms [109, 110] and Green's function [111]. In equation (2.75), one has $\alpha = \frac{k}{C_p}$ and $C = \sqrt{\frac{\alpha}{\tau}}$. This equation was also the

thermal wave equation hypothesized independently by Morse and Feshbach [112].

Equation (2.75) is visibly a wave propagating with damping effect inside it. The quantity C is the thermal wave speed. In an isotropic material this speed can be related to the speed of sound (v_s) as

$$C = \frac{v_s}{\sqrt{3}} \quad (2.76)$$

(with the assumption of no dispersion in the course of phonon collisions and no assumption about the phonon-electron interaction). Such a formula was found without recourse to Landau's two-fluid model [113].

A general and mathematical model to prevent instantaneous propagation of heat transfer was also done by Gurtin and Pipkin [114], based on the continuum mechanics theory. Their procedure is deeply mathematical. However, their approach shows the traces of time lagging models of recent formulation. Their approach is too mathematical to be understood easily, but it can show the temperature waves.

In fact, there are two fine consequences of this type of constitutive equation (2.74). One is the finiteness of the propagation of heat pulses and the other is the second sound in helium II [115]. On the other hand, the CV model, in conjunction with linear thermoelastic formulations, can show propagating stress jumps [116].

The relaxation time is somehow interpreted as the physical instant of time at which the intrinsic length scale in diffusion merges onto that in waves. It is also the time delay between the heat flux vector and the temperature gradient in the fast transient process $\mathbf{q}(\mathbf{r}, t + \tau) = -k \nabla T(\mathbf{r}, t)$ for $\tau > 0$ [117-121]. The last equation is just restricted to the case of the temperature gradient being the cause and the heat flux being the effect.

Recently the dual phase-lagged model is also presented to reconsider the cases in which the heat flux is the cause and the temperature gradient is the effect:

$$\mathbf{q}(\mathbf{r}, t + \tau_q) = -k \nabla T(\mathbf{r}, t + \tau_T), \quad \tau_q > 0, \quad \tau_T > 0. \quad (2.77)$$

The phase lag τ_T measures the thermalization time required for electrons and phonons to achieve thermal equilibrium, whereas the phase lag τ_q absorbs both relaxation times in the electron–phonon system [122].

One thing is debatable about all these models: the Taylor series is the tool to analyze and unfortunately to approximate these constitutive equations. No delay differential analysis (or functional analysis) is used. This can be a good further research topic. However, it is believed that the linearized equation can reveal most of the behaviors of the phenomena, as long as the time delays are of the order of femto and picoseconds. As an example, the linearized phase-lagged models introduce apparent heat sources [123], which might cause temperature resonance. Again, an emphasis is added that if a more thorough analysis is considered, higher order modes of energy transportation might exist which also could reveal more physical unknown areas.

In general, the lagging behavior in the transient process is caused by the finite time required for the sub-structural interaction to occur. The inert behavior of molecules, at extremely low temperatures, is another cause for the *possible* lagging response. One example, for the latter, is the liquid helium at extremely low temperatures.

From these discussions, the new kind of constitutive equations for superfluidity, both phase-lagged heat and stress equations might be needed.

The thermodynamic admissibility (a constitutive law to be approved by second law of thermodynamics) of the phase-lagged model has been approved [68]. However, it seems that a continuum mechanics approach can be found.

The molecular dynamic calculations suggest a time-temperature principle, well known in polymer physics, in which long times at low temperatures are equivalent to short times at high temperatures [115]. This is the idea that if phase-lagged models are apparently acceptable at low temperatures, they can also be useful at high temperatures but with emphasis on short time phenomenon.

Recently a new model of superfluidity was presented by Kulish and Chan [106], in which their formulation was based on the fact that there is a finite time between the onset of energy and the propagation. In other words, there is a finite time lag between the onset of the shear stress and the corresponding velocity gradient. As it was observed, this is not the first time that this idea is at stage (the idea about concerns over infinite speed of energy propagation). In that article, it was shown that when the size of the channel was of the order of nanometers the start-up flow would show the effect of superfluidity at picoseconds after the start-up. As the velocity field is the gradient of the phase of the wave function associated with the wave packet of the molecules, it can be a good motivation to apply their method to examine start-up flow in a nano channel [124]. Kulish and Chan [106] have declared that their model is the extended version of the classical Navier-Stokes and unlike the latter is valid at all scales. Assuming an incompressible, Newtonian fluid with constant physical properties their formulation starts with the momentum equation of motion for incompressible fluid,

$$\frac{\partial \mathbf{v}(\mathbf{x}, t)}{\partial t} + [\mathbf{v}(\mathbf{x}, t) \cdot \nabla] \mathbf{v}(\mathbf{x}, t) = \frac{1}{\rho} \nabla \cdot \boldsymbol{\varphi}(\mathbf{x}, t) + \mathbf{g}(\mathbf{x}, t) \quad (2.78)$$

where $\mathbf{v}$ is the velocity field, ρ represents the density of the fluid, φ is the stress tensor and the $\mathbf{g}$ is the body force. Afterwards, to eliminate the paradox of instantaneous propagation of momentum transfer, it is proposed a time lag between the onset of velocity gradient and the stress caused by it.

$$\varphi(\mathbf{x}, t + \tau) = -\mathbf{p}(\mathbf{x}, t) + \mu \nabla \mathbf{v}(\mathbf{x}, t) \quad (2.79)$$

$\mathbf{p} = p\mathbf{I}$ is the pressure tensor, μ denotes the dynamic viscosity and τ is the *relaxation time* or *time lag*. After such preliminaries, the truncated form of (2.79) up to second order of the Taylor series is put in (2.78) and the result is

$$\begin{aligned} \tau \left[\frac{\partial^2 \mathbf{v}}{\partial t^2} + (\mathbf{v} \cdot \nabla) \frac{\partial \mathbf{v}}{\partial t} + \left(\frac{\partial \mathbf{v}}{\partial t} \cdot \nabla \right) \mathbf{v} \right] + \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = \\ - \frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{v} + \mathbf{g} + \tau \frac{\partial \mathbf{g}}{\partial t}, \end{aligned} \quad (2.80)$$

in which, ν is the kinematic viscosity. They, finally, claimed that, at the start up flows, one can observe the phenomena of superfluidity⁶. One has to mention that, their approach does show the wave motion of the fluid, but it has to be combined with the energy equation to show superfluidity. In fact, it is not believed to be a formulation for superfluidity by its own. It is recommended that this equation must be engaged with the time lagged energy equation. There is also another peculiar point in their paper; the small diameter of the nano-pipe seems to break down any continuous phenomena. As an example, $\partial v_j / \partial x_i$ seems to cease its meaning at those scales.

In a subsequent paper, Kulish and Chan, by the use of kinetic theory, could explicitly suggest that both time lags in propagation of temperature and momentum are

⁶ As by their formulation, one part is transferred by waves and the other by diffusion.

proportional to $1/T$ (T is the temperature.). A prominent achievement in that paper is the effective thermal diffusivity

$$\alpha_{eff} \approx \alpha \left[1 + \frac{\tau}{4t} + \frac{9\tau^2}{2!(4t)^2} + \dots \right]^2. \quad (2.81)$$

In (2.81), α is the thermal diffusivity and α_{eff} is its effective value. According to this formulation, there are two cases when the apparent (or effective) thermal conductivity is huge: 1- τ is big (low-temperature), 2- t is small (ultra-short flows). Finally, with respect to quantum mechanics, they argued that no BEC is required to justify the superfluid action of the flow.

One thing that has to be mentioned about Kulish and Chan's model is that, up to first term approximation in Taylor's series of the equation (2.79), the equations look similar to Maxwell fluids constitutive equations; a class of viscoelastic materials. A general equation for viscoelasticity was presented in [125]. However, this similarity is due to the approximation made in the Kulish and Chan's model. The Maxwell fluid does not show any time lag between the onset of information impulse and its propagation and it only has another inherent physical meaning. The relaxation time appearing in Maxwell viscoelasticity is due to dual nature of the fluid as being a Hookean solid and a viscous fluid. Although the meanings of the terms in Maxwell fluid are totally different, their mathematical procedure [126-129] to solve such flow can be used for approximations in Kulish and Chan's model. To bury any kind of confusion between the Maxwell fluids and the Kulish and Chan model, the general formulation of all viscoelastic fluids is brought here

$$\lambda \frac{\Delta_{abc}\tau}{\Delta t} + \tau = 2\eta \left[\mathbf{D} + \Lambda \frac{\Delta_{abc}\mathbf{D}}{\Delta t} \right] \quad (2.82)$$

in which

$$\begin{aligned}
 \frac{\Delta_{abc} \mathbf{J}}{\Delta t} &= \frac{\partial \mathbf{J}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{J} - (\boldsymbol{\omega} \cdot \mathbf{J} - \mathbf{J} \cdot \boldsymbol{\omega}) + \\
 &a(\mathbf{D} \cdot \mathbf{J} + \mathbf{J} \cdot \mathbf{D}) + b \mathbf{I} \text{trace}(\mathbf{D} \cdot \mathbf{J}) + c \mathbf{D} \text{trace}(\mathbf{J}), \\
 \mathbf{D} &= 1/2[\nabla \mathbf{v} + (\nabla \mathbf{v})^T] \\
 \boldsymbol{\omega} &= 1/2[\nabla \mathbf{v} - (\nabla \mathbf{v})^T]
 \end{aligned} \tag{2.83}$$

and the τ is the stress tensor. In case that $\Lambda = 0$, the constitutive equation is called *Maxwell* [125]. Hence, the Kulish and Chan model is not Maxwell fluid at all.

Before closing this chapter, according to the literature survey, it is possible to express a new definition of superfluidity. Low-temperature superfluidity is a class of flow situations in which microstructure of the material (quantum aspects) manifests itself in the macroscopic behavior of the fluid. This phenomenon is accompanied with second sound, NCRI and special ordering of the particles at atomic level. The addition of quantum aspects, of the fluid, increases the degrees of freedom of the substance.

In the next chapter, the high-temperature model of superfluidity will be explained in detail. It will be shown how a physically correct modification in the Navier-Stokes (NS) will result in high-temperature model of superfluidity.

Chapter 3 : Theoretical Background

In this chapter, the basic idea and full formulation of the superfluid phase-lagged model is presented. It was originated by Kulish and Chan [106]. The first section is about the Kulish-Chan original method and model. The second section is devoted to the Extended Kulish-Chan (EKC) full formulation and mathematical model. The third section describes important physical and mathematical similarities between the EKC model and ET model provided by Mongiovi [102, 103]. In the latter, one can observe approximations and their applicability to finding the thermomechanical effect. In the forth section, a 1-D formulation (and also its approximation) of the model is presented. Finally, this chapter is finished by expressing the results arising from the new formulation and also the qualitative aspects of it.

This chapter is devoted to the basics and foundation of the new continuum model. These basics are, generally, accompanied with continuum aspects of the modeling. Molecular aspects will be discussed in later chapters.

3.1- Original Kulish-Chan Model (Physical Concepts)

The novel idea by Kulish and Chan [106, 130], about the unphysical assumption in energy transport phenomena, is physical and realistic. No one has considered phase-lagged fluid motion before. This model will be shown to be completely different from Maxwell fluids (discussed later in the chapter).

However, this is not the first time that this problem (instantaneous propagation of energy in the domain) is considered in the literature. Tzou [68] chose the ET to approach the problem of instantaneous propagation of energy, only in the heat equation, and Mongiovi

[102] chose the same approach in both momentum and energy equations. Those models are good but they lack some aspects. For the time being, the focus is on the Kulish-Chan model. As presented, in the last sections of the literature review, the phase-lagged model of Kulish and Chan exactly talks about the paradox of instantaneous propagation of energy and momentum. Their idea is obvious. It takes a while, too short at high temperatures and very long at low, for particles of the fluid to interact and cause the motion of the fluid to be affected by the stress. In what comes next, some illustrative justifications of this philosophy are presented. The reader should be aware that this is just an illustrative justification and not a profound schematic starting point for the model.

Imagine that there is an energy difference (Φ_2 , Φ_1 and $\Phi_2 > \Phi_1$) between two infinitesimal neighboring points (at $\mathbf{x}$ and $\mathbf{x} + d\mathbf{x}$) at time $t - \tau$ (see Figure 9). If the transporters of energy are imagined to be the cause for the energy flux (effect), it is obvious that it takes a time, τ , for the transporter with greater energy to reach the one with smaller amount of energy. This causes the energy flux at $\mathbf{x}$. $\Xi(\mathbf{x}, t)$ is the energy flux (effect). Hence, it can be understood that the flow of energy at $(\mathbf{x}, t)$, which is $\Xi(\mathbf{x}, t)$, is caused by a difference in energy between two neighboring points or

$$\Xi(\mathbf{x}, t) \propto \frac{\Phi(\mathbf{x} + d\mathbf{x}, t - \tau) - \Phi(\mathbf{x}, t - \tau)}{|d\mathbf{x}_i|} = \frac{\Phi_2 - \Phi_1}{|d\mathbf{x}_i|}. \quad (3.1)$$

One might state: why both Φ_2, Φ_1 have not been used at the same place and same time t ? The answer is straightforward: in this case, one could not define a function since a function like Φ cannot have two values at the same point.

Figure 9- Illustrative representation for time-lagged phenomena

One can reformulate (3.1) as $dx_i \rightarrow 0$:

$$\Xi(\mathbf{x}, t) = \wp \nabla \Phi(\mathbf{x}, t - \tau), \quad (3.2)$$

Where $\wp$ is a multiplier that changes the proportionality into the equality.

The same procedure is presented by Kulish and Chan but only considering the phase-lagged phenomenon in the heat transfer. In other words, the energy transporters are phonons. They could find that the time lag of the heat transfer is proportional to the mass of the phonon and it is inversely proportional to the temperature.

It is not only this model highlighting on this history behavior, or history dependence of the material response with respect to its parameters. Truesdell [131] in the concept of **Rational Thermodynamics** confirms such possibilities. Also Gurtin and Pipkin [114] generalized the heat transport equation with history. The EKC model is unique in formulation as only one point in the history of material is considered. The model can be extended for a wider range of **past** history by introducing integral equations, but, for the time being, it would only increase the mathematical cost, procedures and yields less flexibility in conclusion. Also, it would bury the physical meaning of the purpose.

Proceeding further with the original model, Kulish and Chan introduced the time lag into the momentum equation that resulted in the phase-lagged Navier-Stokes equation (2.80).

That was an appropriate action, but the results were not general enough to talk about second sound and superfluid phenomena in general.

The method of Kulish and Chan can show the apparent increase in thermal diffusivity, but it is only for the case of considering an *effective* value. In other words, it means that the concepts which are concerned in that paper is just for time lag τ and not the general equations involved for modeling the flow (field equations and energy equation). In the next section, one way to formulate the superfluid time-lagged model is under study.

3.2- Extended Kulish-Chan (EKC) Model

Up to this section, the deficiencies encountered in previous models were mentioned. One can claim that excluding the Kulish and Chan model, the best model is the model presented by the concepts of ET. On the other hand, it is important to bear in mind that the Kulish and Chan model only considers the phase lags or time lags in the momentum equations. It is true to have the time lags in those equations, but one has to remember that superfluids manifest the effect of thermomechanical coupling, like the thermoelastic behaviors in solid materials. Also, superfluids propagate higher-order sounds (e.g. second sound or temperature waves). As a result, the time lags should also be present in the corresponding energy equation. Only then, one might be confident that the correct phenomena have been modeled.

In this section, the formulation of a new model using the concepts of the *continuum mechanics* is tried. However, at some stages, phenomenological approaches to reduce the amount of mathematics involved were used. Some proofs are given in Appendix 1.

The reader must be familiar with the basic concepts of the tensor calculus as this tool is employed in the derivations. Also, the reader must be familiar with the simple field equations and also thermodynamical laws involved in continuum mechanics.

The formulation is based on the fundamentals of continuum mechanics. The field equations are

$$\dot{\rho} + \rho v_{i,i} = 0 \quad (3.3)$$

$$\rho a_i = \rho b_i + t_{ij,j} \quad (3.4)$$

$$t_{ij} = t_{ji}. \quad (3.5)$$

Equations (3.3), (3.4) and (3.5) are, respectively, the continuity equation, the momentum balance equation and the angular momentum balance equation. All have been written in point form rather than integral forms⁷. The parameters ρ , v_i , b_i and t_{ij} are density, velocity, body force and stress tensor, respectively. The energy balance equation is

$$\rho r - \rho \dot{\varepsilon} + t_{ki} d_{ki} - q_{i,i} = 0 \quad (3.6)$$

where r , ε and q_i are body energy supply (like radiation), the internal specific energy

and the heat flux. The term d_{ij} is equal to $\frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$.

Beside the *field equations* and the energy conservation, there are two other *constraints*.

The first constraint is the second law of thermodynamics and the second one is the principle of material frame indifference. Since the second principle is not acceptable by

⁷ As mentioned earlier, integral forms are more appropriate but more mathematically involved.

all scientists working on continuum aspects of the material, the author will not include this principle in the coming investigation. Instead, heuristic similarities, with respect to Navier-Stokes, are adopted. The second law of thermodynamics is stated according to the Clausius-Duhem inequality,

$$\rho \theta \dot{\eta} - \rho r + q_{i,i} - \frac{q_i g_i}{\theta} \geq 0 \quad (3.7)$$

where θ , η and g_i are absolute temperature, specific entropy and temperature gradient, respectively. Since there are 20 unknowns in these equations and constraints, and only 5 available equations (continuity, linear momentum and energy balance), it is needed to define the independent variables and dependent ones to close the mathematical model. In other words, it is time to define the set of constitutive equations in the functional form. One can introduce the functionalities as:

$$\psi = \hat{\psi}(\rho, \theta) \quad (3.8)$$

$$t_{ij} = \hat{t}_{ij}(\rho, \theta, d_{ij}^{\tau_2}, g_i^{\tau_1}) \quad (3.9)$$

$$\eta = \hat{\eta}(\rho, \theta) \quad (3.10)$$

$$q_i = \hat{q}_i(\rho, \theta, d_{ij}^{\tau_2}, g_i^{\tau_1}) \quad (3.11)$$

where $\psi = \varepsilon - \theta\eta$ is the Helmholtz free energy. And

$$g_i^{\tau} = g_i(\mathbf{x}, t - \tau), \quad (3.12)$$

$$d_{ij}^{\tau} = d_{ij}(\mathbf{x}, t - \tau), \quad (3.13)$$

are the general forms of the time lag equations that is needed in the new formulation. In other words, (3.12) and (3.13) explicitly say that there is a finite time lag between the onset of energy gradient and the corresponding energy flux.

One can suppose that, for thermodynamic processes, the classical thermodynamic relations are still acceptable.

$$\frac{\partial \psi}{\partial \theta} = -\eta \quad (3.14)$$

It is necessary to mention that the above formulation is simplistic. However, extra implementation of mathematics will hide the physics of the formulation. One is now able to state the constitutive equations needed for the system of equations. In fact, the relation between the dependent and independent variables in the proposed functionals is to be found systematically. The general formulations can be simplified further as shown in the coming subsections. For the beginning, only linear relations are considered and nonlinear tedious ones are forbidden.

$$t_{ij} = A_{ij}(\rho, \theta) + B_{ijk}(\rho, \theta)g_j^{\tau_1} + C_{ijkl}(\rho, \theta)d_{ij}^{\tau_2} \quad (3.15)$$

$$q_i = D_i(\rho, \theta) + E_{ik}(\rho, \theta)g_k^{\tau_1} + F_{ikl}(\rho, \theta)d_{kl}^{\tau_2} \quad (3.16)$$

$$\psi = G(\rho, \theta) \quad (3.17)$$

$$\eta = J(\rho, \theta) \quad (3.18)$$

If all the possible symmetries available in the formulation are used, and also some ideas are borrowed from the Navier-Stokes equations with no lag, the tensor coefficients in the constitutive equations are proposed as:

$$\begin{aligned}
 A_{ij}(\rho, \theta) &= -p(\rho, \theta)\delta_{ij} \\
 B_{ijk}(\rho, \theta) &= 0 \\
 C_{ijkl}(\rho, \theta) &= \lambda(\rho, \theta)\delta_{ij}\delta_{kl} + \mu(\rho, \theta)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\
 D_i(\rho, \theta) &= 0 \\
 E_{ik}(\rho, \theta) &= -k(\rho, \theta)\delta_{ik} \\
 F_{ikl}(\rho, \theta) &= 0
 \end{aligned} \tag{3.19}$$

Substituting (3.19) in all the proposed constitutive equations, one can easily find

$$t_{ij} = -p\delta_{ij} + \lambda\delta_{ij}d_{kk}^{\tau_2} + 2\mu d_{ij}^{\tau_2}, \tag{3.20}$$

$$q_i = -kg_i^{\tau_1}, \tag{3.21}$$

in which, like in the case of classical thermodynamics $p(\rho, \theta) \triangleq \rho^2 \frac{\partial \hat{\psi}}{\partial \rho}$.

One can proceed, finally, to the set of equations to describe the phase-lag model for superfluidity. In the next sections, the qualitative concept of the formulation is explained.

It is obvious that the formulation is time-lagged Navier-Stokes equations or a more general formulation of the classical Navier-Stokes equations.

One term in the previous equations might call attention: why is the time lag not present in the pressure-like term, p ? As learned from a literature survey, it is possible that p remains without any time-lag [132] and it is possible to have such a term, in a mathematical formulation, because a linear model with respect to the constitutive equations is chosen, and also, the form of the functionals used is $f(\rho, \theta, d_{ij}^{\tau_2}, g_i^{\tau_1})$. In particular, the functionals in the model are only dependent upon the current values of density and temperature and not upon their histories. In addition, it is possible to refer to the previous section arguments about the transporters of energy and consequently the

fact that the time-lag is only considered for terms involving partial derivatives with respect to space. Finally, this *pressure-like* term is not necessarily the familiar pressure that any one knows in ordinary fluids. For instance, Landau and Lifshitz [14] stated the same discussion for the two-fluid model for the pressure-like term. This definition of pressure for the new formulation needs a more atomistic point-of-view. To close this argument, the pressure, according to kinetic theory, is related to the kinetic energy per molecule. This means, that an average value of energy can be dedicated to all molecules. Hence, this pressure-like term can be a representative of the energy density of each particle in proportion to its density and temperature. Summarizing, the term does not need any time-lag as long as the current temperature of the particle is considered and not its temperature history of any kind.

One can now rewrite all the equations involved in the model in their vector form. In the case of constant diffusion coefficients, these equations become:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (3.22)$$

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{v}^{\tau_2}) + \mu \nabla^2 \mathbf{v}^{\tau_2}, \quad (3.23)$$

$$\rho \left(\frac{\partial \varepsilon}{\partial t} + (\mathbf{v} \cdot \nabla) \varepsilon \right) - k \nabla^2 \theta^{\tau_1} = \mathfrak{R}. \quad (3.24)$$

Clearly, the above equations are only valid in the case of small temperature differences, and also if the body forces and radiation are absent or negligible. In equation (3.24), $\mathfrak{R}$ is the dissipative term of the energy equation and is equal to $t_{ki} d_{ki}$.

In this section, the incompressible phase-lagged superfluidity is considered with the assumption of constant coefficients. This formulation is used because many known fluids

are, to good approximation, incompressible (such as water). Also, it is assumed that the thermodynamical coefficients can be considered as constant for some temperature interval.

For an incompressible fluid, the density is expected to remain constant. With this assumption, the continuity equation (3.22) further simplifies into

$$\nabla \cdot \mathbf{v} = 0. \quad (3.25)$$

The momentum equation becomes

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + \mu \nabla^2 \mathbf{v}. \quad (3.26)$$

Finally, the energy equation reduces to

$$\rho \left(\frac{\partial \varepsilon}{\partial t} + (\mathbf{v} \cdot \nabla) \varepsilon \right) - k \nabla^2 \theta = 2\mu d_{ij} d_{ij}. \quad (3.27)$$

As can be seen, in this case, the momentum and energy equations are now decoupled, that is the momentum equation can be solved independently from the energy equation.

Now, if one assumes that the internal energy is a linear function of temperature with a constant coefficient of heat capacity $\varepsilon = c\theta$ there is one immediate consequence: the energy equation completely describes the temperature field in the problem. It is now possible to derive the equation governing the temperature field in a solid medium.

$$\rho c \frac{\partial \theta}{\partial t} = k \nabla^2 \theta. \quad (3.28)$$

This equation shall be used in the next chapter to find some solutions of the phase-lagged equations. The approximated equation (3.28), by one term on the left hand side using

Taylor series, is exactly the telegraphic equation. In the coming sections, the dissipative term, in 1-D, is presented for more clarifications.

3.3- Similarities of EKC Model with ET Model

As mentioned earlier, excluding the EKC model, the best is the ET model. In this section, the new model will be presented with some approximations. Consequently, it will be shown that, introducing these approximations, it is possible to come up with equations that lead to the ET model. Initially the new model is written in its general form, without the Clausius-Duhem inequality.

$$\begin{aligned}
 \dot{\rho} + \rho v_{i,i} &= 0 \\
 \rho a_i &= t_{ij,j} \\
 t_{ij} &= t_{ji} \\
 -\rho \dot{\varepsilon} + t_{ki} d_{ki} - q_{i,i} &= 0
 \end{aligned} \quad . \quad (3.29)$$

It is obvious that in equations (3.29) the body force and the radiation term have been neglected. Now, the constitutive equations for the stress and heat conduction are

$$t_{ij}(\mathbf{x}, t + \tau_2) = -p(\mathbf{x}, t + \tau_2) \delta_{ij} + \lambda \delta_{ij} d_{kk}(\mathbf{x}, t) + 2\mu d_{ij}(\mathbf{x}, t) \quad (3.30)$$

$$q_i(\mathbf{x}, t + \tau_1) = -kg_i(\mathbf{x}, t). \quad (3.31)$$

In equations (3.30) and (3.31), the terms, containing $t + \tau$, can be expanded into the

Taylor series $\Xi(\mathbf{x}, t + \tau) \approx \Xi(\mathbf{x}, t) + \tau \frac{\partial \Xi(\mathbf{x}, t)}{\partial t}$ (Ξ can be q_i , p and t_{ij}). At the same

time, one can approximate the material time derivative with its corresponding partial

time derivative $\dot{(\cdot)} = \frac{D}{Dt} \approx \frac{\partial}{\partial t}$. In fact, the effect of nonlinear term $v_i \frac{\partial}{\partial x_i}$ has been

neglected since the effect of the convective terms is assumed to be small (e.g. in the case

of the sound propagation). As a result of these approximations, all of the equations governing the fluid motion would result into

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial x_i} = 0, \quad (3.32)$$

$$\rho \frac{\partial v_i}{\partial t} = \frac{\partial t_{ij}}{\partial x_j}, \quad (3.33)$$

$$-\rho \frac{\partial \varepsilon}{\partial t} + \frac{t_{ij}}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{\partial q_i}{\partial x_i} = 0, \quad (3.34)$$

$$\tau_2 \frac{\partial t_{ij}}{\partial t} + t_{ij} = - \left(\tau_2 \frac{\partial p}{\partial t} + p \right) \delta_{ij} + \lambda \frac{\partial v_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad (3.35)$$

$$\tau_1 \frac{\partial q_i}{\partial t} + q_i = -k \frac{\partial \theta}{\partial x_i}. \quad (3.36)$$

Now, if one takes a look on equations (2.65)-(2.70), it is possible to observe that by writing $p_E \delta_{ij} + p_{ij} = -t_{ij}$, $p_V = \frac{1}{3} p_{ii}$, $\lambda_2 = \mu$, $\lambda_0 - \frac{2}{3} \lambda_2 = \lambda$, $\lambda_1 = k$, $p_E = p$ and imposing the conditions $\beta = \beta' = 0$, $\tau_2 = \tau_0$ that the ET model and the EKC model become identical. By imposing $\beta = \beta' = 0$, it is assumed that the heat dissipation is not present (as it can be a part of ET). Setting $\tau_2 = \tau_0$ is believed to be a good approximation considering the small value of these coefficients. In fact, these time-lags should be of the same order of magnitude [132] and one can equate the pressure time-lag to the stress time-lag in ultra-fast processes. A thorough proof is presented in Appendix 2.

The agreement between the two models is not peculiar. The fact is that in both methods the models tend to eliminate the concept of the infinite speed of energy propagation.

However, the new formulation is more acceptable and more rational than the ET method, since the time lags have been considered precisely in the time functional form.

There are some important comments to be made at this point that are to the point to talk about. First of all, consider the linear approximation $(\dot{}) = \frac{D}{Dt} \approx \frac{\partial}{\partial t}$. It is known that this approximation is not an appropriate one at least for the cases in which the velocity field is comparable to other observable parameters. Thus, the linear method of ET, although useful in concluding the results such as second sound, is not a very broad concept. Hence, the new original method with nonlinear terms should be used in future works. The only reason for using such an approximation, was to show the capability of the new model to be reduced to the ET model.

Another debatable approximation, is the Taylor series approximation,

$\Xi(\mathbf{x}, t) + \tau \frac{\partial \Xi(\mathbf{x}, t)}{\partial t} \approx \Xi(\mathbf{x}, t + \tau)$. In general, by introducing such an approximation,

one would neglect some information about the initial conditions (from an infinite “pieces of information” set in the past) of the mathematical problem for the time interval $-\tau \leq t < 0$. This approximation will never cover all the controversies about the instantaneous propagation of energy. It seems that again, by using this kind of approximation, the transporting medium completely loses its memory regarding the past

conserves the observable physical aspects of the problem, while at the same time weakens the mathematics behind the formulation. These equations should be solved with accounting for the full history of the variables in the time interval $-\tau \leq t < 0$. It is believed, nevertheless, that such an approximation is well-justified in the case of τ being

of the order of nano-seconds or even smaller. It might provide a good rough estimation for the solution of the problem. However, for large values of τ , the approximation becomes questionable.

In general, this concept of the relaxation time or time-lag is appropriate, as mentioned in [132], and its use is not only confined to superfluids, but also superconductors whose time-lag or relaxation times are very long with respect to the process time.

As one can establish that the approximated formulations and the ET model are the same, it can be claimed that it is possible to have the second sound effect hidden in the new formulations. Also, higher-order sound waves can be described by this approximation. This has been done previously by Mongiovi [102, 103], where the authors considered a large set of hyperbolic linear equations to calculate the wave speeds arising in the ET formulation.

3.4- One-Dimensional EKC and Fountain Effect

In this section, the 1-D model of the EKC is presented, where the fountain effect is shown (thermomechanical coupling) by using some approximations. If one simplifies equations (3.22)-(3.24) with the assumption of constant diffusive parameters, it is possible to write the equations of continuity, momentum and energy as

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial x} + \rho \frac{\partial v}{\partial x} = 0, \quad (3.37)$$

$$\begin{aligned} \rho \left(\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} \right) &= -\frac{\partial p}{\partial x} + (\lambda + 2\mu) \frac{\partial^2 v}{\partial x^2} + \mu \frac{\partial^2 v}{\partial y^2}, \\ 0 &= -\frac{\partial p}{\partial y} + (\lambda + \mu) \frac{\partial^2 v}{\partial x \partial y}, \end{aligned} \quad (3.38)$$

$$\rho \left(\frac{\partial \varepsilon}{\partial t} + v \frac{\partial \varepsilon}{\partial x} \right) + k \frac{\partial^2 \theta^{\tau_1}}{\partial x^2} = \mathfrak{R}, \quad (3.39)$$

$$\mathfrak{R} = -p \frac{\partial v}{\partial x} + \lambda \left(\frac{\partial v^{\tau_2}}{\partial x} \right)^2 + 2\mu \left(\left(\frac{\partial v^{\tau_2}}{\partial x} \right)^2 + \frac{1}{2} \left(\frac{\partial v^{\tau_2}}{\partial y} \right)^2 \right), \quad (3.40)$$

if it is assumed to have velocity in x direction, only, or $v_y = v_z = 0$.

It is apparent from the formulation that the main contributors in the energy dissipation (velocity gradients) are absent for the time interval $0 \leq t < \tau$. For simplicity, it is assumed that only the velocity gradient in the x direction is present. To show the capability of this new model, one can now discuss a phenomenon predicted by the formulation, which is closely similar to the thermomechanical effect in a superfluid. Imagine that there is a pipe between two reservoirs, filled with a superfluid initially at rest, so $v_x = v_y = v_z = 0$ for $t \leq 0$. If at time interval $[0 - \Delta t]$ and distance $[0 - \Delta x]$ one imposes a temperature difference both in time and space, clearly the formulation shows a kind of thermomechanical effect. To show this phenomenon in a qualitative way, one should proceed as follows. From equations (3.39) and (3.40), it is obvious that if $\Delta t < \tau_1, \tau_2$ the stress and heat flux terms are zero or

$$\mathfrak{R} = -p \frac{\partial v}{\partial x}. \quad (3.41)$$

Consequently, if it is assumed that the internal energy to be a linear function of temperature ($\varepsilon = c\theta$), then, ignoring the body force and considering the 1-D flow ($v_x = v$), the energy balance equation (3.6) reduces to

$$\rho c \left(\frac{\partial \theta}{\partial t} + v \frac{\partial \theta}{\partial x} \right) + p \frac{\partial v}{\partial x} = 0, \quad (3.42)$$

which means that there can be an approximate velocity like

$$v = \frac{-p/\rho(\frac{\partial v}{\partial x}) - c \frac{\partial \theta}{\partial t}}{c \frac{\partial \theta}{\partial x}} \quad (3.43)$$

and it is necessarily unequal to zero.

By this approach, however, it is really hard to find the exact direction of v , also c is assumed to be a constant for the temperature range considered here. But, as an approximation, if $c \frac{\partial \theta}{\partial t}$ is much larger than $p/\rho(\frac{\partial v}{\partial x})$, in absolute value (which is possible for a temperature shock), then it is obvious that the fluid is escaping from the heat source. As a consequence of this reasoning, it can be understood that the fluid might be compressible if the continuity equation and the linear momentum equation are considered jointly. However, it is not known whether this compressibility is local like a sound wave or a general case.

Here, it should be noted that the thermomechanical effect and convection are two different matters. In the case of the thermomechanical effect, it is a transient process that goes on without any external forces (such as gravity). However, in the case of convection, an external force is needed to create the flow of fluid with different local densities.

This formulation shows the capability of the approach in modeling the thermomechanical effect and possibly the second sound. What is mentioned in this section is only a rough approximation. The precise conclusion must be based on the exact analytical solutions or numerical approaches.

3.5- Summarizing Chapter Results

In the beginning of this chapter, the original model proposed by Kulish and Chan [106] was presented. The model is based on the physical properties seen in nature. However, the model lacked two things: first, a good rational formulation and, second, coupling the energy and momentum equations. It was shown that the new model (the EKC) can be converted into one of the models based on the concept of Extended Thermodynamics (ET). The similarity obtained was a great asset to show that the new model is more general than the ET models. Also, one can claim that this similarity is a suggestion for confirmation of the model. Finally, one could observe that the 1-D set of equations can simply show the thermomechanical effect in the model.

In general, in this chapter, it was shown that the new model is a model of a single component fluid, which can predict some peculiar features of superfluids. It was not confined to a range of temperature or to any other physical states such as BEC. Therefore, one can claim that the formulation is valid for all temperature ranges and, consequently, one might perceive superfluidity at high temperatures. In Chapter 7, it will be shown that for high temperatures, the formulations stated here can have a strong justification, with respect to the shifted potentials. However, it is emphasized that the justification can generally cover high temperatures (see Chapter 7).

There are also some future directions with regard to this new formulation. The τ_{ij} is possible instead of the τ in both energy and momentum equations. This approach might be used to consider the anisotropic fluids (see Chapter 7). Also, it is possible to consider the nonsymmetrical stress tensor to deal with other types of anisotropic fluids. The last

two generalizations might be useful for media with richer microstructure. In general, they might be useful for multipolar materials.

In the next chapter, the objective is to solve a subclass of the equations encountered in this chapter: Phase-lagged heat equation solution.

Chapter 4 : Solutions of the 1-D Phase-Lagged Heat Equation (PLHE)

As it was observed, in the previous chapters, the phase-lagged models are more physical than the other models. It is because of simple physical ideas that the model is based upon. Now, the main point is to how the solutions of these equations are and what one can imply from those solutions. There is a vast amount of literature dealing with delay differential equations and considering their stability analytic solutions, in both ordinary and partial form. However, few of them really deal with the equations considered in the previous chapter.

In the case of ordinary delay differential equation (DDE), there are references one might refer to listing appropriate solutions [133]. Also, a common method for solving such equations is called the method of steps [134], especially for the case of constant delays. In general, one can write the simplest form of these DDEs as

$$\begin{aligned} y'(t) &= f(t, y_t), \quad t \geq t_0 \\ y_{t_0} &= y(t_0 + \theta) = \Phi(\theta), \end{aligned} \quad (4.1)$$

Where $y_t = y(t + \theta), \theta \in [-r, 0]$ is a function belonging to the space defined as $C = C^0([-r, 0], \mathbb{R}^d)$. The latter is of continuous functions mapping the interval $[-r, 0]$ into $\mathbb{R}^d$ and $f : \Omega \rightarrow \mathbb{R}^d$ is a given function of the set $\Omega \subset \mathbb{R} \times C$ into $\mathbb{R}^d$. In this context $y'(t)$ stands for the right-hand derivative $y'(t)^+$ and $\Phi(\theta) \in C$ represents the *initial point* or the *initial data*. Equation (4.1) is also called the *Volterra functional differential equation*.

On the other hand, to the author's knowledge, there are only a few solutions to the partial delay differential equations. Considering the new model proposed here, there are only a few cases in which, for example, the phase-lagged heat equation is solved or considered. In this chapter, those solutions are presented and then some numerical codes are shown.

4.1- Dai's Method of Separation of Variables and its Validity

Dai and Nassar [135], in their early works, performed an approximate analytic solution by employing the method of separation of variables. They approximated the coefficients of the series solution by polynomials. Their starting equations were

$$\begin{aligned}\frac{\partial T}{\partial t}(x, t + \tau_q) &= a \frac{\partial^2 T}{\partial x^2}(x, t + \tau_T), \\ T(x, 0) &= \varphi(x), \\ T(0, t) = T(l, t) &= 0,\end{aligned}\tag{4.2}$$

which is the 1-D dual-phase-lagged heat conduction equation without a source term and $a = k / (\rho C_p)$. They later assumed that the solution exists and it is smooth. Employing the method of separation of variables, it was proposed that $T(x, t) = \Gamma(t)X(x)$. Finally, they ended up with equations of the form

$$\begin{aligned}X''(x) + \lambda X(x) &= 0, & X(l) = X(0) &= 0 \\ \Gamma'(t + \tau_q) &= -a\Gamma(t + \tau_T)\end{aligned}\tag{4.3}$$

The solution of the first set of equations in (4.3) is simple. It is a Sturm-Liouville problem. However, the second set in (4.3) is not an easy one. To overcome this difficulty, Dai and Nassar introduced a solution of the form $\Gamma(t) = \sum_{i=0}^M C_i t^i$, in which M is finite. They proceeded with this approximate solution, found the coefficients, and

showed some numerical results for their approximate solutions with respect to $\varphi(x) = \sin(\pi x)$. Their mathematical approach is talented; however, there are two great debates about their solutions.

- 1- As it will be shown later, not all delay heat equations are separable.
- 2- No history of the past has been used in their solutions (only time zero has been used), which means that again the approximated equations lacks the basic fundamental aspects of the physical problem. Their approach is acceptable, if and only if, the Taylor series is used to approximate (4.2).

Dai has also solved [136] the Taylor approximation of (4.2) (with respect to proofs that clearly shows the well-posedness of the approximated equation [137]).

Recently, Su *et al.* [138] and Su and Dai [139] presented a new method to compare the phase-lagged heat equation with damped wave heat equation (telegraphic equation). After these attempts, making the heat equation non-dimensional, they come up with the equations

$$\begin{aligned}
 Q(x, t) + \frac{\partial^2 u(x, t)}{\partial x^2} &= \frac{\partial u(x, t)}{\partial t} + \tau_0 \frac{\partial^2 u(x, t)}{\partial t^2} \\
 (x, t) &\in (0, 1) \times (0, \infty) \\
 u(0, t) &= 0, \quad u(1, t) = 0, \quad t > 0; \\
 u(x, 0) &= \sin(\pi x), \quad \partial u(x, 0) / \partial t = 0
 \end{aligned} \tag{4.4}$$

$$\begin{aligned}
 Q(x, t) + \frac{\partial^2 u(x, t - \tau_0)}{\partial x^2} &= \frac{\partial u(x, t)}{\partial t}, \\
 (x, t) &\in (0, 1) \times (0, \infty); \\
 u(0, t) &= 0, \quad u(1, t) = 0, \quad t > 0; \\
 u(x, 0) &= \sin(\pi x), (x, t) \in (0, 1) \times [-\tau_0, 0]
 \end{aligned} \tag{4.5}$$

Solving (4.4) is an easy task⁸. Dai, there, proposes an assumption, which the correctness will be proven to be correct, in only a few special cases. Dai assumes that the solution can be written as $u(x, t) = T(t) \sin(\pi x)$ (a separation of variables solution). After this assumption one can easily write a DDE

$$\begin{aligned} T'(t) + \pi^2 T(t - \tau_0) &= 0, \\ T(t) &= 1 \text{ for } t \in [-\tau_0, 0] \end{aligned} \quad (4.6)$$

After this, the Laplace transform technique was used to find the solution of (4.6) and, consequently, the analytic solution of (4.5). This time, these solutions were correct and really to the point. He finally compared the numerical results and reaches the fact that it is possible to use an approximate first-order Taylor series solution for small time delays. At this point, the author will present a theorem in which Dai's method of separation of variables will be proven. In the coming theorems and lemmas (if not stated explicitly), one should remember that the functions $u(x, t), q(x), p(t), g(t), f(x)$ are all assumed to be smooth and continuous, and in particular, $f(x)$ and $q(x)$ to be infinite time differentiable with respect to their arguments. In addition, all equations are non-dimensional. In fact, in the original equation,

$$\alpha \frac{\partial^2 \theta(x, t - \tau)}{\partial x^2} = \frac{\partial \theta(x, t)}{\partial t} \quad (4.7)$$

if one writes $u = \frac{\theta}{\theta_0}, X = \frac{x}{l}, T = \frac{t\alpha}{l^2}$ (where θ_0 is a positive constant), it is possible to

come up with the non-dimensional form of the PLHE (with again renaming the variables X, T for x, t) which is

⁸ They did it with the method of separation of variables without the source term. For simplicity and without any loss of generality, one can only consider the heat equations with no source terms.

$$\frac{\partial^2 u(x, t - \tau_0)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t}, \quad (4.8)$$

$$(x, t) \in (0, 1) \times (0, \infty)$$

where $\tau_0 = \frac{\tau\alpha}{l^2}$.

Theorem 1: In the phase-lagged heat equation

$$Q(x, t) + \frac{\partial^2 u(x, t - \tau_0)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t},$$

$$(x, t) \in (0, 1) \times (0, \infty); \quad (4.9)$$

$$u(x, t) = \Phi(x, t), (x, t) \in (0, 1) \times [-\tau_0, 0]$$

If $Q(x, t) = q(x)p(t)$, $\Phi(x, t) = f(x)g(t)$, $f(x) = k_1 f''(x) = k_2 q(x)$ and with no specified boundary conditions, the equation (4.9) is separable and has a unique solution of the form $u(x, t) = N(t)f(x)$ with the assumption of the continuity and smoothness of the $u(x, t), q(x), p(t), g(t), f(x)$.

Proof: Starting with the method of steps, one can write (4.9) for the time interval

$0 \leq t \leq \tau_0$ as $q(x)p(t) + f''(x)g(t - \tau_0) = \frac{\partial u(x, t)}{\partial t}$. Now it is possible to integrate this

equation in the time interval $0 \leq t \leq \tau_0$ to obtain

$$u(x, t) = q(x) \int_0^t p(s) ds + f''(x) \int_0^t g(t - \tau_0) ds + A_1(x).$$

It is known that the solution must be continuous at time $t = 0$. Hence, the constant of integration would become

$$A_1(x) = f(x)g(0).$$

So, if one uses the assumptions stated in the theorem to simplify the answer of the problem, the solution of the problem for the time interval $0 \leq t \leq \tau_0$ would be

$$u_1(x, t) = H_1(t)f(x)$$

where

$$H_1(t) = \frac{1}{k_2} \int_0^t p(s)ds + \frac{1}{k_1} \int_0^t g(t - \tau_0)ds + g(0).$$

The exact procedure can be performed on the consequent intervals and by satisfying the continuity of the solution at the boundary of each interval. As result, one can find the solution

$$\left\{ \begin{array}{l} H_1(t) = \frac{1}{k_2} \int_0^t p(s)ds + \frac{1}{k_1} \int_0^t g(t - \tau_0)ds + g(0) \\ u_1(x, t) = H_1(t)f(x) \\ 0 \leq t \leq \tau_0 \end{array} \right.$$

$$\left\{ \begin{array}{l} H_2(t) = \frac{1}{k_2} \int_{\tau_0}^t p(s)ds + \frac{1}{k_1} \int_{\tau_0}^t H_1(s - \tau_0)ds + H_1(\tau_0) \\ u_2(x, t) = H_2(t)f(x) \\ \tau_0 \leq t \leq 2\tau_0 \\ \vdots \end{array} \right.$$

$$\left\{ \begin{array}{l} H_n(t) = \frac{1}{k_2} \int_{(n-1)\tau_0}^t p(s)ds + \frac{1}{k_1} \int_{(n-1)\tau_0}^t H_{n-1}(s - \tau_0)ds + H_{n-1}((n-1)\tau_0) \\ u_n(x, t) = H_n(t)f(x) \\ (n-1)\tau_0 \leq t \leq n\tau_0 \\ \vdots \end{array} \right. .$$

In the latter, u_j means the solution is for the j^{th} interval of integration. Hence, the general form of the solution is

$$u(x, t) = \left(\sum_{j=1}^{\infty} (U(t - (n-1)\tau_0) - U(t - n\tau_0)) H_j \right) f(x), \quad (4.10)$$

where $U(\cdot)$ represents the unit step function.

As the method of steps was used, it is already proved that the solution is unique. As well, separable solution is proved, since the solution presented is separable on each time interval, or one can write $u(x, t) = \aleph(t)f(x)$. One observes that there is no need for the boundary conditions for this kind of problem; in other words, the boundary condition for this special case is not necessary. $\square$

According to this theorem, one can easily agree that Dai's method is correct, and his assumptions are proved. However, it is clear the case studies he has chosen are special cases. Although special cases were used by him, they can hint some physical understanding into the problem. As a result, the general PLE is not separable. It is tacitly seen that the satisfaction of the boundary conditions depends on the history $f(x)$. From the form of the solution and the theorem presented, it is known that, under the assumptions of the theorem, the system always passes through the trajectories of its own history. The history is preserved.

Finally, it is intended to prove a theorem for homogenous PLE for heat conduction in which the results show that one might use the Fourier series for special cases. The Fourier series can be applied to the separable history function $\Phi(x, t) = f(x)g(t)$. Before that, two lemmas are in need of attention:

Lemma 1: The homogenous PL heat equation (PLHE) is linear.

Proof: It is obvious that if u_i and u_j are the solutions of $\frac{\partial^2 u(x, t - \tau_0)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t}$, then

$$\begin{aligned} \frac{\partial^2 (u_i(x, t - \tau_0) + cu_j(x, t - \tau_0))}{\partial x^2} &= \\ \frac{\partial^2 u_i(x, t - \tau_0)}{\partial x^2} + c \frac{\partial^2 u_j(x, t - \tau_0)}{\partial x^2} &= \\ \frac{\partial u_i(x, t)}{\partial t} + c \frac{\partial u_j(x, t)}{\partial t} &= \\ \frac{\partial (u_i(x, t) + cu_j(x, t))}{\partial t} \end{aligned}$$

It proves that the linear combination of the solutions is also the solution for the homogenous PLHE. $\square$

Theorem 2: The solution of the homogenous PLHE with separable history

$\Phi(x, t) = f(x)g(t)$, $\tau_0 \leq t \leq 0$ on the n^{th} interval of integration can be written as

$$u(x, t) = f^{(2n)}(x)h_1(t) + f^{(2n-2)}(x)h_2(t) + \cdots + f(x)g(0),$$

Where h_i 's are some functions of time.

Proof: Solving $\frac{\partial^2 u(x, t - \tau_0)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t}$ by the method of steps for the first interval

$0 \leq t \leq \tau_0$ and satisfying the continuity of the solution, one can find the solution to be of the shape

$$u(x, t) = f^{(2)}(x) \int_0^t g(s) ds + f(x)g(0).$$

The same thing is possible for the second interval $\tau_0 \leq t \leq 2\tau_0$ and the answer looks like

$$u(x, t) = f^{(4)}(x) \int_{\tau_0}^t \left(\int_0^{s-\tau_0} g(p) dp \right) ds + f^{(2)}(x) g(0) (t - \tau_0) + f^{(2)}(x) \int_0^{\tau_0} g(s) ds + f(x) g(0).$$

As it is implied from the procedure on each interval, the second order spatial operator introduces a $f^{(2i)}, i = 0, 1, 2, \dots$, and the integration over the time interval introduces a functionality of time over the terms. Thus, from what is stated previously the solution can be written as

$$u(x, t) = f^{(2n)}(x) h_1(t) + f^{(2n-2)}(x) h_2(t) + \dots + f(x) g(0)$$

for the n^{th} time interval $((n-1)\tau_0 \leq t \leq n\tau_0)$. $\square$

Corollary 1: A basic conclusion drawn from the last theorem is that if the history of homogenous PLHE is separable and if it can be written as

$$\begin{aligned} \Phi(x, t) &= f(x)g(t), \quad \tau_0 \leq t \leq 0; \\ f(x) &= A(x) + B(x) \end{aligned}$$

then the solution of homogenous PLHE with history $f(x)g(t)$ is equal to the summation of the solutions of homogenous PLHEs with histories of $A(x)g(t)$ and $B(x)g(t)$. There is a direct consequence of this theorem which is stated in the next corollary.

Corollary 2: It is now an easy task to understand that in case of homogenous PLHE with separable history $u(x, t) = f(x)g(t), \tau_0 \leq t \leq 0^9$, it is possible to expand $f(x)$ with

⁹ With finite number of terms or in case of infinite number of terms, not only is important the convergence of the original series, but also the convergence of the second order derivative of the summation.

respect to its expanded history and find the answer for each term and sum them up to find the global solution.

Notes:

- 1- The corollary is an emphasis on the fact that the Fourier series might not be always useful. It will be shown with an example.
- 2- If the history is separable, the solution is not necessarily the same! This will be shown by an example that the solution is not separable by any means.

At this stage the author will present another theorem regarding the separable condition of a PLE. This theorem is a compliment to theorem 1.

Theorem 3: The sufficient condition for the solution of PLE

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t-\tau)}{\partial x^2}$$

$$u(x,s) = p(s)q(x) \quad -\tau \leq s \leq 0$$

to be separable is that $q''(x) = \lambda q(x)$.

Proof: Suppose that the solution can be written as $u(x,t) = U(x)T(t)$. If one puts this equation in the PLE, and without the loss of generality, considers only the first interval of the integration, one would find

$$U(x) \dot{T}(t) = q''(x)p(t-\tau)$$

or

$$\frac{q''(x)}{U(x)} = \frac{\dot{T}(t)}{p(t-\tau)} = \kappa$$

where κ is a constant. From what is written above, it is simple to find that

$$U(x) = \frac{1}{\kappa} q''(x)$$

$$T(t) = \int_0^{t < \tau} p(s - \tau) ds + c$$

then

$$u(x, t) = q''(x) \int_0^{t < \tau} p(s - \tau) ds + \frac{c}{\kappa} q''(x)$$

where c is a constant. One should expect the solution to be continuous at the time zero,

thus

$$\frac{c}{\kappa} q''(x) = p(0)q(x)$$

or

$$q''(x) = \frac{p(0)\kappa}{c} q(x)$$

and, if it is set $\frac{p(0)\kappa}{c} \triangleq \lambda$, the theorem is proved. Although the first interval was considered, it is possible to redo above procedures for all intervals. $\square$

It is seen, from the first and last theorems, that the necessary and sufficient condition for the solution of the PLE to be separable is that the second order derivative of the spatial part of the history should be proportional to itself. Also, it is possible to construct the solution of the PLE according to the first theorem. Now, it is seen that in [138, 139] the solutions are just special cases and not general ones. On the other hand, what was presented here clearly shows that the separation of variables is a weak method to find the

global solutions of these problems. Hence, the methods presented in [140, 141] should be reconsidered.

For more clarification let us present an example.

Example: It is intended to solve

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} &= \frac{\partial^2 u(x, t - \tau)}{\partial x^2} \\ u(x, s) &= -x(x - 1) \quad -\tau \leq s \leq 0 \\ 0 &\leq x \leq 1 \end{aligned} \quad (4.11)$$

by the following methods, only for one interval:

1-Method of steps

2-Fourier series expansion combined with the method of steps.

1- *Method of steps:* for the first interval $0 \leq t \leq \tau$ one has

$$\begin{aligned} \frac{\partial u(x, t)}{\partial t} &= \frac{\partial^2 (-x(x - 1))}{\partial x^2} = -2 \\ \Rightarrow u(x, t) &= -2t + q(x) \end{aligned} \quad (4.12)$$

The continuity of the solution at time zero must be satisfied,

$$u(x, t) = -2t - x(x - 1). \quad (4.13)$$

What is clear here is the fact that predefined boundary conditions, including the Dirichlet, will not be satisfied. The latter was also mentioned by Domoshnitsky [142]. Hence, a conclusion from this part of the example is the fact that not all histories are acceptable in the physical sense. If one tries to continue the solution of (4.13) further it would be seen that the solution is completely unbounded.

2- *Fourier series*: In this part, the Fourier series is used to show that the general concept of separation of variables is unsatisfactory. First of all, one should expand the history in terms of the full Fourier series in the interval $0 \leq x \leq 1$

$$-x(x-1) = \frac{1}{6} + \sum_{n=1}^{\infty} \frac{-\cos(2n\pi x)}{(n\pi)^2}. \quad (4.14)$$

Now, performing the method of steps on each cosine term one has

$$\begin{aligned} u_0(x, t) &= \frac{1}{6} \\ u_n(x, t) &= \left(4t - \frac{1}{(n\pi)^2}\right) \cos(2n\pi x) \end{aligned} \quad (4.15)$$

It is obvious that there is no convergence for the summation of all terms in (4.15). Or, in other words, the series presented as $\frac{1}{6} + \sum_{n=1}^{\infty} \left(4t - \frac{1}{(n\pi)^2}\right) \cos(2n\pi x)$ will never converge to $u(x, t) = -2t - x(x-1)$. The reason is obvious: the history is separable, but the second order derivative of (4.14) is not convergent. Hence, the solution is not separable (it violates the theorems). Consequently, the test solutions and, in general, the solutions presented in [138, 139] are special cases.

It is worth to mention that the convergence of the Fourier terms is not the only problem in the separation of variables method. The stability of the terms is also important.

Consider an equation such as $\dot{f}(t) = -\lambda^2 f(t - \tau)$. A simple stability around the zero point shows that the critical time lag for the stability of the equation is $\tau_{cr} = \frac{\pi}{2\lambda^2}$. As a

result, in the Fourier series, since λ is increasing at each term, the critical time lag decreases and many terms would become unstable. Domoshnitsky [142] found that the

oscillation in the PLHE (in his proposed Dirichlet BVP) would occur when $\tau_{cr} > \frac{w^2}{e\pi^2}$,

where w is the length of the boundary.

In the next section, some numerical tools will be presented by which it is tried to directly model the PLE. There will be a comparison between the numerical solution of PLHE and the corresponding solution of the classical (no phase-lag) heat equation.

4.2- Numerical Results

Up to now, some pure mathematical theorems were presented. Some of them were based on the methods presented in recent papers and some were derived intuitively from the methods available in ordinary DDEs. The main points, in those theorems and formulas, were the possibility of separability, which were based on the continuity and differentiability of the initial (history) functions.

However, in many applications, one is not able to completely model the problem where one might not be able to observe continuous initial or history functions. As an example, one can mention a thermal input which might appear in the form of step function or, even worse, in the form of the Dirac delta function. As a result, one has to adapt some numerical tools (even relatively simple and primitive) to overcome these situations and gain some reasonable answers for the new model.

Numerical works, in this area, are neither deep nor new. For example, analogous to the approaches presented by Tzou [68], one might be able to apply the Laplace transforms on both sides of the real PLHE and employ appropriate inverse numerical Laplace transforms. However, Tzou never considered PLHE and he has always considered the approximated equations for his procedure. But those approaches might be hard, in

applying to the case, when one wants to solve all the equations in the model of superfluidity simultaneously and work with the non-linear momentum terms. Separable numerical methods by Dai and Su [135, 136, 138, 139] also seem to depend on an initial condition which is separable. As a result, their approach cannot be applied to those cases, in which there is a kind of discontinuous initial (history) condition. Hence, they might not be good methods for the beginning and are also far technical than simple difference schemes.

In this section, a difference scheme is presented that is based on a simple idea of discretion of variables like in the heat equation with no lag. With respect to the simulations for small time lags, the method is, stable and accurate.

4.2.1- Difference Scheme

The work here begins with the dimensional form of PLHE without source term. One can again rewrite the equation

$$\frac{\partial u(x, t)}{\partial t} = \alpha \frac{\partial^2 u(x, t - \tau)}{\partial x^2}. \quad (4.16)$$

In fact, by doing this, one is able to work with both dimensional form and non-dimensional form at the appropriate stage. The space and time are to be made discrete. It is chosen that $u(x_j, t_n) = u_j^n$ for the value of the function at point $x_j = j\Delta x$ and $t_n = n\Delta t$. In this case, one should choose $\Delta x = l / h$ and $\Delta t = \tau / p$, where, h is the total number of spatial meshes and p is the number of time marches in the interval $[0, \tau)$.

Then, one has to write appropriate difference schemes for all the partial derivatives presented in the problem. The time derivative is approximated by using the Euler formula as

$$\frac{\partial u(x_j, t_n)}{\partial t} = \frac{u_j^{n+1} - u_j^n}{\Delta t} \quad (4.17)$$

and the spatial derivative as

$$\frac{\partial^2 u(x_j, t_n - \tau)}{\partial x^2} = \frac{u_{j-1}^{n-p} - 2u_j^{n-p} + u_{j+1}^{n-p}}{(\Delta x)^2}. \quad (4.18)$$

With this way of discretization, it is possible to write a code to analyze the response of the system with discontinuous initial and history functions.

In general, one has to solve the matrix equation written in the form

$$\mathbf{u}^{n+1} = \mathbf{u}^n + q\mathbf{A}\mathbf{u}^{n-p} \quad (4.19)$$

Where $q = \frac{\alpha \Delta t}{(\Delta x)^2}$, $(\mathbf{u}^n)^T = (u_1^n, u_2^n, \dots, u_h^n)$ and

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & & \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ & & & 1 & -2 & 1 \\ 0 & \dots & & 0 & 0 & 0 \end{pmatrix} \quad (4.20)$$

is a tridiagonal matrix. Finally, the problem is closed by putting some appropriate initial (history) condition and also appropriate boundary condition for the matrix equation.

From the comparison conducted with Dai's numerical approaches, it is found that the method used here is precise and stable for small values of τ . In fact, although a scheme really similar to the explicit method is used for the Fourier heat transfer, one has to mention that it is hard to find the region of stability of the answer with respect to both time-lag and time-space meshes. However, it has to be mentioned that this numerical approach is consistent with the original equation, which is a PLHE. As stated earlier, the precision of the numerical method is satisfactory compared to separable cases done by others. However, one has to mention that this area would be of great interest for applied and computational mathematicians. There are references, such as [143-145], in which some kind of numeric solutions for some classes of partial delay differential equations were introduced. None of them is about the PLHE that is solved here. Other approaches are also possible. However, for the time being, it is better to confine the results to what has been presented in this subsection.

4.2.2- Helium-4 Example

In this subsection, the concentration is on the values of helium-4 at low temperatures. With respect to the measurements by Fairbank and Wilks [146], at temperature $0.2K$, the main contributor to heat transfer are phonons and not rotons. Also, the wave length of photons is of the order of $500 \text{ \AA}$. However, this wave length is not a measure of mean free path between phonon collisions. Hence, in the formulation for small size specimen, in which it is intended to employ (4.19), one has to use the distances between phonons as Δx in the formulation. For the purpose of this example, a one dimensional specimen, with the length $l = 3 \times 10^{-5} m$, of liquid helium is chosen (in fact, the liquid helium was chosen, because its properties at small temperatures are known). It is supposed that the

motions of liquid particles are tiny, so one is able to ignore them when the temperature gradients are applied. In fact, one can assume the fluid with its boundary as a slab. One end is imagined to be fixed at zero temperature and the other is supposed to be fixed at $1K$ after $t = 0$. The history, in the domain, is also considered to be zero for $t < 0$. The Schematic picture of the problem is shown in Figure 10.

Figure 10- Schematic drawing of the simulated problem

Referring to the measurements of Peshkov [59], Ackerman *et al.* [147] and the data provided by Tzou [68], one can adopt these approximate values for the example. In fact, one can show the differences between the Fourier heat model and PLHE. The values that are chosen are

$$\tau \approx 10^{-9} \text{ sec} \quad c_p \approx 300 \text{ m/s} \quad \alpha \approx 10^{-6} \text{ m}^2/\text{sec}$$

where the values are the time lag, the phonon speed and the diffusion coefficient, respectively. As it is known, *for heat transfer*, the time lag, in the macro-scale viewpoint, is the mean free time which can be found by dividing the mean free path of phonons to the phonon speed. Hence, Δx is equal to $3 \times 10^{-7} \text{ m}$. One can use the non-dimensional parameters as follows:

$$\begin{aligned} x_{new} &= \frac{x}{l} \\ t_{new} &= \frac{t\alpha}{l^2} \\ u_{new} &= \frac{u - u_0}{u_0} \end{aligned} \quad (4.21)$$

These values would simplify (4.16) into

$$\frac{\partial u_{new}(x_{new}, t_{new})}{\partial t_{new}} = \frac{\partial^2 u_{new}(x_{new}, t_{new} - \tau_{new})}{\partial x_{new}^2} \quad (4.22)$$

where $\tau_{new} = \frac{\tau\alpha}{l^2}$. From now on, these new dimensionless values are used and the *new*

index is dropped. With the physical values and dimensionless groups introduced, one can now solve (4.22) numerically using (4.19). The same thing is done for the Fourier heat transfer equation, whereas and the method to discretize it is the simple implicit finite difference scheme [148]. It is the nearest method for modeling non-steady heat transfer which preserves the infinitely fast propagation of heat. The code, used to perform the calculations, is presented in Appendix 3.

If one simultaneously plots the temperatures obtained for the Fourier model and PLHE with respect to the dimensionless length for different time steps, it is not possible to perceive anything special from the graphs. One only sees very small deviations from the Fourier heat transfer law. In fact, almost no deviation from each other! For example, if one looks at Figure 11, no big differences are seen and, actually, it seems that both graphs are located at the same position. This is true at a first glance. However, if one plots the differences between the temperatures calculated in the PLHE and the Fourier models, it is possible to observe some significant differences.

As it is seen from Figure 12, Figure 13 and Figure 14 (which are plotted at different times), one can easily perceive that at the beginning of the process there is no apparent temperature rise in the PLHE model. The dominant negative part of the graph clearly shows that the PLHE temperature is less than its counterpart (Figure 12). After some time (Figure 13), it is observed that some parts of the graph are becoming positive. As

time goes on, it is observe that this wave motion happens in the domain, but with smaller amplitude (Figure 14). To the author's judgment, it can be a good representation for the wave transport phenomenon hidden in the PLHE model. As expected, the wave front loses its amplitude as the wave propagates through the domain.

Figure 11- PLHE model Vs Fourier model after 60 ns

Figure 12- The difference of temperatures of the two models at 60 ns

Figure 13- *The difference of temperatures of the two models at 600 ns*

Figure 14- *The difference of temperatures of the two models at 6000 ns*

Although it is possible to justify the results qualitatively, one must take care about some important quantitative issues regarding these graphs.

- 1- Some might state that the orders of magnitude of the temperature difference in the last three figures are really small and they might be ignored and what has been stated is merely error propagation in the computational domain. The answer is as follows. It is known that one could not change the spatial mesh as it has to be fixed according to physical interpretations in the problem. On the other hand,

the last three graphs were checked by reducing the time steps from 100 time steps between $[0, \tau]$ to 1000 and even 2000 time steps. Not only the shape of the graphs did not change, but also the local values remain the same. Consequently, according to this mesh test, one cannot say that this phenomenon is only a matter of error propagation.

- 2- The heat transfer at small spatial scales (submicron) is necessarily with small time scales (Nano to Pico seconds). At those scales, the spatial meaning of continuous temperature difference is not clear. However, the discretization chosen is physical and not continuous. Hence, the PLHE might have the potentiality to be converted to a microscopic set of equations. This would be one of the future goals in research, considered in Chapter 6.
- 3- If one had reduced the specimen size, one had to expect more wavy behavior and more discontinuous temperature in the spatial domain.

In the next chapter, the main course of the thesis will be followed again. High-temperature superfluid flow in nano-annular domain will be considered. The main motivation of such a solution is Leggett's paper [11]. The author is trying to mimic the conditions of NCRI in the high-temperature case.

Chapter 5 : Solution of the Approximate Equations in an Annular domain:

In this chapter, the focus is on the solution of equation (3.26) when one uses the first term Taylor series approximation. The chapter aims at the possibilities of wavy motion inside the domain. The possible wavy solution is directly related to the superfluid phenomena at high temperatures. This wavy motion is similar to the superfluid state at low temperatures [11]. Showing the wavy motion to exist, at high temperature, is sufficient to prove that the proposed model predicts high-temperature superfluidity similar to the low-temperature superfluidity.

The author does not intend to propose a general solution for (3.26). The objective is to extract some of the physical characteristics of the new formulation. In this chapter, the velocity of the fluid particles is denoted by $\mathbf{u}$.

5.1- Problem Formulation

It is assumed that the fluid is confined in a circular annulus cylinder. The inner radius of the annulus is R_1 and the outer radius is R_2 . It is assumed that, at startup, the outer cylinder starts to rotate with velocity V . Prior to start up, both the walls and fluid are stationary. The following conditions are assumed:

- 1- Constant diffusion coefficients, which means that the temperature variations are small.
- 2- The flow is assumed to be incompressible.
- 3- There is no flow in the radial and axial directions. The flow is only circumferential. In other words, one has $u_z = u_r = 0$.

4- According to the symmetries present at the problem it is also assumed

$$\frac{\partial u_\theta}{\partial \theta} = \frac{\partial u_\theta}{\partial z} = 0$$

$$\frac{\partial p}{\partial \theta} = 0$$

Using all these simplifying assumptions equation (3.26) would become

$$\frac{\rho}{\mu} \frac{\partial u(r, t + \tau)}{\partial t} = \frac{1}{r} \frac{\partial u(r, t)}{\partial r} + \frac{\partial u^2(r, t)}{\partial r^2} - \frac{u(r, t)}{r^2}$$

$$\rho \frac{u^2(r, t)}{r} = \frac{\partial p}{\partial r} \quad (5.1)$$

in which $u = u_\theta = \hat{u}(r, t)$ and the pressure also has the same functionality.

Using the Taylor series on the left hand side of the first equation of (5.1) would result in

$$\frac{\rho \tau}{\mu} \frac{\partial^2 u}{\partial t^2} + \frac{\rho}{\mu} \frac{\partial u}{\partial t} = \frac{1}{r} \frac{\partial u(r, t)}{\partial r} + \frac{\partial u^2(r, t)}{\partial r^2} - \frac{u(r, t)}{r^2} \quad (5.2)$$

with the following boundary conditions

$$u(r, 0) = 0 \quad u(R_1, t) = 0$$

$$\frac{\partial u(r, 0)}{\partial t} = 0 \quad u(R_2, t) = V \quad (5.3)$$

5.2- Problem Solution

In order to solve (5.2), considering the specified boundary conditions (5.3), one should use an auxiliary function $P(r)$, such that

$$u(r, t) = v(r, t) + P(r). \quad (5.4)$$

which results in the following system of equations:

$$\begin{aligned}
 av_{tt} + bv_t &= v_{rr} + \frac{1}{r}v_r - \frac{1}{r^2}v \\
 v(r, 0) &= -P(r) \quad v(R_1, t) = 0 \\
 v_t(r, 0) &= 0 \quad v(R_2, t) = 0
 \end{aligned} \tag{5.5}$$

$$\begin{aligned}
 P'' + \frac{1}{r}P' - \frac{1}{r^2}P &= 0 \\
 P(R_1) &= 0 \\
 P(R_2) &= V
 \end{aligned} \tag{5.6}$$

where $a = \frac{\rho\tau}{\mu}$ and $b = \frac{\rho}{\mu}$. The solution of (5.6) is

$$P(r) = \frac{VR_2}{R_2^2 - R_1^2} \left[r - \frac{R_1^2}{r} \right] \tag{5.7}$$

In order to solve (5.5), one can set $v(r, t) = R(r)T(t)$ which would result in

$$a \frac{\ddot{T}}{T} + b \frac{\dot{T}}{T} = \frac{R''}{R} + \frac{1}{r} \frac{R'}{R} - \frac{1}{r^2} = -f^2 \tag{5.8}$$

in which f is assumed to be a positive coefficient that must be found. The solution of the spatial part of (5.8) is

$$R(r) = C^1 J_1(fr) + C^2 Y_1(fr) \tag{5.9}$$

where J_1 and Y_1 are the Bessel functions of the first and second kind, respectively. Both are first order Bessel functions. Now, using the boundary conditions in (5.5) one would have

$$\begin{aligned}
 0 &= C^1 J_1(fR_1) + C^2 Y_1(fR_1) \\
 0 &= C^1 J_1(fR_2) + C^2 Y_1(fR_2)
 \end{aligned} \tag{5.10}$$

to have implicit answers for (5.10) one must set the determinant of the multipliers to zero, or in mathematical terms

$$0 = J_1(fR_1)Y_1(fR_2) - J_1(fR_2)Y_1(fR_1) \quad (5.11)$$

in which, one would be able to find the eigen-values or f 's. These values are denoted as f_n . The resulting eigen-functions would be

$$R_n(r) = Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \quad (5.12)$$

Now, considering (5.8) and $v(r, t) = R(r)T(t)$ together one will find that

$$v(r, t) = \sum_{n=1}^{\infty} \left(\zeta_n^1 e^{K_n^1 t} + \zeta_n^2 e^{K_n^2 t} \right) \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) \quad (5.13)$$

where

$$\begin{aligned} K_n^1 &= \frac{-b + \sqrt{b^2 - 4af_n^2}}{2a} \\ K_n^2 &= \frac{-b - \sqrt{b^2 - 4af_n^2}}{2a} \end{aligned} \quad (5.14)$$

Finally, it is necessary to find ζ_n^1 and ζ_n^2 with respect to the initial conditions in (5.5).

This is done

$$-P(r) = \sum_{n=1}^{\infty} (\zeta_n^1 + \zeta_n^2) \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) \quad (5.15)$$

$$0 = \sum_{n=1}^{\infty} (\zeta_n^1 K_n^1 + \zeta_n^2 K_n^2) \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) \quad (5.16)$$

in which the corresponding ζ_n^1 and ζ_n^2 satisfy the following set of equations.

$$0 = \zeta_n^1 K_n^1 + \zeta_n^2 K_n^2 \quad (5.17)$$

and also

$$\zeta_n^1 + \zeta_n^2 = \frac{\int_{R_1}^{R_2} (-P(r)) r \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) dr}{\int_{R_1}^{R_2} r \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right)^2 dr} \quad (5.18)$$

If one solves (5.17) and (5.18) simultaneously, the corresponding final solution will be

$$u(r, t) = \sum_{n=1}^{\infty} \left(\zeta_n^1 e^{K_n^1 t} + \zeta_n^2 e^{K_n^2 t} \right) \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) + \frac{VR_2}{R_2^2 - R_1^2} \left[r - \frac{R_1^2}{r} \right] \quad (5.19)$$

It is also possible to find the shear stress at every point inside the domain using equation

(5.19). It is noteworthy to state that one should expect $t_{r\theta} = t_{\theta r} = \frac{\partial u}{\partial r} - \frac{u}{r}$, or in other

words, since there are some symmetries available in the domain, the shear stress is only in the $r - \theta$ direction.

$$t_{\theta r} / \mu = \sum_{n=1}^{\infty} H_n(t) \left(f_n \left(Y_1'(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1'(f_n r) \right) + \frac{1}{r} \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) \right) + \frac{2VR_2}{R_2^2 - R_1^2} \left[\frac{R_1^2}{r^2} \right] \quad (5.20)$$

where H_n is $\zeta_n^1 e^{K_n^1 t} + \zeta_n^2 e^{K_n^2 t}$.

In the next section, the consequences of the solution will be further analyzed using numerical approaches. It will be shown how the wavy motion can be extracted from the formulas presented in this chapter.

5.3- Solution Analysis

It is clear that the solution can exhibit wave-like behavior. In fact, the term H_n is an attenuating oscillatory term. Actually, the terms K_n^1 and K_n^2 inherently involve complex conjugate terms and this will force the exponential term to be converted into decaying oscillatory ones. A straightforward way to view this fact is to plot the velocity profile with respect to radial distance for some values of viscosity and time-lag. In this text, the values adopted by Kulish [106] are used for which $\nu = 1.55 \times 10^{-5} m^2/sec$ and $\tau = 3.87 \times 10^{-10} sec$.

Figure 15- Velocity profile at 10^{-11} seconds

In order to mimic the Nano-channel behavior presented in [106], one can take $R_1 = 0.1m$ and $R_2 = R_1 + 3 \times 10^{-9}m$. In Figure 16 and Figure 17, the velocity profile (blue line), is plotted with respect to the steady-state velocity profile (green line) and also the radial distance between the mentioned digits stated above. The initial condition was such that the outer wall was jerked with the speed $1m/sec$. Notice that because of the small radial distance between the cylinder walls the x-axis of the figures might be misleading. However, the distance is between $0.1m$ and $0.1m + 3 \times 10^{-9}m$. The wavy motion of the profile is more obvious if one tries to plot the velocity profile at other times.

Figure 16- Velocity profile at 10^{-10} seconds

From the figures, it is possible to ascertain the wavy behavior inside the domain. However, if one plots the consecutive velocity profile it will be seen that the steady-state is obtained at time roughly 5×10^{-9} sec .

Figure 17- Velocity profile at 1.5×10^{-10} seconds

Another observation can be made when plotting the solution of the phase-lagged Navier-Stokes equation and the original one without time delays for the same problem. The results, in Figure 18 and Figure 19, show that for the original solution of the NS equation it is hard to grasp the correct physical response to the input. In the case of the original solution of the NS equation it is observed that the steady-state condition is reached at early moments after the input. The green lines in the following figures are the velocity profile of the original NS equation. The solution of the original NS looks like

$$u(r, t) = \sum_{n=1}^{\infty} \left(\zeta_n^1 e^{-f_n^2 t/b} \right) \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) + \frac{VR_2}{R_2^2 - R_1^2} \left[r - \frac{R_1^2}{r} \right] \quad (5.21)$$

Where

$$\zeta_n^1 = \frac{\int_{R_1}^{R_2} (-P(r)) r \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right) dr}{\int_{R_1}^{R_2} r \left(Y_1(f_n r) - \frac{Y_1(f_n R_1)}{J_1(f_n R_1)} J_1(f_n r) \right)^2 dr} \quad (5.22)$$

Figure 18- Velocity profile comparison of the models at 10^{-14} seconds

Figure 19- Velocity profile comparison of the models at 10^{-13} seconds

In the case of the solution of the original NS, the steady-state condition is obtained in 10^{-12} sec. At last, it has to be mentioned that the Taylor series approximation solely tries to cover some of the physical aspects of the problem. It will never cover the mathematics behind the original phase-lagged formulation. Obviously, because of the viscosity, the original NS solution is damped faster.

This approximate solution shows that the equations are able to predict the wavy transport of the matter. A concept that is believed to be necessary for high-temperature superfluidity [106, 149]. It is to be mentioned that for a low-temperature version, the thermomechanical effect, mentioned in Chapter 3, is more crucial to show the capabilities of the equations. The latter is derived directly from the phase-lagged equations. For low-temperature, the Taylor series approximation is not recommended at all, since the time-lag in the equations might be large.

In the next chapter, a new phenomenological approach to the heat transfer is explained. The transport formulations, from a macroscopic world to the microscopic one, are substituted with a formulation of the microscopic world from a microscopic perspective.

Chapter 6 : New Phenomenological Discrete Nanoscale Phase-Lagged Heat Transfer Model

In previous chapters, the failure of the Fourier heat transfer law in nano scales and short times was mentioned. It was also mentioned that the phase-lagged heat transfer law is the best substitute for the Fourier law at small scales and short times. However, defining the temperature at that scale is challenging. On the other hand, the PLHE is a view to micro-scale from a macro-scale point-of-view. Obviously, the model, even strong in generalities, will ignore some of the micro-scale features. Some scientists have clearly stated that the classical definition of the temperature would not be acceptable with respect to the classical point-of-view [150]. There have been treatments to tackle the problem of Temperature Definition (TD), at very small scales. Few have adopted the phonons to explain temperature. Different models have been developed from the phonon approach; e.g. the Lattice Boltzmann Method (LBM) and the Equation of Phonon Radiative Transfer (EPRT) [151-153]. At the same time, few others have adopted the classical molecular dynamics approaches [154, 155]. This adoption is believed to be erroneous since the macro-scale statistical mechanics definition of temperature is used to explain the temperature at micro-scale. Even the models, which are able to calculate few of the small scale features of the heat transfer, are not able to face the very short time phenomena involved, in great details [152].

In this chapter, a new phenomenological model of heat transfer is presented. It will be shown that this discrete model can be converted into the Fourier law under some assumptions. Furthermore, the slip temperature boundary condition is also shown to be a consequence of the model. There are, also, some more features of this model that will be

mentioned in the coming sections and subsections. This model has the ability of expressing some unexplained phenomena at the small scales.

6.1- A Review of TD and heat transfer models

The classical definition of the temperature is as follows. Temperature is an intensive property of a system. In order to define this property, in a medium in which different parts energies deviate from the average value, one should assume the Local-Equilibrium Assumption (LEA). Based on LEA, the Fourier law can be derived. More accurately, the Fourier law and the EPRT can be derived under the LEA.

In the Kinetic theory, the temperature is directly related to the kinetic energy of the molecules. This temperature is called the kinetic temperature and, in molecular dynamics, is presented as

$$\frac{3}{2} k_B T = \frac{1}{2} m \bar{v}^2. \quad (6.1)$$

In (6.1), k_B is the Boltzmann constant, T is the temperature, m is the molecular mass and $\bar{v}$ is the average of the velocity of some N particles. The averaging period must be much longer than the Mean Free Time (MFT) of the particles. The MFT is the time that shows how fast the system restores to equilibrium locally [156]. As a result (6.1) cannot be used for very fast, or pico- and atto-second processes. This formula is the basis of the Molecular Dynamics (MD) simulations. However, since the MD only considers atoms and not electrons, the field of applicability of this definition is limited.

A better scientific way to tackle the TD problem at small scales, and also short times, is the use of Boltzmann Transport Equation (BTE). The basic formula of BTE is

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{a} \cdot \frac{\partial f}{\partial \mathbf{v}} = \left(\frac{\partial f}{\partial t} \right)_{\text{collision term}}. \quad (6.2)$$

In (6.2), f is the distribution function. This parameter can be related to the energy and consequently to the temperature [152], though the relation is not general. In solids, the Debye's model states that all atoms are vibrating together. Then, the quanta of lattice vibration are named phonons. Finally, the Bose-Einstein (BE) statistics is assumed to be the mechanical statistics of the system, and the distribution function is consequently found. The distribution function is converted into internal energy. The Debye's model seems to be only acceptable in a range of specified temperature. Another weak point of the model is that it can only be used for equilibrium cases.

The main difficulty in the solution of (6.2) is the "collision term", especially in the case of non-equilibrium physics. The correct definition of this term can bring hints to unknown fields of the physics. However, little is known about this term. The latter causes EPRT formulations to be a good approximation of the real phenomena in heat transfer at nano-scales and small times, but not an accurate and completely physical one. The nonlinear, integro-differential equation form of the collision term will make it even harder to be solved.

The main problem in TD is that at very small scales the continuum assumption breaks down. As a result, the local velocity (or temperature) definition would be unreliable. As it was observed, in Chapter 4 examples, even if a continuum model is used in numeric solutions, the domain of solution must be physically discretized. The best phenomenological model that deals with TD is the CV (Cattaneo-Vernotte) model. However, some scientists believe that CV is not experimentally justified and also the assumptions behind the formulation produce unphysical results. Another

phenomenological model is the two-temperature model. In this model, at non-equilibrium cases, one temperature is assumed for atoms and one for the electrons. Some scientists believe that the two-temperature model is more physical. It is worth mentioning that the PLHE never talks about TD. It is because temperature is like an axiom in continuum mechanics. It is a mathematical definition, not a physical one.

All in all, there is a fundamental issue about the correct definition of the temperature at non-equilibrium nanoscale systems [150]. One has to keep in mind that the following model, in this chapter, is all about conduction in solid materials. Further extension of the model can be done to convert it into a complete model for all states of the matter.

6.2- Assumptions of the New Model

Here, the temperature is not defined based on other physical properties. It is directly assumed that temperature is a linear portion form of the internal energy of each atom, lattice point, or molecule. The temperature that is defined here is valid for both non-equilibrium and equilibrium. The following assumptions and comments are the philosophy behind the new formulation of heat transfer:

- 1- Temperature is a pointwise variable. Despite the localized definition in previous models, in this model the temperature is not continuous in the entire space. It is assumed that this variable is located at the most probable position of an atom, or a lattice point. The most probable position of the atom can be found with the help of the Schrödinger equation. As a result, in a solid crystal medium, the temperature can be specified at to the position of the lattice points.
- 2- Whatsoever the definition of the temperature is, in this model, one should expect that the equilibrium temperature must quantitatively agree with other models. In

order to test this characteristic, one can measure the steady-state temperature of the medium.

- 3- The Fourier law must be a limit case of the new model, when the coarse graining is applied to the new model. The coarse graining procedure must be conducted for spatial and temporal domains, simultaneously. It is solely due to the fact that the Fourier law is a macroscopic phenomenon, both in space and time.
- 4- Quantum mechanical effects, like tunneling, must be present in the heat transfer formulation.
- 5- The propagation, or transportation, of energy or temperature is not with an infinite speed. There is a time delay between the transportation of energy from one point to another. It takes a finite amount of time for the carriers of energy to travel from one lattice point to the other. Also, the model must be capable of including the assumption that any change of properties at each lattice point can be observed at the neighboring points of the lattice with a time delay.
- 6- The energy always flows from a high level to a low level. However, this effect is not simultaneous. By the latter, it is meant that if an atom observes that one of its neighbors has a lower level of energy, this observation belongs to a past time. This is a consequence of the previous assumption.
- 7- The thermal energy is linearly proportional to temperature. However, the proportionality coefficient is not necessarily constant. This assumption relates the energy definition to the temperature in a direct way.

8- The change of thermal energy in time is an order-one linear differential operator

as $\frac{d}{dt}$ (this is solely an assumption)¹⁰.

9- The conservation of energy is valid.

The above statements are the basic assumptions, by which the formulation for the Pointwise Heat Transfer Model (PHTM) would be constructed.

6.3- PHTM Phenomenology

One would start constructing the model by considering a two-atom case. Later on, the model can be extended to many body systems.

Figure 20- Two atoms

If the atoms are in thermal contact, see Figure 20, the conservation of energy must be valid. Denoting e_a as the energy of atom a , and e_b as the one for b , the conservation of energy states that the change of energy of the atom a (or b) is equal to the amount of input energy, minus the output. In mathematical terms it is

$$\frac{d(e_a)}{dt} = -q_{a \rightarrow b} + q_{b \rightarrow a} \quad (6.3)$$

The $q_{a \rightarrow b}$ is the amount of energy flowing from a to b . Since nothing is simultaneous, atom a observes that atom b is at the lower energy level after a time delay. Hence, when

¹⁰ In fact, whether it is truly of order one or not, depends on the experimental and numerical results.

the energy is lower the transport of energy from a to b starts. It is assumed that this flow is linearly dependent on the differences in temperatures. The proportionality coefficient is denoted as k_{ab} , which is “ a to b conductivity”. As a result, the linear relationship for $q_{a \rightarrow b}$ is

$$q_{a \rightarrow b} = k_{ab} u(T_a(t) - T_b(t - \tau)) \quad (6.4)$$

in which

$$u(A - B) \triangleq \begin{cases} A - B & \text{if } A > B \\ 0 & \text{if } A < B \end{cases}.$$

Equation (6.4) states that when atom (lattice point) a observes that atom (lattice point) b is at a lower energy (temperature), the former transports energy to the latter. Also, the observation of the temperature of atom b , for atom a , is after a time delay, τ .

At the same time, atom a might have had some input of energy from atom b . It is shown by $q_{b \rightarrow a}$. It is assumed that this transportation, like in previous case, is linearly dependent on the temperature differences. The proportionality coefficient is denoted as k_{ba} , which is “ b to a conductivity”. This time, the transportation time delay from b to a must also be considered. If this delay is called energy transport time delay, τ' , the equation for $q_{b \rightarrow a}$ is

$$q_{b \rightarrow a} = k_{ba} u(T_b(t - \tau') - T_a(t - \tau - \tau')). \quad (6.5)$$

Finally, if one considers the energy of atom a to be $e_a = \chi_a T_a$, the energy balance (for the PHTM) would be as the following equation. χ_a is the linear coefficient of the

temperature proportionality to energy. By this assumption of linear proportionality, the energy and temperature almost become the same in definition.

$$\frac{d(\chi_a T_a)}{dt} = -k_{ab} u(T_a(t) - T_b(t - \tau)) + k_{ba} u(T_b(t - \tau') - T_a(t - \tau - \tau')). \quad (6.6)$$

In general, equation (6.6) shows that one atom transports the energy whenever it *observes* that its energy is higher. The *observation* and the *transportation* both involve time delays. The fact that the response, in the atomic scales, also involves some time delays has been shown recently [157-161]. As a result, it is not far from reality to consider the time lags. This illustration paves the way for the general form of the PHTM, presented in the next section.

6.4- General PHTM

The previous sections, acting as an introduction, allow us to present the complete form of the model. Here, one should distinguish between electron and lattice transport of energy. It is necessary to mention that the PHTM can be extended for cases in which more mechanisms exist in the transportation of the energy, or temperature. The temperature transport can be related to mechanisms like spin changes of the particles. However, in this report, the author has confined the model to the mechanisms stated in this section. As a result, despite the formula in the previous section, equation (6.6), there will be two terms for the conduction of energy. One pair would be by electrons and the other for the conduction by the means of lattice vibration. In the coming formulation, the “electron neighbors” means the atoms or lattice points that are in thermal energy transfer by electrons. The same is considered for lattice points, “lattice neighbors”. The lattice and electron neighbors might be different. In fact, the electrons might pass through the

barriers of energy by the tunneling effect. The τ_a^i is supposed to be equal to τ_i^a . The latter is the time-lag in the observation of the status of atom a by atom i and vice-versa. The ${}^e\tau_a^i$ is the time delay in the electron transporters of energy. Similar to that, ${}^l\tau_a^i$ is the time that it takes for the transporter of the lattice energy to travel from i to a . Here, ${}^e k_i^j$ is the electron conductivity from j to i and ${}^l k_i^j$ is the lattice conductivity from j to i . It is supposed that all conductivities are positive. The positive conductivity is the correct way to satisfy the assumption of the energy flux direction from a higher level to a lower one. Summarizing, the formula is

$$\begin{aligned}
 \frac{d(\chi_a T_a)}{dt} = & - \sum_{\substack{\text{electron} \\ \text{neighbors} \\ i \neq a}} {}^e k_i^a \left(T_a(t) - T_i(t - \tau_a^i) \right) \\
 & + \sum_{\substack{\text{electron} \\ \text{neighbors} \\ i \neq a}} {}^e k_a^i \left(T_i(t - {}^e\tau_a^i) - T_a(t - \tau_i^a - {}^e\tau_a^i) \right) \\
 & - \sum_{\substack{\text{lattice} \\ \text{neighbors} \\ i \neq a}} {}^l k_i^a \left(T_a(t) - T_i(t - \tau_a^i) \right) \\
 & + \sum_{\substack{\text{lattice} \\ \text{neighbors} \\ i \neq a}} {}^l k_a^i \left(T_i(t - {}^l\tau_a^i) - T_a(t - \tau_i^a - {}^l\tau_a^i) \right)
 \end{aligned} \quad (6.7)$$

The conservation of energy is already satisfied in (6.7). However, one has to mention that despite the Fourier law, the temperature itself is not conserved. In later sections it will be shown that because of the delay in the transport of energy, the temperature is not conserved in the PHTM, in transient situations.

6.4.1- General PHTM with Source Term

When the source term is present, everything is like equation (6.7), except the fact that some lattice points can have a source term of energy. This source term can be due to the chemical reactions, or radiation. The tunneling effect in radiation can also be

incorporated in the formulation. However, at this stage, only, the general form is presented, $w_i(t)$. The latter needs a constitutive equation for more clarification. For sure, quantum mechanics can be helpful.

$$\begin{aligned}
 \frac{d(\chi_a T_a)}{dt} = & - \sum_{\substack{i \neq a \\ \text{electron} \\ \text{neighbors}}}^{\text{electron}} k_i^a u \left(T_a(t) - T_i(t - \tau_a^i) \right) \\
 & + \sum_{\substack{i \neq a \\ \text{electron} \\ \text{neighbors}}}^{\text{electron}} k_a^i u \left(T_i(t - \tau_a^i) - T_a(t - \tau_i^a - \tau_a^i) \right) \\
 & - \sum_{\substack{i \neq a \\ \text{lattice} \\ \text{neighbors}}}^{\text{lattice}} k_i^a u \left(T_a(t) - T_i(t - \tau_a^i) \right) \\
 & + \sum_{\substack{i \neq a \\ \text{lattice} \\ \text{neighbors}}}^{\text{lattice}} k_a^i u \left(T_i(t - \tau_a^i) - T_a(t - \tau_i^a - \tau_a^i) \right) + w_i(t)
 \end{aligned} \tag{6.8}$$

Later on, the effect of this term is studied in a few simulations.

6.5- Simplified 1-D PHTM

Further basic investigation of the model needs a simplified version of the equations. In order to show the non-existence of negative temperature, temperature waves (heat waves), inhomogeneous media properties and also conservation of energy a one-dimensional model is introduced. It is known that in reality 1-D materials do not necessarily exist; however this simplification can be a good approximation to verify the model.

Suppose there is a line-like lattice. See Figure 21. For such a lattice, if one solely assumes that the neighbors are the nearest lattice points, equation (6.7) would be

$$\begin{aligned}
\frac{d(\chi_i T_i)}{dt} = & -{}^e k_{i-1}^i u \left(T_i(t) - T_{i-1}(t - \tau_i^{i-1}) \right) - {}^e k_{i-1}^i u \left(T_i(t) - T_{i+1}(t - \tau_i^{i+1}) \right) \\
& + {}^e k_i^{i-1} u \left(T_{i-1}(t - \tau_i^{i-1}) - T_i(t - \tau_{i-1}^i - \tau_i^{i-1}) \right) \\
& + {}^e k_i^{i+1} u \left(T_{i+1}(t - \tau_i^{i+1}) - T_i(t - \tau_{i+1}^i - \tau_i^{i+1}) \right) \\
& - {}^l k_{i-1}^i u \left(T_i(t) - T_{i-1}(t - \tau_i^{i-1}) \right) - {}^l k_{i-1}^i u \left(T_i(t) - T_{i+1}(t - \tau_i^{i+1}) \right) \\
& + {}^l k_i^{i-1} u \left(T_{i-1}(t - \tau_i^{i-1}) - T_i(t - \tau_{i-1}^i - \tau_i^{i-1}) \right) \\
& + {}^l k_i^{i+1} u \left(T_{i+1}(t - \tau_i^{i+1}) - T_i(t - \tau_{i+1}^i - \tau_i^{i+1}) \right)
\end{aligned} \quad (6.9)$$

Figure 21- 1-D lattice

More simplification is done in the next subsection, when the non-dimensional formula of the model is derived. Before continuing further, it is worth mentioning something in relation to equation (6.9). If, for example, all the left to right conductivities are omitted, then the heat can only propagate in only one direction, which is from right to left. This case might occur when there is an electromagnetic field imposed on the material. The latter, in case of metallic materials, can obviously hamper the electrons in a few directions, or at least reduce their mobility. This electron mobility reduction can result in one-dimensional and one-directional heat transfer. The justification of this proposition will be left upon experimental results in future researches.

6.5.1- Non-dimensional Form of 1-D Simplified PHTM

Here some simplifying assumptions are made to convert (6.9) into a simplified non-dimensional form that can be used in numeric simulations. The assumptions are as follow

$$1- {}^e k = {}^l k = k / 2 \equiv Cte .$$

$$2- \chi_a = \chi = Cte .$$

$$3- k / \chi \triangleq K .$$

$$4- \tau_j^i = \tau_i^j = \tau .$$

$$5- {}^e \tau_i^j = {}^e \tau_j^i = {}^e \tau = {}^l \tau_i^j = {}^l \tau_j^i = {}^l \tau .$$

Two non-dimensional forms are introduced as $t' = \frac{t}{\tau}$ and $\theta_i = \frac{T_i - T_{\min}}{T_{\max} - T_{\min}}$. In the

latter, the minimum and maximum expressions are more useful when the boundaries of the problem are clearly set. In other cases, those terms will not have the proper literal meaning and are solely used to make the main equation non-dimensional. The non-dimensional form of the equation (6.9) would be

$$\begin{aligned} \frac{d(\theta_i(t'))}{dt'} = & \tau K [-u(\theta_i(t') - \theta_{i-1}(t' - 1)) - u(\theta_i(t') - \theta_{i+1}(t' - 1)) \\ & + u(\theta_{i+1}(t' - 1) - \theta_i(t' - 1 - \frac{{}^l \tau}{\tau})) \\ & + u(\theta_{i-1}(t' - 1) - \theta_i(t' - 1 - \frac{{}^l \tau}{\tau}))] \end{aligned} \quad (6.10)$$

If, further on, one assumes ${}^l \tau = \tau$, the equation (6.10) would be

$$\begin{aligned} \frac{d(\theta_i(t'))}{dt'} = & \tau K [-u(\theta_i(t') - \theta_{i-1}(t' - 1)) - u(\theta_i(t') - \theta_{i+1}(t' - 1)) \\ & + u(\theta_{i+1}(t' - 1) - \theta_i(t' - 2)) \\ & + u(\theta_{i-1}(t' - 1) - \theta_i(t' - 2))] \end{aligned} \quad (6.11)$$

These non-dimensional forms will be used later for numerical simulations, especially in the concept of the Slip Boundary Condition (SBC).

6.5.2- Simplified non-dimensional PHTM with Source Term

According to the previous sections, the simplified non-dimensional form of PHTM is

$$\begin{aligned} \frac{d(\theta_i(t'))}{dt'} = & \tau K \left[-u(\theta_i(t') - \theta_{i-1}(t' - 1)) - u(\theta_i(t') - \theta_{i+1}(t' - 1)) \right. \\ & + u(\theta_{i+1}(t' - 1) - \theta_i(t' - 1 - \frac{l\tau}{\tau})) \\ & \left. + u(\theta_{i-1}(t' - 1) - \theta_i(t' - 1 - \frac{l\tau}{\tau})) \right] + \frac{\tau w_i(t')}{\chi(T_{\max} - T_{\max})} \end{aligned} \quad (6.12)$$

6.6- Concept of Negative Temperature

In this section, it will be shown that, under certain assumptions, the temperature will never get negative. The assumptions made, in this section, are that χ_a and all conductivities are constant. On the other hand, all $\tau_j^i = \tau_i^j = \tau$ are equal, in equation (6.7). The second assumption makes the proof stricter. At this stage, it is supposed that the temperatures for all lattice points are constant, T_0 . Suddenly, if the temperature of all neighboring points of the i^{th} lattice point is set to zero, the dynamical equation for the i^{th} lattice point, after τ , would be

$$\dot{T}_i = \frac{1}{\chi_i} \left(\sum_{j \neq i}^{electron \ neighbors} {}^e k_j^i + \sum_{j \neq i}^{lattice \ neighbors} {}^l k_j^i \right) T_i(t). \quad (6.13)$$

This equation clearly shows that the solution

$$T_i = T_0 e^{-\frac{1}{\chi_i} \left(\sum_{j=1}^{\text{electron neighbors}} e k_j^i + \sum_{j=1}^{\text{lattice neighbors}} l k_j^i \right) (t-\tau)} \quad (6.14)$$

is both stable and non-negative, since $\frac{1}{\chi_i} \left(\sum_{j=1}^{\text{electron neighbors}} e k_j^i + \sum_{j=1}^{\text{lattice neighbors}} l k_j^i \right)$ is a positive constant. This

simple proof shows that, as long as the temperature on the boundaries are above, or equal to zero, the dynamics of the system never predicts a negative temperature. As stated previously, this simple procedure, inherently, is showing that equation (6.7) can be stable. Also, the stability could be exponential.

This section shows despite other models, in which the stability and negative temperature issues are concerning problems [156, 162], the PHTM ,by the stated assumptions, is capable of showing non-negative temperature and possible stability. The physical nature of the assumptions, in the model, makes it capable of showing stability and non-negative temperature.

Landau [163] has claimed that negative temperature can exist in a system. However, the statement never implies that a material with negative temperature is colder than a material with a positive one. In fact, a material with negative temperature is hotter than the material with positive temperature. This conflict comes from the temperature definition in statistical physics. The definition of temperature in this chapter is as abstract as the definition of energy. This is why the non-negative temperature is a consequence of the formulation.

In statistical mechanics, since most of the equations are coming from the equilibrium assumption, the non-equilibrium definitions remain unclear. As a result, when a non-equilibrium case occurs, the peculiarities of these definitions arise in the concept, e.g.

negative temperature. In fact, high concentration of energy at a local point combined with the fast transport of energy, in the present chapter, is similar to the negative temperature stated by Landau. In both cases, non-equilibrium exists and energy is transported from a hotter place to the colder one. It is to the point to mention that, in both cases, the relaxation times (time lags) are the causes of non-equilibrium situations.

6.7- Conversion of PHTM into the Fourier Law

In order to convert the PHTM into the Fourier law, the following assumptions are taken into account:

1- ${}^e k = {}^l k = k / 2 \equiv Cte.$

2- Neighbors are the nearest atoms.

3- The lattice is homogeneous.

4- $\chi_a = \chi = Cte.$

5- $k / \chi \triangleq K.$

6- $\tau_j^i = \tau_i^j = \tau.$

7- ${}^e \tau_i^j = {}^e \tau_j^i = {}^e \tau.$

8- ${}^l \tau_i^j = {}^l \tau_j^i = {}^l \tau.$

9- There is no large heat flux in the domain. This implies that there exists no large temperature difference in the domain as well.

The last assumption will result in a slow-changing temperature at each lattice point. In other words:

$$\begin{aligned} T_i(t - \tau) &\approx T_i(t) \\ T_i(t - \tau - {}^l\tau) &\approx T_i(t - \tau - {}^e\tau) \approx T_i(t). \\ T_i(t - {}^l\tau) &\approx T_i(t - {}^e\tau) \approx T_i(t) \end{aligned} \quad (6.15)$$

In the following sections, it is shown by examples (though not proved), that equations (6.15) are direct consequences of the last assumption. At this stage, it is assumed that N atoms, or lattice points, are in a cubic box of length L . This box is named “B”. From equation (6.7), by using the assumptions stated in this section, one can write the summation for the lattice points inside B:

$$\sum_a \dot{T}_a = -K \sum_a \sum_{i \neq a}^{\text{neighbors}} u(T_a(t) - T_i(t)) + K \sum_a \sum_{i \neq a}^{\text{neighbors}} u(T_i(t) - T_a(t)) \quad (6.16)$$

Some terms, in the right hand side of the equation (6.16), are zero. They are the points with all the neighbors inside the box. This is because the energy from i to a is compensated by the energy of a to i in the summation. The only terms that remain in the RHS of (6.16) are the terms that involve the temperature of the points outside B. Those points that are outside B, and are present in the RHS of (6.16), are shown by a prime superscript and ia script.

$$\sum_a \dot{T}_a = -K \sum_a^{\text{on the boundary of B}} u(T_a(t) - T'_{ia}(t)) + K \sum_a^{\text{on the boundary of B}} u(T'_{ia}(t) - T_a(t)). \quad (6.17)$$

A new temperature is defined here, denoted as cell average temperature,

$$\frac{\sum_a T_a}{N} = \bar{T}_{IJK}. \quad (6.18)$$

One should use a new assumption

$$\sum_a^{\text{on the boundary of } B} T_a = pn \bar{T}_{IJK}. \quad (6.19)$$

In (6.19), n is the number of all lattice points in B that have neighbors outside B . p is a phenomenological constant, that is assumed to present the uniformity of the cell average temperature. If $p \approx 1$, the cell average temperature is almost the individual lattice point temperatures. This coefficient is assumed to be the same for all neighboring cells. Finally, using all of these assumptions, equation (6.17) will be like the following. The numerical indices show the neighboring cells of the IJK cell. For example, $I+1, J, K$ is the next cell on the right side of IJK cell, in the Cartesian coordinate system.

$$\begin{aligned} \frac{d(\bar{T}_{I,J,K})}{dt} = \frac{K}{N} & \left[-\frac{pn}{6} \{ \bar{T}_{I,J,K} - \bar{T}_{I+1,J,K} \} - \frac{pn}{6} \{ \bar{T}_{I,J,K} - \bar{T}_{I-1,J,K} \} \right. \\ & - \frac{pn}{6} \{ \bar{T}_{I,J,K} - \bar{T}_{I,J+1,K} \} - \frac{pn}{6} \{ \bar{T}_{I,J,K} - \bar{T}_{I,J-1,K} \} \\ & \left. - \frac{pn}{6} \{ \bar{T}_{I,I,K} - \bar{T}_{I,J,K+1} \} - \frac{pn}{6} \{ \bar{T}_{I,J,K} - \bar{T}_{I,J,K-1} \} \right] \end{aligned} \quad (6.20)$$

If the distance between lattice points, the diameter of the atoms, are d , then n would be

$$n \simeq \left(\frac{L}{d} \right)^2 \quad \text{and} \quad \frac{n}{N} \simeq \frac{d}{L}. \quad (6.21)$$

Using (6.21) in (6.20) and consequently rearranging the terms, one will find

$$\begin{aligned} \frac{d(\bar{T}_{I,J,K})}{dt} = \frac{-Kpd}{L} \bar{T}_{I,J,K} + \\ \frac{Kpd}{6L} [\bar{T}_{I+1,J,K} + \bar{T}_{I,J+1,K} + \bar{T}_{I,J,K+1} + \bar{T}_{I-1,J,K} + \bar{T}_{I,J-1,K} + \bar{T}_{I,J,K-1}] \end{aligned} \quad (6.22)$$

If one sets $\frac{Kpd}{6L} = \frac{\alpha}{\Delta x^2}$ and $\Delta x = L$, equation (6.22) is identical to the discrete form of the Fourier law. This shows that

$$K = \frac{6\alpha}{pdL}. \quad (6.23)$$

Since α , K and d are fixed variables, the important issue is how to find L . This characteristic length must be chosen, in a way that satisfies all the assumptions. The most important of these assumptions, is the constant and near to unity value of p . This assumption guarantees the existence of the $\bar{T}_{JK}$. Hence, in a region in which this characteristic length cannot be found, the Fourier law is essentially not satisfied. This can happen in very small scales. Not only can small scales break down all these assumption, but also high energy fluxes, e.g. laser pulses, in short period of times, can have the same effect: the failure of the Fourier law.

6.8- Slip Boundary Condition Concept

One of the main topics in micro-scale heat transfer is the concept of Slip Boundary Condition (SBC) [152]. In this section, it is shown that this concept is clearly deductable from the simplified PHTM equation. The SBC is more observable when the steady state condition is achieved by the system. Here, the model is one-dimensional and equation (6.11) is used. In the steady-state condition, the temperature derivative, with respect to

time, is zero. It is assumed that the non-dimensional temperature is $\theta_i = \frac{T_i - T_{BR}}{T_{BL} - T_{BR}} \cdot T_{BR}$

is the temperature at the right boundary and T_{BL} is the temperature at the left boundary.

Hence, $\theta_{BL} = 1$ and $\theta_{BR} = 0$. There are N lattice points in the middle. It is also

assumed that $T_{BL} > T_{BR}$. The latter emphasizes on the fact that the heat transfer is from left to right and $\theta_i > \theta_{i+1}$ for $i = 1, \dots, N-1$. It is further assumed that all the points inside the domain are the same with the same K . Both of the boundaries are connected to the rest of the domain with K_B .

For $i = 1, N-1$ the equation (6.11) would be

$$\begin{aligned} (1+x)\theta_1 - \theta_2 &= x \\ (1+x)\theta_N - \theta_{N-1} &= 0 \end{aligned} \quad (6.24)$$

where $x = \frac{K_B}{K}$. For other $i = 2, \dots, N-1$ the equations are

$$\theta_{i-1} - 2\theta_i + \theta_{i+1} = 0. \quad (6.25)$$

If one defines $m_i \triangleq \frac{\theta_{i+1} - \theta_i}{i+1-i}$, then according to equation (6.25), one has

$$m_1 = m_2 = \dots = m_{N-1}. \quad (6.26)$$

The latter emphasizes that all the non-dimensional temperatures, inside the domain, are on the same line.

In order to find a quantitative measure for the SBC, one needs to find θ_1 . If the $N-1^{th}$ equation is multiplied by $1+x$, the $N-2^{th}$ by $1+2x, \dots$, and the first one by $1+(N-1)x$, and then summing up all the equation the θ_1 is found.

$$\theta_1 = \frac{1+(N-1)x}{2+(N-1)x} < 1 = \theta_{BL} \quad (6.27)$$

The slip at the left boundary is defined as $\theta_{BL} - \theta_1 \triangleq S$.

$$S = \frac{1}{2 + (N - 1)x} \quad (6.28)$$

This equation shows that the slip at the boundaries depends on two factors: the first one is the number of lattice points; and the second one is the conductivity ratio of the medium to the boundary. While the latter acts exactly like a boundary resistance, the former shows that the slip boundary condition exists, necessarily, at nano- and micro-scales as the number of lattice points are limited.

6.9- Numerical Methods and Simulations

In all the simulations presented in this section, equations (6.11) and (6.12) are used. As a result, all simulations are one-dimensional. The first issue, in the numerical approach to this problem, is to define the time derivative. There are plenty of good and accurate numerical approaches to DDEs [164]. However, in this section, the time derivative is approximated with the simplest, and also most physical, possible approximation. Here, the Euler method is used.

$$\frac{df_i^j}{dt} = \frac{f_i^{j+1} - f_i^j}{\Delta t} \quad (6.29)$$

In this formula, the value of the derivative of f at the j^{th} time step, and the i^{th} lattice point position, is approximated by the right hand side of (6.29). The time step, as it is seen in (6.29), is Δt . Using equation (6.29), the numeric system of equations for the dimensionless temperature is

$$\theta^{j+1} = (\mathbf{A} + \mathbf{B})\theta^{j-h} + \mathbf{C}\theta^j + \mathbf{D}\theta^{j-2h}. \quad (6.30)$$

In this equation,

$$\underline{\theta}^j = (\theta_1^j, \theta_2^j, \dots, \theta_i^j, \dots, \theta_N^j)^T. \quad (6.31)$$

The h is the number of time steps, in one time lag. In other words $h = 1/\Delta t$. The matrices are, for the case that the boundary conditions are specified,

$$\mathbf{A} = a \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 0 & & \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ & & & 1 & 0 & 0 \\ 0 & \dots & & 0 & 0 & 0 \end{pmatrix}_{N \times N} \quad (6.32)$$

$$\mathbf{B} = b \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 0 & 1 & & \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ & & & 0 & 0 & 1 \\ 0 & \dots & & 0 & 0 & 0 \end{pmatrix}_{N \times N} \quad (6.33)$$

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1+c & 0 & 0 & \dots & 0 \\ 0 & 0 & 1+c & 0 & & \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ & & & 0 & 1+c & 0 \\ 0 & \dots & & 0 & 0 & 0 \end{pmatrix}_{N \times N} \quad (6.34)$$

$$\mathbf{D} = d \begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 1 & 0 & & \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ & & & 0 & 1 & 0 \\ 0 & \dots & & 0 & 0 & 0 \end{pmatrix}_{N \times N}. \quad (6.35)$$

If one defines $\tau K \Delta t \triangleq q$ then

$$\begin{aligned}
 a &= q \left(U(\theta_i^j - \theta_{i-1}^{j-h}) + U(\theta_{i-1}^{j-h} - \theta_i^{j-2h}) \right) \\
 b &= q \left(U(\theta_i^j - \theta_{i+1}^{j-h}) + U(\theta_{i+1}^{j-h} - \theta_i^{j-2h}) \right) \\
 c &= -q \left(U(\theta_i^j - \theta_{i-1}^{j-h}) + U(\theta_i^j - \theta_{i+1}^{j-h}) \right) \\
 d &= -q \left(U(\theta_{i+1}^{j-h} - \theta_i^{j-2h}) + U(\theta_{i-1}^{j-h} - \theta_i^{j-2h}) \right)
 \end{aligned} \tag{6.36}$$

Finally,

$$U(x - y) = \begin{cases} 1 & \text{if } x > y \\ 0 & \text{if } x < y \end{cases} \tag{6.37}$$

If the boundary conditions are not specified, it means that the lattice points are connected to no boundaries. Therefore, the matrices will be the same, except

$$\begin{aligned}
 A_{N,N-1} &= a \\
 B_{1,2} &= b \\
 C_{1,1} &= 1 - q \left(U(\theta_1^j - \theta_2^{j-h}) \right) \\
 C_{N,N} &= 1 - q \left(U(\theta_N^j - \theta_{N-1}^{j-h}) \right) \\
 D_{1,1} &= -q \left(U(\theta_2^{j-h} - \theta_1^{j-2h}) \right) \\
 D_{N,N} &= -q \left(U(\theta_{N-1}^{j-h} - \theta_N^{j-2h}) \right)
 \end{aligned} \tag{6.38}$$

The question might arise in the reader's mind of why other difference operators are not used instead of equation (6.29). The response is that other difference equations, or even operators like Adam's method operators [164], are nonphysical. This is because those equations and operators use the information of more than two points in time. The other problem is that they are more mathematically involved and the accuracy will be hindered by the computational cost. In the next subsection the results of the simulations are presented based on the numerical approaches of this chapter. The coming simulations are based on the physical concepts stated in the previous parts.

6.9.1- Simulation without Boundary Condition

In the coming numerical simulation, it is assumed that $N = 50$ lattice points are released from a random initial condition. All the lattice point temperatures are between zero and one. The value of τK is set to be unity. This simulation roughly shows how energy is conserved. At the start of the process, the average of dimensionless temperature is $\bar{\theta} = 0.4915$. When the process starts the average temperature drops. This can be seen in Figure 22 and Figure 23.

Figure 22- Dimensionless temperature distribution and average temperature @ $t / \tau = 4$

At this stage, the energy is being transferred by the means of the carriers of the energy. It shows that a great portion of the energy is in transfer. Later on, when these carriers of energy are reduced in magnitude of the energy that they transport, the temperature average reaches the initial value exponentially. At the beginning of this limiting regime,

one can say that the heat transfer has entered the slow regime. The temperature propagation is now diffusive. This slow transport was one of the main assumptions in deriving the Fourier law. This is when the concept of the quasi-equilibrium is present. In this numeric example, the quasi-equilibrium happens after ten phase delays. One important factor is that the steady-state condition of the temperature average does not mean the steady-state of the temperature itself. This can be observed clearly in Figure 24.

Figure 23- Dimensionless temperature distribution and average temperature @ $t / \tau = 9$

The simulations in this subsection clearly show that after a while, the process becomes slow. When there is no large heat flow rate, the process ceases its rapid speed of change. In other words, the heat propagation becomes diffusive rather than ballistic.

Figure 24- Dimensionless temperature distribution and average temperature @ $t / \tau = 99$

6.9.2- Heat Wave

A consequence of (6.7) is the heat wave. In the following simulation, 5 out of 50 lattice points are excited from a neutral state, $\theta = 0$. The governing equations for the system are stated in equation (6.12). The value of τK is assumed to be 10. The source term is only applied for one phase-lag and the system is released afterwards. There is no boundary condition for the problem. The boundaries are thermally free. After the imposition of the source term, two temperature waves are propagating in the system. The waves are propagated in two different directions. The heat waves reach the free boundaries of the system and are reflected back into it. The heat is reflected from the free boundaries since, for a short time, there is energy accumulation at the boundaries. This accumulation must be smoothed. As a result the energy flows back from the boundaries

as it cannot flow out. At the centre of the system at $t / \tau = 55$, again, the waves meet each other. As can be seen in the figures, the temperature wave is damped as time goes on.

This simulation clearly shows how the PHTM is capable of predicting the heat wave.

This model can clearly be used in cases like laser pulses.

6.9.3- Approximate Equation

When the average temperature reaches a constant value, in the domain, one can assume that the system has lost its memory. It is all due to the fact that the process has become slow. If the system is large enough, the Fourier law would be acceptable. However, in small scales one can devise a memory-less form of (6.11). This assumption is like

$$\theta_i(t') \approx \theta_i(t' - 1) \approx \theta_i(t' - 2). \quad (6.39)$$

With respect to this assumption one has

$$\begin{aligned} \frac{d(\theta_i(t'))}{dt'} \approx \tau K [& -u(\theta_i(t') - \theta_{i-1}(t')) - u(\theta_i(t') - \theta_{i+1}(t')) \\ & + u(\theta_{i+1}(t') - \theta_i(t')) \\ & + u(\theta_{i-1}(t') - \theta_i(t'))] \end{aligned} \quad (6.40)$$

In the following simulation, $N = 50$ lattice points are released from a random initial condition. All temperatures are between zero and one. The τK is set to be 10. The system is first solved for 23 time delays. The first plot in Figure 25 shows the asymptotic approach for the temperature average. At this point, when the average temperature steady-state condition is reached, the approximate equation (6.40) and the exact one are solved for 1000 time delays. In order to define the errors involved in the approximate equation, one can define two quantities. The average error and maximum error are defined as following to show the severity of the error. The first one shows the error produced and averaged over all lattice points. The *norm* defined in the following formula is the L^2 norm for a $N \times 1$ vertical vector $\underline{\theta}$.

$$\begin{aligned}
 \text{Average Error} &\triangleq \frac{\text{norm}(\theta_{\text{exact}} - \theta_{\text{approximate}})}{\text{norm}(\theta_{\text{exact}})} \times 100 \\
 \text{Maximum Error} &\triangleq \frac{\text{Max}(\theta_{\text{exact}} - \theta_{\text{approximate}}) \times N}{\text{norm}(\theta_{\text{exact}})} \times 100
 \end{aligned}
 \tag{6.41}$$

Figure 25- Average temperature at 23τ

As can be seen in the following figure, Figure 26, the differences between the two equations are small.

Figure 26- Temperature distribution at 998τ

The errors, for the example simulation, are

$$\text{Average Error} = 0.1798$$

$$\text{Maximum Error} = 1.9295$$

These results clearly show that when the process is slow, the memory is lost.

6.9.4- Numeric Results of the Slip Boundary Condition

In this subsection, equations (6.24) and (6.25) are solved for a few numerical cases. At the beginning, the value x is under study. For a fixed value of N , which is chosen to be $N = 50$, the results are shown in Figure 27.

Figure 27- Steady-state dimensionless temperature for different x 's

As it has been seen, the lower the x is, the larger the slip is observed. This suggests that different materials may result in different slips. The stronger the boundary bond is, the less the slip will be present.

In the following example, the effect of the boundary slip is examined. Equation (6.28) is plotted for different values of x . As it is obvious, in all cases the Slip approaches zero as

the number of lattice points is increased. By increasing the number of lattice points, the system approaches its continuum regime. Hence, the Slip eventually fades at that area.

Figure 28- The slip effect

In the next section, the conclusions of this chapter are presented.

6.10- Summary and Conclusion

In this chapter, a full phenomenological pointwise heat transfer model was presented. This model, at the first stage, is based on fundamental physics basis. The model was presented in its general form. Later on, the one-dimensional form of it was derived.

The consequences of this new modeling are numerous:

- 1- Derivation of the Fourier law
- 2- Heat wave
- 3- Memory effect of the material
- 4- Slip Boundary Condition

5- Non-negative temperature

- 6- In this model, the heat transfer is a direct effect, and the temperature difference is the cause of it.

One shortcoming of this chapter is that no real value of the physical quantities is presented. This is due to the fact that the experimental values of the properties which are defined, in this chapter, were not available to the author.

Last, but not least, there is no definition of entropy here. Despite statistical physics that the temperature can be defined through entropy, here the entropy must be related to the temperature. In fact, in this chapter the temperature is an axiom directly connected to the energy. Consequently, the definition of the entropy can be a future work in this area of research.

The next chapter is a logical flow of the current idea. The idea of phase lag will be brought to the molecular domain to justify the origins of the high-temperature model of superfluidity.

Chapter 7 : On the Origins of High-Temperature Model of Superfluidity

In this chapter, the origins of the high-temperature model of superfluidity will be discussed. However, applying the same procedure presented in the previous chapter to the fluid case can be too complicated. This is due to the fact that the molecules are all moving with different velocities. As a result, defining the most probable position for a particle is not applicable in parallel to what was done in the case of heat transfer in solid bodies. Hence, a phenomenological approach might completely spoil the physical picture of the problem. Consequently, the phenomenological approach will not be adopted in this chapter. In the coming section, the author first tries to see where the time-lag modifications can be implemented. It is logical to seek possible modifications in fundamental approaches and models to show the possibilities of the high-temperature model of superfluidity. In fact, in this chapter, it is shown how the concept of phase-lag can improve the understanding of some physical phenomena. Also, it will suggest that this approach can be implemented in areas like Quantum mechanics.

7.1- Possible Modifications

There are four major fundamental models that one might be able to modify to find the origins of high-temperature superfluidity. They are the Liouville equation, the Boltzmann equation, the ballistic-diffusive treatment, and finally, the molecular dynamics. These four approaches are the most fundamental ones in the microscopic treatment of the matter at the atomic level. In the following, each formulation is considered. It will be shown that molecular dynamics is the most appropriate model to address high-temperature superfluidity.

7.1.1- The Liouville Equation

The Liouville equation is one of the most fundamental formulas in mechanics. The equation relates the time derivative of the distribution function f to the “phase-space” derivatives as follows.

$$\frac{\partial f^{(N)}}{\partial t} + \sum_{i=1}^n \dot{\mathbf{r}}^{(i)} \frac{\partial f^{(N)}}{\partial \mathbf{r}^{(i)}} + \sum_{i=1}^n \dot{\mathbf{p}}^{(i)} \frac{\partial f^{(N)}}{\partial \mathbf{p}^{(i)}} = 0. \quad (7.1)$$

In the formula, n is the number of degrees of freedom, N is the number of the atoms (particles), and $f^{(N)} = f^{(N)}(t, \mathbf{r}^{(n)}, \mathbf{p}^{(n)})$. Also, $\mathbf{r}^{(n)}$ is the generalized coordinate of the system and $\mathbf{p}^{(n)}$ is the generalized momentum.

This equation is one of the most fundamental equations in science; however, its direct solution is impossible for a non-equilibrium system. In fact, finding a proper functionality for f , even in equilibrium, is harder than the solution itself. Truly, this fundamentality is paid off in non-solvability. As previously mentioned, the situation would be exacerbated if the non-equilibrium condition is involved.

7.1.2- The Boltzmann Equation

This equation is an averaged form of the Liouville equation. The distribution function, in this case, is an average of the N -particle distribution function over the rest of the other $N - 1$ particles of the system. This averaging tries to reduce the number of independent variables, though at a cost of introducing a collision term. As hard as defining the distribution function, in the Liouville equation, the collision term is also hard to be defined. The proposed collision terms in literature are mostly differo-integral equations, being one of the hardest equations to be solved. In fact, in order to tackle this issue, a

relaxation time approximation is usually used. This will result in a quasi-equilibrium constitutive equation, mentioned in the previous chapter. The approximation, obviously, makes the non-equilibrium considerations dim.

As one can observe, neither the Liouville equation nor the Boltzmann equation are suitable for any consideration in the phase-lag formulations. They can only provide approximate solutions. It worth mentioning that, the Boltzmann equation is most suitable for dilute systems assuming no volume for particles, and considering the interactions to be limited to the instance of collision [165]. It is also assumed that the collision time is much smaller than the free travelling time of particles. The latter is violated for liquids.

7.1.3- The Ballistic-Diffusive Treatments

Since ballistic-diffusive treatments are based on the relaxation time approximation of the Boltzmann equation, it is doubtful to try to implement phase-lagged formulation into this field. The phase-lagged formulation tries to capture the non-equilibrium features. As a result, its use is, to great extent, not for a quasi-equilibrium case. In addition, since the relaxation time approximation is completely based on the elastic collision of the particles, the use of phase lags seems to be fruitless here as well.

7.1.4- The Molecular Dynamics

Molecular dynamics is about the potential (force) field between the molecules in a system [166, 167]. The molecular dynamics equations, up to the knowledge of the author, are all functions of relative positions of the particles. This relative functionality is not a function of time. The equations governing the motion are all derived, originally, from electrostatics. In electromagnetism, one knows that the moving charged particle

imposes an electromagnetic field. The produced fields are propagated at the speed of light in vacuum [168]. As a result, any reaction to the field at any point is a function of other particles positions in the past. This fact is clearly ignored in molecular dynamics. However, this ignorance can be a good place for the modification of the molecular dynamics formulas to show the origins of the high-temperature superfluidity. It is worth mentioning that the delay time for information propagation is ,already, a solved problem in electromagnetism [169]. Interestingly, this effect has both Newtonian and Relativistic formulations. Consequently, the time-lag in conveying of the “news” must be included in the molecular dynamics. As it is known to the author, no molecular dynamics formulation is based on this fact. In other fields of physics, few authors have, recently, mentioned this phase-lag [170-173]. All in all, the molecular dynamics is the best place to implement the phase-lag idea. This implementation will show whether there is any foundation for the high-temperature superfluidity or not. In the next section, the study will start from the basic and simple ideas of time delay in the transportation of the information.

7.2- Shifted Potential Fields

It is known that, in molecular dynamics of the soft-sphere models, it is the potential field by each atom that is responsible for all the interactions. The classical force field and potential function are functions of position. The force is an “action in a distance” force type. Here, the author tries to formulate a potential that is both dependent on position of the particles affected and the particle position itself in the past. The position of the particle, at the instance of interaction, is found at the time needed for the signals to travel from the particle to the specified interaction position. Some similar attempts have been conducted in electromagnetism [169], though no attempts in molecular dynamics.

As can be seen in Figure 29, one can suppose that the position of the particle at time t is $\mathbf{r}_p(t)$. Vector position $\mathbf{r}$ is the position of an arbitrary point in space. The effect of the particle at position $\mathbf{r}$ is felt after a time τ when the position of the particle had been $\mathbf{r}_p(t - \tau)$. As a result the force field at position $\mathbf{r}$ is dependent on the position of the particle at $\mathbf{r}_p(t - \tau)$. If one names the potential field as Φ , its functionality is like $\Phi(\mathbf{r}, \mathbf{r}_p(t - \tau))$. The time delay τ is the positive root of the equation

$$\tau = \frac{|\mathbf{r} - \mathbf{r}_p(t - \tau)|}{c} \quad (7.2)$$

in which, c is the speed of the information propagation. This speed can be the speed of light in case of electromagnetism. In other systems, this speed is different. Since in reality, particles cannot travel faster than the speed of light, the positive solution of (7.2) is unique.

Figure 29- Delay force field

In the next part, a simple example is presented to show the consequence of such a delay in distortion of the force and potential fields. It will be shown how the potential field is squeezed (or expanded) because of the finite speed of information transport.

7.2.1- Example 1, constant velocity

Let's imagine that there is a 1-D space. In other words, there is only x direction in this space. Suppose that a particle is at rest at time $t = 0$. It is assumed that the particle is suddenly moved from rest to a velocity v along the positive direction of the axis. It is assumed that the potential field produced by the particle, at rest, is

$$\Phi(x) = \begin{cases} 0 & x < 0, x > x_0 \\ 1 - \frac{x}{x_0} & 0 < x < x_0 \end{cases} \quad (7.3)$$

Figure 30- Example potential

It is intended to find the potential field as the particle is moving. The shape of the potential is shown in Figure 30. In the figure, x_0 is unity.

As the particle is at rest and suddenly starts to move from the rest position, at $x = 0$, the position of the particle is $x_p(t) = vt$ for all $t \geq 0$. The new potential field is proposed to involve the effect of finite speed of the information propagation:

$$\Phi(x, t) = \begin{cases} 0 & x < x_p(t), x > x_p(t - \tau) + x_0 \\ 1 - \frac{x - x_p(t - \tau)}{x_0} & x_p(t) < x < x_p(t - \tau) + x_0 \end{cases} \quad (7.4)$$

It is also known that

$$x - x_p(t - \tau) = c\tau, \quad (7.5)$$

where c is the speed of the information propagation. Now, for the time $t > 0$ at which the situation is $x_p(t) < x < ct < x_0$, the potential field is

$$\Phi(x, t) = 1 - \frac{x - x_p(t - \tau)}{x_0}. \quad (7.6)$$

Equation (7.6) can be simplified further according to equation (7.5). The procedure is

$$x - x_p(t - \tau) = c\tau \rightarrow x - v(t - \tau) = c\tau$$

$$\Rightarrow \begin{cases} \tau = \frac{x - vt}{c - v} \\ x_p(t - \tau) = \frac{ct - x}{\frac{c}{v} - 1} \end{cases}.$$

As a result, equation (7.6) would become

$$\Phi(x, t) = 1 - \frac{x - x_p(t)}{\left(1 - \frac{v}{c}\right)x_0}, x_p(t) < x < ct < x_0 \quad (7.7)$$

The displaced potential field is shown in Figure 31. As can be seen from the figure, at the position that the information has just arrived, there is a jump in the slope of the line (in the Figure 31 $x = 0.5$ for $v = c/2$). The proof of continuity of the potential is easy. If

one sets $x = ct$ in (7.7) and (7.3), the continuity is satisfied. However, the slope of the potential at $x = ct$ is not continuous. The gradient is $((1 - v / c)x_0)^{-1}$ from the left and $(x_0)^{-1}$ from the right. As the particle moves and the information completely propagates beyond x_0 the shape of the potential is totally shrunk. The final shape of the potential field is shown in Figure 32.

Figure 31- Displaced potential

Figure 32- Steady state squeezed potential

It can be deducted that the characteristic length, x_0 , in the direction of motion is squeezed by a factor of $1 - v/c$ and expanded by $1 + v/c$ in the opposite direction. Later, it will be shown that if one assumes that the force is the gradient of the potential field, the force is increased and squeezed in the direction of motion and decreased and expanded in the opposite direction. In the next subsection, by an example, it will be shown that the discontinuity, in the slope of the potential field, or the discontinuity, in the force field, can be alleviated by a continuous velocity for the particle.

7.2.2- Example 2, continuous velocity

In the previous part, the sudden shock to the particle imposed a discontinuous potential slope. In this part, the potential field is (7.4), however, the position of the particle is given by $x_p(t) = at^2 / 2$. As a result, the acceleration of the particle remains the same.

The rest of the procedure is like in the previous section:

$$x - x_p(t - \tau) = c\tau \rightarrow x - a.(t - \tau)^2 / 2 = c\tau \quad (7.8)$$

The only accepted root is the positive one, hence one has

$$\tau = \frac{at - c + \sqrt{c^2 + 2a(x - ct)}}{a} \quad (7.9)$$

$$x_p(t - \tau) = \frac{1}{a} \left[c^2 + a(x - ct) - c\sqrt{c^2 + 2a(x - ct)} \right] \quad (7.10)$$

The potential field is

$$\Phi(x, t) = 1 - \frac{c(\sqrt{c^2 + 2a(x - ct)} + at - c)}{ax_0}. \quad (7.11)$$

At $x = ct$ the continuity is satisfied from the left and right sides. The gradient of (7.11)

at $x = ct$ from the left and right are

$$\left. \frac{\partial \Phi_-}{\partial x} \right|_{x=ct} = \frac{-c}{x_0} \frac{1}{\sqrt{c^2 + 2a(x - ct)}} \bigg|_{x=ct} = \frac{-1}{x_0} = \left. \frac{\partial \Phi_+}{\partial x} \right|_{x=ct}. \quad (7.12)$$

Hence, as long as the motion is smooth and the position is derivable with respect to time, at least once, the force field will be continuous.

7.2.3- Lennard-Jones Potential

The Lennard-Jones (LJ) potential is the major potential used to consider the motion of the atoms and molecules in molecular dynamics simulations. The original LJ model is

$$\Phi(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (7.13)$$

where r is the distance between the particles and, ε and σ are the specific values for the particle force field. It is to the point to mention that, after all the formulations that will be stated in this subsection, there will be a direct deviation from the classical mechanics. This means that Newton's third law of motion will not be applicable any more.

Let's assume that a particle has been travelling for a long time (the steady-state condition is considered), with a constant velocity v , in the x direction, with respect to an observer.

In other words $\mathbf{r}_p(t) = vt\mathbf{i}$, where $\mathbf{i}$ is the unit vector, in the x direction. The new potential field is now defined as

$$\Phi(\mathbf{r}, \mathbf{r}_p(t - \tau)) = 4\varepsilon \left[\left(\frac{\sigma}{|\mathbf{r}_p(t - \tau) - \mathbf{r}|} \right)^{12} - \left(\frac{\sigma}{|\mathbf{r}_p(t - \tau) - \mathbf{r}|} \right)^6 \right]. \quad (7.14)$$

As in previous sections, $\mathbf{r}_p(t - \tau)$ is the position of the particle in the past time $t - \tau$.

There is also an equation relating the time-lag and speed of the propagation of information c :

$$|\mathbf{r}_p(t - \tau) - \mathbf{r}| = c\tau. \quad (7.15)$$

For a better reference one can refer to the Figure 29. Equation (7.15) can now be written like below since the motion is in the x direction.

$$(c\tau)^2 = (x - v(t - \tau))^2 + y^2 + z^2 \quad (7.16)$$

For simplicity it is possible to consider the moment that the particle is at the origin, or setting $t = 0$ in (7.16). If one solves for the positive solutions of the equation (7.16), the results for the time delay and particle position would be

$$\tau = \frac{xv + \sqrt{x^2v^2 + r^2(c^2 - v^2)}}{c^2 - v^2} \quad (7.17)$$

$$\mathbf{r}_p(-\tau) = -\frac{x + \sqrt{x^2 + r^2(c^2 / v^2 - 1)}}{c^2 / v^2 - 1} \mathbf{i}. \quad (7.18)$$

In the above equations, one has $r^2 = x^2 + y^2 + z^2$. Equation (7.18) shows that, for any point $\mathbf{r} = (x, y, z)$ in space, the position of the particle at the moment of the information propagation is defined by (7.18). It is also deductable from (7.18) that the spheres of information are not symmetrical with respect to the current position of the particle,

any more. Taking (7.18) into spherical coordinates, partially, will effectively reduce further calculations

$$\mathbf{r}_p(-\tau) = -r \frac{\sin \varphi \cos \theta + \sqrt{\sin^2 \varphi \cos^2 \theta + (c^2 / v^2 - 1)}}{c^2 / v^2 - 1} \mathbf{i}. \quad (7.19)$$

As a result the $|\mathbf{r}_p(-\tau) - \mathbf{r}| = R$ will be calculated as

$$R^2 = r^2 \left[1 + \left(\frac{\sin \varphi \cos \theta + \sqrt{\sin^2 \varphi \cos^2 \theta + (c^2 / v^2 - 1)}}{c^2 / v^2 - 1} \right)^2 + 2 \sin \varphi \cos \theta \frac{\sin \varphi \cos \theta + \sqrt{\sin^2 \varphi \cos^2 \theta + (c^2 / v^2 - 1)}}{c^2 / v^2 - 1} \right]. \quad (7.20)$$

Before finding the complete form of the delay potential, it is wise to see what happens to the equal-potential surfaces for a moving particle. The equal-potential surfaces are the ones that make equation (7.14) constant. In other words, these surfaces are the ones that keep (7.20) constant.

In Figure 33, it can be seen that for two different values of R , $R = 1$ is the outer sphere and $R = 0.5$ is the inner one, the spheres are not at all symmetric with respect to the origin, which is the current particle location. The value of v / c has been assigned as 0.8, in (7.20), to clearly show the asymmetric propagation of the information spheres. It is also possible to observe the XY sketch of Figure 33, in Figure 34. As the particle moves, the spheres are left back. The smaller is the sphere's radius, the more symmetry with respect to the current particle position.

Figure 33- Displaced information spheres

Figure 34- XY projection of Figure 33

From the above figures, one can find the position at which the particle had been at the instant of information propagation. In the next figure, Figure 35, it is possible to compare the classical view of the equal-potential surfaces and the new one. Both surfaces are plotted for $R = 1$. The new model has the parameter $v / c = 0.8$. The dashed sphere is the classical potential view and the meshed one is the new one. Obviously, the new one, as can be seen, in Figure 35 and Figure 36, is highly shifted to the left. Again, the current position of the particle is at the origin.

Figure 35- Equal-potential comparison; old and new models

Figure 36- XY projection of Figure 35

Since all the information surfaces are spheres, the volume in which the information is confined remains constant and it does not depend on the velocity.

At this point, if one defines the force field produced by the potential field as $\mathbf{F} = -\nabla\Phi$, in which the del operator is only spatial, the force field would be

$$\mathbf{F} = 24 \frac{\varepsilon}{\sigma} \left(2 \left(\frac{\sigma}{R} \right)^{13} - \left(\frac{\sigma}{R} \right)^7 \right) (\nabla R). \quad (7.21)$$

The function R is defined as (7.20). The first conclusion that can be drawn from (7.21) is that there exists no more symmetry in the force field. In the following graphical

sketches for simplicity σ is set to be unity and all plots are not the force $\mathbf{F}$ but $\frac{\sigma \mathbf{F}}{24\epsilon}$. As mentioned, the force is not symmetric any more. Since the functionality of $\mathbf{F}$ is not simple and its calculation is complicated, a computer program handles the situation (Appendix A3.3). A consequence of the latter is that there will be a resulting moment field $\mathbf{M} = \mathbf{r} \times \mathbf{F}$ with respect to the current position of the particle. Figure 37 shows a moment field on a circular path ($|\mathbf{r}| = 1$) in the $z = 0$ plane around the current position of the particle $(0, 0, 0)$ shown by a green star at the centre of the plot. As it is observable, the moment field presence is higher at the back of the moving particle. This existence of the moment field is solely a consequence of the new model and the classical models cannot indicate such an effect.

Figure 37- Moment field on a circular path for $v / c = 0.8$

The shape of the force field is also interesting and can be used for further justifications about the possible existence of the high-temperature superfluidity. In the next figure, see Figure 38, the force field is plotted in the x direction.

Figure 38- x -directional force fields

The blue curve, in Figure 38, is the original LJ force field. It is completely symmetrical in all directions. The red curve, in Figure 38, is the shifted force field of the new model for $v/c = 0.8$. The position of the particle is illustrated by a green circle. As can be seen, in the direction of motion, the force field is highly squeezed and intensified. The characteristic length is reduced in this direction. In the opposite direction of motion the force field is stretched and its strength is reduced. The characteristic length is also stretched. A consequence of the new modeling is that, in the direction of the motion, the $\text{range of influence}$ is reduced at the expense of higher

7.2.3.1- A Classical Relativistic Phenomenon

The classical LJ potential can be rearranged to have a functionality of R/σ . In other words, the functionality is of the form

$$\Phi = \bar{\Phi}\left(\frac{r}{\sigma}\right). \quad (7.22)$$

In the new model, the functionality is direction-wise. For example in the x direction the functionality is of the form $\Phi = \bar{\Phi}\left(\frac{r}{(1 - v/c)\sigma}\right)$ and in $-x$ direction it is of the form

$\Phi = \hat{\Phi}\left(\frac{r}{(1 + v/c)\sigma}\right)$. In all above formulas, r is the distance from the current particle

position. If one tries to simplify (7.14) for the potentials in the $x = 0$ plane the result is

$$\Phi = \hat{\Phi}\left(\frac{r}{\sigma\sqrt{1 - v^2/c^2}}\right). \quad (7.23)$$

One might ask whether it is accidental or something relativistic. The answer is that, it is completely relativistic. Although the $x = 0$ plane potential is mentioned here, the measurements to find σ are all carried out in the x -direction. This formulation completely shows that if the characteristic lengths of the particle are measured simultaneously, the length reduction of special relativity is obvious in the formulation.

This formula shows that the lengths are all reduced by a factor of $\sqrt{1 - v^2/c^2}$, if and only if, they are measured simultaneously.

7.3- A Justification for High-temperature Superfluidity

At first it is assumed that every potential field, or force field, has an effective range of influence beyond which no interaction occurs. It is physically true. Another assumption is that a particle only reacts to the other particle force field. By the latter, the Newton's third law of motion is not satisfied, similar to the forces in special relativity. In other words, if $\mathbf{F}_{ij}$ is the force exerted by particle i on the j^{th} one, it is not equal to $\mathbf{F}_{ji}$.

Let's assume that, at the beginning, all of the particles have a random distribution expressed by Boltzmann's distribution. Later on, some of the particles are highly excited in a way that they acquire very high velocities, which are not necessarily in one direction. As a result, the force fields of the particles shift in the opposite direction of

motion. There are two regimes of collisions between the particles. The first one is called a Head to Head (HH) collision, in which, the particles have the same direction of motion. This collision is very sparse. The other collision, which is rife, is called Side by Side (SS) collision. The latter will be completely different from its classical counterparts. By an SS collision it is meant that the directions of the velocities are not the same at all anymore, for the particles.

In an SS collision, since the highly excited particles have a shifted effective range, they first experience the force field of a non-excited particle and later influence the non-excited one. Because of this reaction mechanism, the non-excited particle only experiences the force field of the highly excited one in a very short period of time. The latter will result in a low energy transfer from the highly excited particle to the non-excited one. Hence, the non-excited particle will not have a major distortion in its trajectory, when compared to the classical cases, both because of the shifted force field and short period of influence. On the other hand, the highly excited particle will also have little distortion in its trajectory not only because of short period of influence of non-excited one, but also due to relativistic phenomena. In special relativity, the force on a particle can be related to its momentum according to

$$\mathbf{F} = \frac{d}{dt} \left(\frac{m_0 \mathbf{v}}{\sqrt{1 - |\mathbf{v}|^2 / c^2}} \right). \quad (7.24)$$

In the above formula, $\mathbf{v}$ is the velocity of the particle and m_0 is the rest mass of the particle. Obviously, if the particle has velocity high enough for a specified $\mathbf{F}$, the trajectory will not change much, in contrast to the classical case. The particle seems to be heavier and any change in its momentum is harder. All in all, because of these

statements, the highly excited particle can penetrate more than an ordinary non-excited one in a medium. The lighter the particle is, the higher the penetration length will be. For particles like electrons, the penetration length would be higher since they are lighter than many of the known particles, and consequently can have higher velocities. Hence, in case of solid heat transfer, the highly excited electrons (for example by laser pulses) can travel into the bulk of the material (mostly metals), carry the energy deep inside, and transfer the heat like a wave for some distance.

The particles, because of this high velocity, become more and more elusive to the force fields. In fluid cases, the highly excited particles get out of equilibrium and penetrate further in the bulk of material compared to the classical case. The penetration length is higher than the diffusion characteristic length of the material. It is transport of energy by means of wave fronts. It is nothing but high-temperature superfluidity. Since the particles are travelling fast, for the short period that they are passing through the other particles, the viscosity tends to be zero.

All in all, superfluidity is a possible phenomenon in high temperatures, if and only if some of the particles are highly jerked. Depending on the shock and input energy, the life and penetration length of the superfluidity differs.

This justification partly supports the EKC model presented in the first chapters of this thesis. In fact, in those formulations, in order to simplify the mathematics involved in the formulation, the time lags were assumed to be constant. However, the justification presented in this chapter shows that the time lags can depend on the boundary conditions. As a result, the model, in Chapter 3, should be considered as a good general sample model of all the other models. It is to the point to mention that anisotropic superfluidity is also possible. Since the orientation of the force field of an anisotropic fluid is arbitrary,

in general, to observe a high-temperature version of superfluidity, the existence of external fields, e.g. magnetic one, is necessary.

As observed in these justifications, the superfluidity only needs some highly excited particles in high temperatures in order to be triggered. There is no need, at least, for quantum mechanical effects in high temperatures to support the superfluidity physics.

7.4- Conclusion and Future Work Remarks

In this chapter, the effect of the time-lag, in the potential and force fields, was studied. It could be shown that the time-lag will result in shifted and distorted fields. The shift and distortion will provide a justification for superfluidity at high temperatures. All the topics, in this chapter, were based on a simple physical assumption: the speed of the propagation of any field is considered to be constant. This constant speed should be the speed of light. As a consequence of this assumption the Newton's third law is not valid any more.

Further investigations, on this topic, can be extended in to the new formulation of molecular dynamics. The equations, needed to solve high energy particles, should be accompanied by the considerations about the shifted potential fields combined with the relativistic mechanics.

Chapter 8 : Closing Remarks

8.1- Summary and Conclusion

The research, in this report, is consisted of seemingly diverse though interconnected models. The impact of the physical assumptions, made by Kulish and Chan [106, 149], have been profound. This chapter is devoted to a summary and conclusion debate. Later, few future tasks are mentioned. As mentioned earlier, the author never expected that the idea of this research would penetrate deep, in numerous fields of physics.

In Chapter 2, a thorough literature review, about the superfluid models, was presented. It was mentioned that BEC has been proposed, by some scientists, as a possible source of superfluidity, at low temperatures. At the same time, it was mentioned that the best single-fluid models are the Mongiovi ET model of superfluidity and the Kulish and Chan phase-lagged formulation.

In Chapter 3, the emphasis was on a new model, extended from the Kulish and Chan model of superfluidity, predicting high-temperature superfluidity. The mathematical and physical ideology behind the problem was to consider a time lag between the onset of energy gradient and the corresponding energy flux. The model could predict a thermomechanical effect. In Chapter 5, the approximate equations of Chapter 3 were shown to be able to simulate a wavy behavior that is known to be inherent in the supertransport of energy. The main idea of that problem was motivated by Professor Leggett's paper to find the behavior of the new model with respect to its low-temperature counterpart. Chapter 4 was another ground for the explanation of more superfluid phenomena, namely the heat waves. The numerical simulations clearly showed that a wave must propagate in the domain that involves temperature shock. In that chapter, few

mathematical solutions for the original phase-lagged heat transfer were proposed. Those solutions were able to explain the behavior of a subclass of PDDEs.

In Chapters 6 and 7, an idea was under scrutiny that the superfluidity is not the sole consequence of the time delay in information, or energy, transport. Specifically, in Chapter 6, it was shown that some phenomena of the nano scale heat transfer and non-equilibrium heat transport can be modeled by the idea of the phase-lagged discrete heat transfer. The model had similar results to the one stated in Chapter 4. However, since the methodology was more micro-scale-based, the results were more general and global. Also, because ordinary delay differential equations were imposed to a discontinuous medium, the number of phenomena that could be covered was much higher than the heat transfer model used by the partial delay differential equations.

Chapter 7 was a breakthrough for the justifications needed for high-temperature superfluidity. The modified shifted potentials of this chapter could state that, at high temperatures, the superfluidity is possible if a few of the molecules acquire much more energy than the others. The model of shifted potentials stated that at high temperatures BEC is not required to explain the possibility of superfluidity.

All in all, the idea that, at first, was assumed to be a good cornerstone of the superfluidity turned out to cover other phenomena.

8.2- Future Works

The Extended Kulish and Chan (EKC) model of superfluidity is proved to be a robust model in predicting high-temperature superfluidity. The experimental approach to observe superfluidity at high temperatures is needed to convert the model into a theory. This part is a challenging but promising work. In this research, nothing explicit about the

boundary conditions was stated. As observed in Chapter 4, the partial delay differential equations, need a special kind of treatment on the boundary conditions. Also, as mentioned in Chapter 7, the time-lag might depend on boundary conditions. These topics need further investigation.

The model in Chapter 6 needs more attention. The further development can be in areas like convection, radiation and tensorial formulation of the new nano-discrete model of heat transfer. The case of fluid flow, of this new model, should be viewed with the help of what is considered in Chapter 7. It will provide a better understanding of the phase-lagged fluid transport equations. Moreover, this model still needs to be further investigated. As an example, nothing was mentioned about the entropy. Finally, a rigorous mathematical approach is needed to find the connection between PLHE and PHTM. One should not expect a direct transformation between them, since they are derived from two different points of view.

Last but not least, the potential shifts portrayed in Chapter 7 need more investigation. As stated there, more attempts are needed to formulate the new physical laws. What was mentioned in that chapter was completely introductory. The field is open and full of vacant research areas. In complement to the ideas of Chapter 7, one truly needs to bring the effect of the phase lag down to quantum world. It seems possible researches, at that area, will shed light on the less-understood accepted axioms of the physics. The author is pointing out the vast research needed to mention the reality behind the space and time. At this stage, one might even come up with a unifying field theory.

By this work, a door to understand more physical phenomena is opened. As a result, one can consider it as a general perspective that is needed to be magnified more.

Appendix 1

In this part, a mathematical approach, for the formulations in the second section of Chapter 3, is presented. It has to mentioned that this part can be ignored (by the reader) without besmirching the physical importance of the methodology and presented physical ideas. This appendix is solely devoted to show the beautiful mathematical concepts hidden behind the formulations.

One can start with writing all the available field equations and also thermodynamics laws.

$$\begin{aligned}
 \dot{\rho} + \rho v_{i,i} &= 0 \\
 \rho a_i &= \rho b_i + t_{ij,j} \\
 t_{ij} &= t_{ji} \\
 \rho r - \rho \dot{\varepsilon} + t_{ki} d_{ki} - q_{i,i} &= 0 \\
 \rho \theta \dot{\eta} - \rho r + q_{i,i} - \frac{q_i g_i}{\theta} &\geq 0
 \end{aligned} \tag{A1.1}$$

As mentioned earlier, one has only 5 equations and 20 unknowns. To overcome the problem and close the mathematical part of the problem one needs to have some knowledge about the constitutive equations. In fact, finding the appropriate approach of finding constitutive relations seems to be like a matter of design. Here, one can present these functionals as primitive shapes of the expected constitutive equations.

$$\begin{aligned}
 \psi &= \hat{\psi}(\rho, \theta, d^{\tau_2}_{ij}, g^{\tau_1}_i) \\
 t_{ij} &= \hat{t}_{ij}(\rho, \theta, d^{\tau_2}_{ij}, g^{\tau_1}_i) \\
 \eta &= \hat{\eta}(\rho, \theta, d^{\tau_2}_{ij}, g^{\tau_1}_i) \\
 q_i &= \hat{q}_i(\rho, \theta, d^{\tau_2}_{ij}, g^{\tau_1}_i)
 \end{aligned} \tag{A1.2}$$

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Also, for simplicity and without destroying the generality, one can imagine that the body forces and body energy supplies are zero. In other words, it is $r = 0, b = 0$. What is written, in (A1.2), is based on one of the principles in *Rational Thermodynamics* and that is the *principle of equipresence* [131]. Later, one might refute some dependencies in the proposed functionals, but for the start it is necessary to present them as done above.

Up to this stage, the form of mathematical problem has been closed, but for the case of applied fluid mechanics one has to be aware of the correct shape of equations in (A1.2). First of all, one should implement equation (A1.2), in the last equation presented in (A1.1); or to more technical language, one has to validate the proposed constitutive equations with respect to the first constraint¹¹.

If one uses the Helmholtz free energy and uses it at the same time in energy equation and implement the results into the entropy inequality, one would have the following.

$$-\rho(\dot{\psi} + \eta \dot{\theta}) + t_{ki} d_{ki} - \frac{q_i g_i}{\theta} \geq 0 \quad (\text{A1.3})$$

It is now a good time to write

$$\dot{\psi} = \frac{\partial \hat{\psi}}{\partial \rho} \dot{\rho} + \frac{\partial \hat{\psi}}{\partial \theta} \dot{\theta} + \frac{\partial \hat{\psi}}{\partial d_{ij}^{\tau_2}} \dot{d}_{ij}^{\tau_2} + \frac{\partial \hat{\psi}}{\partial g_j^{\tau_1}} \dot{g}_j^{\tau_1} \quad (\text{A1.4})$$

and to remind in mind the fact that the continuity equation can be written as $\dot{\rho} = -\rho d_{ii}$.

The equation (A1.3) can now be expressed as

$$(\rho^2 \frac{\partial \hat{\psi}}{\partial \rho} \delta_{ik} + t_{ki}) d_{ki} - \rho (\frac{\partial \hat{\psi}}{\partial \theta} + \eta) \dot{\theta} - \rho \frac{\partial \hat{\psi}}{\partial d_{ij}^{\tau_2}} \dot{d}_{ij}^{\tau_2} - \rho \frac{\partial \hat{\psi}}{\partial g_j^{\tau_1}} \dot{g}_j^{\tau_1} - \frac{1}{\theta} q_i g_i \geq 0. \quad (\text{A1.5})$$

¹¹ Clausius-Duhem inequality in rational mechanics is exclusively a constraint and not a new equation.

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as the independent values can acquire any value, if one puts $\dot{\theta} = 0, \dot{d}_{ij}^{\tau_2} = 0, \dot{g}_j^{\tau_1} = 0$ one can easily come up with the following inequality.

$$(\rho^2 \frac{\partial \hat{\psi}}{\partial \rho} \delta_{ik} + t_{ki}) d_{ki} - \frac{1}{\theta} q_i g_i \geq 0 \quad (A1.6)$$

Now if one considers equations (A1.6) and (A1.5) together, it would not be hard to understand that the necessary and sufficient condition for (A1.5) to be true is that the coefficients of the rate of independent variables must be equal to zero. It is simply possible to find this result as the following equations.

$$\begin{aligned} \frac{\partial \hat{\psi}}{\partial \theta} &= -\eta \\ \frac{\partial \hat{\psi}}{\partial d_{ij}^{\tau_2}} &= 0 \\ \frac{\partial \hat{\psi}}{\partial g_j^{\tau_1}} &= 0 \end{aligned} \quad (A1.7)$$

On the other hand, one can investigate more in inequality (A1.6). It is known that one might encounter materials in which the velocity field is equal to zero or the temperature gradient is zero. A consequence of these is

$$\begin{aligned} -\frac{1}{\theta} q_i g_i &\geq 0 \\ (\rho^2 \frac{\partial \hat{\psi}}{\partial \rho} \delta_{ik} + t_{ki}) d_{ki} &\geq 0 \end{aligned} \quad (A1.8)$$

At this stage, it is easily seen that the (3.8) is a direct consequence of (A1.7).

Now, it is possible to propose two important factors needed to describe the flow motion. One is the constitutive representation of stress tensor and the second one is the heat

equation constitutive relation. One can choose the relations to be linear with respect to

$g_j^{\tau_1}, d_{ij}^{\tau_2}$. One can write them as

$$\begin{aligned} t_{ij} &= A_{ij}(\rho, \theta) + B_{ijk}(\rho, \theta)g_j^{\tau_1} + C_{ijkl}(\rho, \theta)d_{kl}^{\tau_2} \\ q_i &= D_i(\rho, \theta) + E_{ik}(\rho, \theta)g_k^{\tau_1} + F_{ikl}(\rho, \theta)d_{kl}^{\tau_2} \end{aligned} \quad (\text{A1.9})$$

The time is for using the symmetry. It is known that $t_{ij} = t_{ji}, d_{ij} = d_{ji}$ which implies that the following must be obeyed.

$$\begin{aligned} A_{ij} &= A_{ji} \\ C_{ijkl} &= C_{jikl} = C_{ijlk} \\ B_{ijk} &= B_{jik} \\ F_{ikl} &= F_{ilk} \end{aligned} \quad (\text{A1.10})$$

Here, the rest of the formulation is going to be derived heuristically. It has to be explained that this is the only physical, and not mathematical, approach chosen to complete the problem. It is assumed that the possible functionality of equations (A1.9) is similar to the Navier-Stokes constitutive equations. It would be explicitly visible that many classes of material behavior can completely be ignored by the bilinear relations defined in (A1.9).

$$\begin{aligned} A_{ij}(\rho, \theta) &= -p(\rho, \theta)\delta_{ij} \\ B_{ijk}(\rho, \theta) &= 0 \\ C_{ijkl}(\rho, \theta) &= \lambda(\rho, \theta)\delta_{ij}\delta_{kl} + \mu(\rho, \theta)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ D_i(\rho, \theta) &= 0 \\ E_{ik}(\rho, \theta) &= -k(\rho, \theta)\delta_{ik} \\ F_{ikl}(\rho, \theta) &= 0 \end{aligned} \quad (\text{A1.11})$$

Simplifying all equations would lead into

$$\begin{aligned} t_{ij} &= -p\delta_{ij} + \lambda\delta_{ij}d_{kk}^{\tau_2} + 2\mu d_{ij}^{\tau_2} \\ q_i &= -kg_i^{\tau_1} \end{aligned} \quad (A1.12)$$

So, the general form of the model is now built. However, there are some notes to be added here regarding the mathematical procedure chosen:

- 1- There is only one point in the derivation making the whole approach physical-mathematical one. It is the resemblance adopted in equation (A1.11).
- 2- If one had ignored the time lags in the formulations (if one had considered a compressible viscose fluid), it could be talked more about the signs of k, μ, λ .

But now, as the time lags are present, one is not able to use the Clausius-Duhem inequality. As a result, one can accept the following constraints as sufficient

$$\begin{aligned} k &\geq 0 \\ \mu &\geq 0 \\ \lambda + \frac{2}{3}\mu &\geq 0 \end{aligned} \quad (A1.13)$$

to have the appropriate case for the limiting case of $\tau_1, \tau_2 \rightarrow 0$.

Appendix 2

In this appendix, the step by step procedure that showed the similarity of the ET model with the EKC is explained.

One can again rewrite the ET model after Mongiovi [102, 103, 174] by ignoring the phenomenological terms she proposed to consider the thermal dissipation $\beta = \beta' = 0$.

In fact, even Mongiovi has ignored these terms in her derivations in some cases. On the other hand, it is believed that there is no dissipation with regard to heat transfer in a way that she has proposed.

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial x_i} &= 0 \\
 \rho \frac{\partial v_i}{\partial t} + \frac{\partial}{\partial x_j} [(p_E + p_V) \delta_{ij} + p_{<ij>}] &= 0 \\
 \rho \frac{\partial e}{\partial t} + \frac{\partial q_j}{\partial x_j} + [(p_E + p_V) \delta_{ij} + p_{<ij>}] \frac{\partial v_i}{\partial x_j} &= 0 \\
 \tau_0 \frac{\partial p_V}{\partial t} + \lambda_0 \frac{\partial v_i}{\partial x_i} &= -p_V \\
 \tau_2 \frac{\partial p_{<ij>}}{\partial t} + 2\lambda_2 \frac{\partial v_{<i}}{\partial x_{j>}} &= -p_{<ij>} \\
 \tau_1 \frac{\partial q_i}{\partial t} + \lambda_1 \frac{\partial T}{\partial x_i} &= -q_i
 \end{aligned} \tag{A2.1}$$

If one puts $p_E \delta_{ij} + p_{ij} = -t_{ij}$ the first three equations in (A2.1) would become

$$\frac{\partial \rho}{\partial t} + \rho \frac{\partial v_i}{\partial x_i} = 0$$

$$\rho \frac{\partial v_i}{\partial t} = \frac{\partial t_{ij}}{\partial x_j}$$

$$-\rho \frac{\partial \varepsilon}{\partial t} + \frac{t_{ki}}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{\partial q_i}{\partial x_i} = 0.$$

where they are exactly the linearized equations (3.32)-(3.34). The last equation in (A2.1) is again exactly the same as (3.36) if one puts $\lambda_1 = k$. Hence, the only remaining dilemma is to bring the fourth and fifth equations in (A2.1) to one equation, namely (3.35). To do so, one should add the fourth and fifth equations in (A2.1) together. There would be the following equation.

$$\begin{aligned} \tau_2 \frac{\partial t_{ij}}{\partial t} + t_{ij} = & - \left(\tau_2 \frac{\partial p_E}{\partial t} + \tau_2 \frac{\partial p_V}{\partial t} - \tau_0 \frac{\partial p_V}{\partial t} + p_E \right) \delta_{ij} + \\ & \left(\lambda_0 - \frac{2}{3} \lambda_2 \right) \frac{\partial v_k}{\partial x_k} \delta_{ij} + \lambda_2 \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \end{aligned} \quad (\text{A2.2})$$

A comparison between (A2.2) and (3.35) shows that it is possible to come to (3.35) if one puts $\lambda_2 = \mu$, $\lambda_0 - \frac{2}{3} \lambda_2 = \lambda$, $\tau_2 = \tau_0$ and

$$\tau_2 \frac{\partial p_E}{\partial t} + \tau_2 \frac{\partial p_V}{\partial t} - \tau_0 \frac{\partial p_V}{\partial t} + p_E = \tau_2 \frac{\partial p}{\partial t} + p.$$

It is possible to simplify the above results by assuming $\tau_2 = \tau_0$ and considering the consequences of this assumption: $p_E = p$ and $p_V = \frac{1}{3} p_u$. The last assumption made is not a weird one at least according to the order of time lags presented in texts of extended irreversible thermodynamics. With respect to all these simplifications, the Mongiovi model and the one presented in chapter 3 are clearly interchangeable for special cases. The cases are like the propagation of waves.

Appendix 3

A3.1

In this appendix, the code written to justify the model in Chapter 4 is explained.

In the *inputs* part, it is possible to define the dimensionless length and diffusion coefficient side by side with the number of time steps per time lag and also the number of the spatial meshes. In the *parameters* part, the code defines the needed values for q , Δx and Δt . Afterwards, two functions are used to produce the matrices needed for solving (4.19), (4.20) and a simple implicit finite difference scheme for the Fourier heat transfer. They are named as *delay matrix generator* and *Fourier matrix generator*, respectively. The *initial conditions* (history) are the next lines defined in the code. After all, the *solving engine* solves both equations (PLHE and the Fourier heat transfer) simultaneously. Finally the *plotting engine* produces all the graphs and plots needed for the justification.

The reader should be reminded that in the solving engine, unlike ordinary solvers, one has to save all the values in any time lag interval, since the domain needs the memory of some past events.

```
function AD=Delay_matrix_generator(h)
AD=sparse(h,h);
B=sparse(h,h);
C=sparse(h,h);
D=sparse(h,h);
B(2:h-1,1:h-1)=eye(h-2,h-1);
C(2:h-1,3:h)=eye(h-2,h-2);
D(2:h-1,2:h-1)=-2*eye(h-2,h-2);
AD=B+C+D;


---


function AF=Fourier_matrix_generator(h,q)
AF=sparse(h,h);
B=sparse(h,h);
C=sparse(h,h);
D=sparse(h,h);
```

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```

B(2:h-1,1:h-1)=eye(h-2,h-1);
C(2:h-1,3:h)=eye(h-2,h-2);
D(2:h-1,2:h-1)=-2*eye(h-2,h-2);
AF=-q*B-q*C-.5*(1+2*q)*D;
AF(1,1)=1;
AF(h,h)=1;

```

```

clc
clear
tic
% Inputs
alpha=1;
tau=10^(-6);
k=60;
% Time steps per time lag interval
p=100;
% Spatial mesh
h=100;
L=1;
% Parameters
T=[];
TF=[];
delt=tau/(p);
delx=L/h;
x=0:delx:L;
q=alpha*delt/(delx)^2;
% Matrices
AD=Delay_matrix_generator(h+1);
AF=Fourier_matrix_generator(h+1,q);
%Initial Conditions
T(1:h+1,1:p)=0;
TF(1:h+1,1:p)=0;
% Solver engine
Hh = waitbar(0,'Please wait...');
for j=1:k
    for n=(p+1):(2*(p))

        T(:,n)=T(:,n-1)+q*AD*T(:,n-(p));
        T(1,n)=1;
        T(h+1,n)=0;

        TF(:,n)=AF\TF(:,n-1);
        TF(h+1,n)=0;
        TF(1,n)=1;

    end

    waitbar(j/k)

    T(:,(1:p))=T(:,(p+1):(2*(p)));
    TF(:,(1:p))=TF(:,(p+1):(2*p));
end
close(Hh)
% Plotting engine
plot(x,T(:,n)-TF(:,n));

% plot(x,T(:,n));
% hold on
% plot(x,TF(:,n),'r');
% plot(time,Temp);
% hold on

```

```
% plot(time,TempF,'r');
% hold off
xlabel('Dimensionless Length of Specimen');
ylabel('Difference of Temperatures');
% legend('PLHE model','Fourier heat model')
toc
```

A3.2

The code is for numeric solution of equations system in (6.11).

```
function [N,tau,k,h,delt,n]=input_function
%% number of lattice points
N=50;
%% time delays
tau=1;
%% conductivity
k=1;
%% number of time marches in one time dealy
h=300;
%% Calc
delt=tau/h;
%% number of iterations (n*tau)
n=5;

function [A,B,C,D]=matrix_function(T,k,delt,N,h,j)
%%
A=sparse(N,N);
B=sparse(N,N);
C=sparse(N,N);
D=sparse(N,N);
%%
for i=2:N
    A(i,i-1)=k*delt*(step_function(T(i,j),T(i-1,j-
h))+step_function(T(i-1,j-h),T(i,j-2*h)));
end
% A(N,N-1)=0;
%%
for i=1:N-1
    B(i,i+1)=k*delt*(step_function(T(i,j),T(i+1,j-
h))+step_function(T(i+1,j-h),T(i,j-2*h)));
end
% B(1,2)=0;
%%
for i=2:N-1
    C(i,i)=1-k*delt*(step_function(T(i,j),T(i-1,j-
h))+step_function(T(i,j),T(i+1,j-h)));
end
C(1,1)=1-k*delt*(0+step_function(T(1,j),T(1+1,j-h)));
C(N,N)=1-k*delt*(step_function(T(N,j),T(N-1,j-h))+0);
%%
for i=2:N-1
    D(i,i)=-k*delt*(step_function(T(i+1,j-h),T(i,j-
2*h))+step_function(T(i-1,j-h),T(i,j-2*h)));
end
D(1,1)=-k*delt*(step_function(T(1+1,j-h),T(1,j-2*h))+0);
```

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```

D(N,N)=-k*delt*(0+step_function(T(N-1,j-h),T(N,j-2*h)));
function [A,B,C]=matrix_function_first_set(T,k,delt,N,h,j)
%%
A=sparse(N,N);
B=sparse(N,N);
C=sparse(N,N);
D=sparse(N,N);
%%
for i=2:N
    A(i,i-1)=k*delt*(step_function(T(i,j),T(i-1,j-h)));
end
% A(N,N-1)=0;
%%
for i=1:N-1
    B(i,i+1)=k*delt*(step_function(T(i,j),T(i+1,j-h)));
end
% B(1,2)=0;
%%
for i=2:N-1
    C(i,i)=1-k*delt*(step_function(T(i,j),T(i-1,j-
h))+step_function(T(i,j),T(i+1,j-h)));
end
C(1,1)=1-k*delt*(0+step_function(T(1,j),T(1+1,j-h)));
C(N,N)=1-k*delt*(step_function(T(N,j),T(N-1,j-h))+0);

```

```

function u=step_function(a,b)
if a>b
    u=a-b;
else
    u=0;
end

```

```

tic
clc
clear
%% reading input
[N,tau,k,h,delt,n]=input_function;
%% History
T(1:N,1:3*h+2)=0;
T(1:N,1)=1*rand(N,1);
for i=2:h+1
    T(1:N,i)=T(1:N,1);
end
M1 = mean(T(1:N,1));
% T=ones(N,3*h+2);
% T(1,1:3*h+2)=10;
% T(N,1:3*h+2)=0;
%% First Set Solver & Plotter
wait = waitbar(0,'Please wait...');
p=1;
for j=h+1:2*h
    [A,B,C]=matrix_function_first_set(T,k,delt,N,h,j);
    T(:,j+1)=A*T(:,j-h)+B*T(:,j-h)+C*T(:,j);
end
%% Solver & Plotter
while p<n
    for j=2*h+1:3*h+1
        [A,B,C,D]=matrix_function(T,k,delt,N,h,j);
        T(:,j+1)=A*T(:,j-h)+B*T(:,j-h)+C*T(:,j)+D*T(:,j-2*h);
    end
    M(p)=mean(T(:,j));
    p=p+1;
end

```

```

T(:,1:2*h+1)=T(:,h+2:3*h+2);
waitbar(p/n)
end

toc
subplot(2,1,1)
plot(1:p-1,M)
ylabel('Average Dimensionless Temperature');
xlabel('Time March');
subplot(2,1,2)
plot(1:N,T(:,3*h+2),'LineWidth',2);
ylabel('Dimensionless Temperature');
Axis([1 N 0 1]);
title(['Temp @ ', ' t/',texlabel('tau'),'=',num2str(p-1)]);

close(wait)

```

A3.3

This is the code that has been used to calculate F in (7.21). The symbolic toolbox of Matlab was used.

```

function F=force(x,y,z,beta)
sigma=1;
R=radius(x,y,z,beta);
[Rx,Ry,Rz]=grdintR(x,y,z,beta);
F=(2*(sigma/R)^13-(sigma/R)^7)*[Rx;Ry;Rz];
function [Rx,Ry,Rz]=grdintR(x,y,z,beta)
gama=1/beta;
Rx=1/(x^2*gama^2+y^2*gama^2-z^2*gama^2-
z^2)^(1/2)*(x*(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2)+2*x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2+x*(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2)*gama^2)/(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2+x^2+2*x*(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2))^(1/2)*(gama/(gama^2-1));
Ry=y*(x+(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2))/(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2)/(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2+x^2+2*x*(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2))^(1/2)*(gama^2-1)*(gama);
Rz=z*(x+(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2))/(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2)/(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2+x^2+2*x*(x^2*gama^2+y^2*gama^2-y^2+z^2*gama^2-
z^2)^(1/2))^(1/2)*(gama^2-1)*(gama);
function R=radius(x,y,z,beta)
gama=1/beta;
r2=x^2+y^2+z^2;
R2=r2+((x+(x^2+r2*(gama^2-1))^0.5)/(gama^2-
1))^2+2*x*(x+(x^2+r2*(gama^2-1))^0.5)/(gama^2-1);
R=R2^0.5;

```

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