OBJECTIVE

*Heat Transfer Physics* is a graduate course describing atomic-level kinetics (mechanisms and rates) of thermal energy storage, transport (conduction, convection, and radiation), and transformation (various energy conversions) by principal energy carriers. These carriers are: **phonon** (lattice vibration wave also treated as quasi-particle), **electron** (as classical or quantum entity), **fluid particle** (classical particle with quantum features), and **photon** (classical electromagnetic wave also as quantum-particle), as shown in figure below.

The approach combines fundamentals (through survey and summaries) of following fields. Molecular orbitals/potentials, statistical thermodynamics, computational molecular dynamics (including lattice dynamics), quantum energy states, transport theories (e.g., the Boltzmann and stochastic transport equations and the Maxwell equations), solid-state (including semiconductors) and fluid-state (including surface interactions) physics, and quantum optics (e.g., spontaneous and stimulated emission, photon–electron–phonon couplings). These are rationally connected to atomic-level heat transfer (e.g., heat capacity, thermal conductivity, photon absorption coefficient) and thermal energy conversion (e.g., ultrasonic heating, thermoelectric and laser cooling).

The course presents a unified theory, over fine-structure/molecular-dynamics/Boltzmann/macrosopic length and time scales (as shown in figure below), of the heat transfer kinetics which are the transition rates and relaxation times. The fundamentals are also related to modern applications (including nano- and microscale size effects).

The prerequisite is ME 335 (Heat Transfer) or consensus of the instructor.
1 Introduction and Preliminaries
1.1 Phonon, Electron, Fluid Particle, and Photon
1.2 Combinatorial Probabilities and Energy Probability Distribution Functions
1.3 Particle, Wave, Wave Packet, and Quasi-Particle
1.4 A History of Contributions towards Heat Transfer Physics
1.5 Energy in Classical and Quantum Mechanics
1.6 Periodic Table of Elements
1.7 Heat Transfer Physics
1.8 Scope

2 Molecular Orbitals-Potentials-Dynamics, and Quantum Energy States
2.1 Interatomic Forces and Potential Well
2.2 Orbitals and Interatomic Potential Models
2.3 Molecular Ensembles, Temperature, and Thermodynamic Relations
2.4 Classical Mechanics, Hamiltonian, and Partition Function
2.5 Molecular Dynamics Simulations
2.6 Schrödinger Equation and Quantum Mechanics

3 Carrier Energy Transport and Transition Theories
3.1 Boltzmann Transport Equation
3.2 Energy Transformation Kinetics and Fermi Golden Rule
3.3 Maxwell Electromagnetic Wave Propagation Equations
3.4 Onsager Transport Coefficients
3.5 Stochastic Particle Dynamics and Transport
3.6 Green–Kubo Transport Theory
3.7 Macroscopic Fluid Dynamics Equations
3.8 Macroscopic, Elastic Solid Mechanics

4 Phonon Energy Storage, Transport and Transition Kinetics
4.1 Phonon Dispersion in One-Dimensional, Classical Lattice Vibration
4.2 Phonon Density of States
4.3 Reciprocal Lattice and Brillouin Zone
4.4 Three-Dimensional Lattice Dynamics and Dispersion Relation
4.5 Quantum Theory of Lattice Vibration
4.6 Examples of Phonon Dispersion and DOS
4.7 Debye Lattice Specific Heat Capacity
4.8 Atomic Displacement in Lattice Vibration
4.9 Phonon BTE and Callaway Conductivity Model
4.10 Einstein and Cahill–Pohl Minimum Conductivities
4.11 Phonon Conductivity at High Temperatures
4.11 Phonon Conductivity from MD and G–K Autocorrelation
4.12 Quantum Corrections to MD Predictions
4.13 Phonon Conductivity from BTE: Variational Method
4.14 Optical Phonon Contribution to Conductivity
4.15 Experimental Data on Phonon Conductivity
4.16 Phonon Boundary Resistance
4.17 Absorption of Ultrasound Waves in Solids
4.18 Size Effects

5 *Electron Energy Storage, Transport and Transition Kinetics*
5.1 Electron Band Structure in Crystals
5.2 Electronic Energy Bands in One-Dimensional Ionic Lattice
5.3 Three-Dimensional Bands Tight-Band Approximation
5.4 Electron Band Structures for Semiconductors and Effective Mass
5.5 Ab Initio Calculation of Electronic Band Structure
5.6 Electron Gas Model for Metals
5.7 Density of Electronic Energy States for Semiconductors
5.8 Electron Specific Heat Capacity
5.9 Electron BTE for Semiconductors
5.10 Scattering Potential, Fermi Golden Rule, and Relaxation Time
5.11 Average Relaxation Time for Power-Law Energy Dependent Relaxation Time
5.12 Transport Coefficients in Coupled Electrical and Thermal Currents
5.13 Semiconductor Electro-Thermal Transport Properties using $J_e$ and Gradient of $T$
5.14 Magnetic Field and Hall Factor
5.15 Phonon Scattering of Electron
5.16 Electro-Thermal Transport Properties Data for Semiconductors and Metals
5.17 Ab Initio Calculation of TE Properties
5.18 Electron and Phonon Transport Equations under Thermal NonEquilibrium
5.19 Cooling Length in Electron- Lattice Thermal Non-equilibrium
5.20 Electronic Energy States of Rare-Earth Ion Doped Crystals
5.21 Electronic Energy States of Gases
5.22 Size Effects

6 *Fluid Particle Energy Storage, Transport and Transition Kinetics*
6.1 Fluid Particle Quantum Energy States and Partition Functions
6.2 Idea-Gas Specific Heat Capacity
6.3 Dense-Fluid Specific Heat Capacity
6.4 Fluid Particle BTE and Average Molecular Speed
6.5 Elastic Binary Collision Rate of Ideal Gas
6.6 Ideal Gas Mean-Free Path
6.7 Relaxation Time Approximation of Gas BTE
6.8 Thermal Conductivity of Ideal Gas
6.9 Thermal Conductivity of Liquids
6.10 Effective Conductivity with Suspended Particles in Brownian Motion
6.11 Interaction of Fluid Particle and Surface
6.12 Turbulent-Flow Structure and Transport
6.13 Thermal Plasmas
6.14 Size Effects

7 *Photon Energy Storage, Transport and Transition Kinetics*
7.1 Quasi-Particle Treatment: Photon Gas and Planck Emission
7.2 Laser and Narrow-Band Emissions
7.3 Classical and Semi-Classical Treatments of Photon–Matter Interaction
7.4 Photon Absorption and Emission in Two-Level Electron Energy System
7.5 Photon BTE: Scattering, Absorption, and Emission
7.6 Equation of Radiative Transfer
7.7 Wave Treatment: Field Enhancement and Photon Localization
7.8 Continuous and Band Photon Absorption in Solids
7.9 Continuous and Band Photon Emission in Solids
7.10 Spectral Surface Emission
7.11 Radiative and Non-Radiative (with Phonon Emission) Decays and Quantum Efficiency
7.12 Anti-Stokes Fluorescence and Photon–Electron-Phonon Couplings
7.13 Gas Lasers and Laser Cooling of Gases
7.14 Photovoltaic Solar Cell
7.15 Size Effects