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QUANTUM WEAK TURBULENCE
WITH APPLICATIONS
TO SEMICONDUCTOR LASERS.

by
Yuri Victorovich Lvov

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A Dissertation Submitted to the Faculty of the
DEPARTMENT OF PHYSICS
In Partial Fulfillment of the Requirements
For the Degree of
DOCTOR OF PHILOSOPHY
In the Graduate College
THE UNIVERSITY OF ARIZONA

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As members of the Final Examination Committee, we certify that we have
read the dissertation prepared by Yuri Victorovich Lvov
entitled Quantum Weak Turbulence with Applications to
Semiconductor Lasers

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ACKNOWLEDGEMENT.

I am very grateful to my advisor, Alan Newell, for his patient immediate and intercontinental guidance and permanent support from my first steps in the USA and up to now. His ideas, encouragement, and contagious enthusiasm have made the existence of this manuscript possible. My special thanks to Vladimir Zakharov for numerous and elucidative discussions of this and other projects in the field of nonlinear physics. His approach to life and physics has had a profound effect on my view of the world. I am also greatly indebted to my undergraduate mentor, Vadim Gurevich, who's introduction to theoretical physics laid out a necessary foundation for starting this work.

I am very thankful to my collaborator on [1] Rolf Binder. I am also very grateful to Chris Bowman, Roberto Camassa, Ildar Gabitov, Mac Hyman, Robert Indik, Mark Mineev, Jerry Moloney, Sergey Nazarenko and Andrei Pushkarev for immensely useful and intriguing discussions. I am admiring and respecting their intelligent and varied commentary on science and on life in general.

To my dear parents and wife for their loving support and encouragement, and to my little daughter Elizabeth for always keeping the draft pages of this manuscript in perfect order and referring to them as “my dissertation”.

TABLE OF CONTENTS

LIST OF FIGURES	9
ABSTRACT	11
DEFINITIONS.	12
CHAPTER 1. INTRODUCTION AND MOTIVATION	15
1.1. Motivation.	15
1.2. Introduction	16
1.2.1. Many body problems. Statistical description.	16
1.2.2. Brief literature review.	18
1.2.3. Weak turbulence as a tool to decouple BBGKY hierarchy.	19
1.2.4. Kolmogorov Spectra and Semiconductor Lasers.	23
1.2.5. Main results	27
1.3. Outline	30
CHAPTER 2. SETTING UP THE STAGE	34
2.1. Conductors, Semiconductors and Insulators	34
2.2. Schroedinger Equation in Periodic potential.	35
2.2.1. Bravais Lattice.	35
2.2.2. Bloch Theorem.	35
2.2.3. Schroedinger Equation.	36
2.3. Tight-Binding Approximation	37
2.4. Basics of Band Structure.	44
2.5. Description of Semiconductor Media	46
2.5.1. Bosons and Fermions.	46
2.5.2. Second Quantization of a Fermions.	48
2.5.3. Heisenberg Equation of Motion	53
CHAPTER 3. QUANTUM BOLZMANN KINETIC EQUATION	56
3.1. Systematic Derivation of the Kinetic Equation and Evolution equations for Higher Order Cumulants	56
3.1.1. Basic Definitions and Evolution Equation	56
3.1.2. Cumulants and their evolution.	59
3.1.3. Asymptotic Expansions and Closure	68
3.1.4. Long Formulas.	72
3.1.5. Results.	80

TABLE OF CONTENTS—*Continued*

3.2. Analysis of the Kinetic Equation.	84
3.2.1. Conservation Laws, Thermodynamic and Finite-Flux solutions of the Kinetic Equation.	84
3.2.2. Time Flow Theorem - QKE	93
3.2.3. Entropy, Entropy Production and h-Theorem	94
3.2.4. Summary of QKE properties.	94
3.3. Differential Kinetic Equation	95
3.3.1. Derivation of Differential Kinetic Equation	95
3.3.2. Solutions and properties of the DQKE	100
3.3.3. Summary of DQKE properties.	102
3.3.4. DKE - Numerical scheme and boundary conditions.	102
3.3.5. Numerical Results.	106
 CHAPTER 4. DIFFERENTIAL QKE -TWO PARTICLE CASE	 114
4.1. Derivation of the 2-particle DQKE.	114
4.1.1. Effective mass and effective frequency.	116
4.1.2. Derivation.	117
4.2. Properties and solutions of 2-DQKE.	120
4.2.1. Thermodynamic Equilibrium solutions.	120
4.2.2. Role of the "cross" term.	120
4.2.3. Boltzmann H theorem.	122
4.2.4. Conservation Laws.	124
4.3. Boundary conditions.	125
4.4. Numerical Results.	128
4.5. Setup for input-output fluxes for the case of semiconductor.	134
 CHAPTER 5. PHONONS	 138
5.1. System Hamiltonian.	138
5.2. Equation of motion.	139
5.3. Kinetic Equation for carrier-phonon scattering.	139
5.4. Stability of FD distribution.	145
5.5. Phononic conclusion.	145
 CHAPTER 6. LIGHT-MATTER INTERACTION	 147
6.1. Polarization.	147
6.1.1. Classical definition of polarization.	147
6.1.2. The Interband polarization.	147
6.2. Many Body Hamiltonian	149
6.3. Semiconductor Bloch Equations	150

TABLE OF CONTENTS—*Continued*

6.4. Slowly varying Maxwell equations.	152
CHAPTER 7. LASERS	155
7.1. Basic Physics of Lasers.	155
7.2. Different types of lasers.	157
7.3. Few words about applications.	161
7.4. Basic principles of semiconductor laser operation.	165
7.5. Application of Quantum Weak Turbulence to Semiconductor Lasers.	169
7.5.1. One-particle model.	170
7.5.2. Two particle model.	184
7.6. Analysis.	194
CHAPTER 8. CONCLUSION AND REMAINING CHALLENGES	199
REFERENCES	201

LIST OF FIGURES

FIGURE 1.1. “Typical” Fermi-Dirac distribution functions.	25
FIGURE 2.1. Band structure for 2 parabolic bands.	45
FIGURE 3.1. Setup for input-output fluxes.	91
FIGURE 3.2. Numerical solution of DKE in the left transparency window.	107
FIGURE 3.3. Numerical solution of DKE in the right transparency window.	109
FIGURE 3.4. Time evolution of the distribution function as described by DKE (3.78), with boundary conditions $P = Q = 0$ at both ends.	110
FIGURE 3.5. Same as in Figure (3.4), but for $P = 0, Q = Q_1 > Q_0$ at both ends.	111
FIGURE 3.6. The stationary values of fluxes as a functions of ω , as well as pumping and damping profiles.	113
FIGURE 3.7. Verification of formulas for the magnitude of particle and energy fluxes to the right and to the left.	113
FIGURE 4.1. Evolution of electron (a) and hole (b) distribution functions as given by the 2DQKE.	129
FIGURE 4.2. Evolution of electrons and holes “temperature”.	131
FIGURE 4.3. Evolution of electron (a) and hole (b) distribution functions as given by 2DQKE.	132
FIGURE 4.4. Evolution of electrons and holes “temperature”.	133
FIGURE 4.5. Setup for input-output fluxes.	135
FIGURE 7.1. Basic principles of semiconductor laser operation.	165
FIGURE 7.2. Time dependence of distributions (a) and output laser intensity (b) according to (7.6-7.8).	176
FIGURE 7.3. Same as in Figures (7.2) but for increased pump rate. Broad-band pumping case.	178
FIGURE 7.4. Same as in Figure (7.2) and with same pump rate as in Figure (7.3). Narrow band pumping.	179
FIGURE 7.5. The output power as a function of pumping strength for narrow-band and broad-band pumping, one particle model.	182
FIGURE 7.6. Time dependence of distributions (a) and output laser intensity (b) according to (7.18-7.20). Narrow pumping case.	190
FIGURE 7.7. Same as on Figure (7.6) for increased pumping rare. Broad band pumping case. $\mu_h/\mu_e = 2$	191

LIST OF FIGURES—*Continued*

FIGURE 7.8. Same as on Figure (7.6) for narrow band pumping. Pumping rate is the same as in Figure (7.7). $\mu_h/\mu_e = 2$	192
FIGURE 7.9. The output power as a function of pumping strength for narrow-band and broad-band pumping. $\mu_h/\mu_e = 2$	193
FIGURE 7.10. Same as on Figure (7.6) for broad pumping case. $\mu_h/\mu_e = 6$	195
FIGURE 7.11. Same as on Figure (7.6) for narrow pumping case. Pumping rate is the same as on Figure (7.10). $\mu_h/\mu_e = 6$	196
FIGURE 7.12. The output power as a function of pumping strength for narrow-band and broad-band pumping. $\mu_h/\mu_e = 6$	197

ABSTRACT

Based on a model Hamiltonian appropriate for the description of fermionic systems such as semiconductor lasers, we describe a natural asymptotic closure of the BBGKY hierarchy in complete analogy with that derived for classical weak turbulence. The main features of the interaction Hamiltonian are the inclusion of full Fermi statistics containing Pauli blocking and a simple, phenomenological, uniformly weak two particle interaction potential equivalent to the static screening approximation. The resulting asymptotic closure and quantum kinetic Boltzmann equation are derived in a self consistent manner without resorting to a priori statistical hypotheses or cumulant discard assumptions.

We find a new class of solutions to the quantum kinetic equation which are analogous to the Kolmogorov spectra of hydrodynamics and classical weak turbulence. They involve finite fluxes of particles and energy across momentum space and are particularly relevant for describing the behavior of systems containing sources and sinks. We explore these solutions by using differential approximation to collision integral.

We make a *prima facie* case that these finite flux solutions can be important in the context of semiconductor lasers. We show that semiconductor laser output efficiency can be improved by exciting these finite flux solutions. Numerical simulations of the semiconductor Maxwell Bloch equations support the claim.

DEFINITIONS.

Here we present the list of definitions used through this manuscript. We will try to be consistent whenever possible.

- $a_k^\dagger, a_k$ are creation/annihilation operators of electrons.
 $\hat{\phi}_s^\dagger(\mathbf{r}), \hat{\phi}_s(\mathbf{r})$ are field operators;
- $b_k^\dagger, b_k$ are creation/annihilation operators of holes;
- $c_k^\dagger, c_k$ are creation/annihilation operators of phonons;
- $n_k = \langle a_k^\dagger a_k \rangle$ is the distribution function of electrons;
- $m_k = \langle b_k^\dagger b_k \rangle$ is the distribution function of holes;
- $p_k = \langle b_{-k} a_k \rangle$ is the polarization of state k . $\mathbf{P}(t)$ is the total polarization (6.3);
- $g_k = \langle c_k^\dagger c_k \rangle$ is the distribution function of phonons;
- $\mathcal{H}$ is a Hamiltonian;
- $\mathcal{P}_{1234}, \mathcal{Q}_{123456}, \mathcal{R}_{12345678}$ are cumulants of fourth, sixth and eighth order;
- $\tilde{\omega}_k$ is the optical transition energy between hole and electron with momentum $\mathbf{k}$, $\hbar\tilde{\omega}_k = \epsilon_{e,k} + \epsilon_{h,k} + \epsilon_{gap}$;
-

$$\epsilon_{ek} = \frac{\hbar^2 k^2}{2\mu_e}$$

is electron energy measured from the bottom of conduction band, μ_e is the electron mass.

$$\epsilon_{hk} = \frac{\hbar^2 k^2}{2\mu_h}$$

is the hole energy measured from the top of valence band, μ_h is the hole mass;

- ω generally refers to reduced mass kinetic energy, (4.5);
- $\epsilon_{gap} \approx 1400\text{meV}$ is the bangap energy;
- $T_{k,k_1;k_2,k_3}$ is the general form of carrier-carrier interaction matrix element, V_q is the particular form of $T_{k,k_1;k_2,k_3}$ corresponding to the screened Coulomb potential;
- $S_{\omega,\omega_1;\omega_2,\omega_3}$ is the angular averaged $|T_{k,k_1;k_2,k_3}|^2$ written in frequency space;
- G_q is the carrier-phonon interaction matrix element, (5.2);
- $S_{\omega,\omega_p,\omega_q}^{\text{phon}}$ is the angular averaged $|G_q|^2$ written in frequency space;
- e is electrical field envelope;
- d_k is dipole matrix element, in this manuscript taken to be

$$d_k = \frac{d_{k=0}}{(1 + \epsilon_k/\epsilon_{\text{gap}})};$$

- Q is the flux of particles, Q_0, Q_L, Q_R are input flux, flux to the left, flux to the right respectively. In Chapter 4 we will introduce Q^e, Q^h - flux of electrons and holes along with $Q_0^\alpha, Q_L^\alpha, Q_R^\alpha, \alpha = e, h$;
- P is the flux of energy, we also introduce P_0, P_L, P_R - input energy flux, energy flux to the left, energy flux to the right respectively;

- I is the one-particle interaction strength, I_1 is two-particle interaction strength, I_2 is electron-hole interaction strength;
- Λ_k is the injection current pumping strength.

$$\dot{n}_k = \dots + \Lambda_k(1 - n_k)$$

as the manifestation of Pauli exclusion principle. If one wants to model electrons and holes separately, then $\Lambda_k^{(e)}$ ($\Lambda_k^{(h)}$) are the electron (hole) injection current pumping strengths.

$$\dot{n}_k = \dots + \Lambda_k^{(e)}(1 - n_k), \quad \dot{m}_k = \dots + \Lambda_k^{(h)}(1 - m_k);$$

- Ω_0 is the surface area of the unit sphere in d dimensions;
- Ω is the laser cavity frequency taken to be $1440 \text{ meV} = \epsilon_{gap} + 40 \text{ meV}$
- S - entropy;
- T - temperature, T^e , T^h - temperatures of electrons and holes.

Commonly used abbreviations:

- KE - kinetic equation;
- QKE - quantum kinetic equation;
- $DQKE$ - differential quantum kinetic equation;
- $2DQKE$ - 2 species differential quantum kinetic equation;
- FD - Fermi Dirac, usual context - FD distribution;
- $BBGKY$ hierarchy -
Born-Bogoliubov-Green-Kirkwood-Yvon hierarchy.

Chapter 1

INTRODUCTION AND MOTIVATION

1.1 Motivation.

Kinetic equations describe the evolution of statistical properties of a system of many interacting particles or waves. It has been known since 1968 (see, for example, [2]) that the kinetic equation corresponding to the case of classical wave turbulence has two classes of stationary solutions, thermodynamical equilibria and Kolmogorov spectra. The former corresponds to the case when the system of interest does not exchange energy with the external world. But physical systems are rarely in isolation. Imagine the situation where the interactions of the system with external world are characterized by some length scales. Suppose the system gets energy from external world at length scale L_1 and returns the same amount of energy to the world at another scale L_2 . Then the stationary (but not equilibrium !) situation can be realized when energy is transferred by the system from one scale L_1 to the other scale L_2 . Such a solution is called the Kolmogorov spectrum of wave turbulence (see, for example, [2]). In the theory of wave and hydrodynamic turbulence, the solution corresponding to thermodynamical equilibrium has little relevance; the Kolmogorov spectra is the one seen in numerous numerical and real-world experiments.

For the case of interacting quantum particles one may also derive the corresponding quantum Boltzmann kinetic equation. This kinetic equation also has thermodynamical spectra as a steady solution. I was asked by my PhD advisor back in 1993: *does the quantum kinetic equation have a steady solution analogous to a Kolmogorov spectra of classical wave turbulence?*

One physical situation where the quantum Boltzmann kinetic equation is particularly relevant is semiconductor lasers.

Is it then possible to use the (at that time hypothetical) quantum Kolmogorov distribution to design a better semiconductor laser?

Later I learned that classical wave systems are sometimes described by using the concept of weak turbulence. I asked myself, *is it possible to generalize the concept of weak turbulence to include quantum systems?*

That's how all this manuscript started. We found the "quantum Kolmogorov Spectra" and answered "yes" to the above questions.

1.2 Introduction

1.2.1 Many body problems. Statistical description.

Suppose that one needs to characterize and predict the behavior of a system, consisting of billions of interacting particles. There is no hope for an analytical or numerical solution of a billion coupled Newton's equations for a case of classical system. In quantum mechanics, the situation is even more hopeless, as one has operators and Schroedinger equations instead of numbers and Newton's equations.

If, by some miracle, the above problem were to be solved, so that trajectories or time-dependent wave functions would be available, it would not bring us closer to understanding of the properties of the system of interest. Indeed, what would you do with these terra bytes of information? In order to proceed, we would need to extract some statistical information about the system from particle trajectories/wave functions. We might as well derive evolution equations for these statistical quantities from first principles.

One of quantity which proved itself to be extremely useful in describing

many-body systems is the so called distribution function. Extremely useful means that many other quantities of interest depend on distribution function. For example, semiconductor laser output power depends on the carrier (the common name for both electrons and holes) distribution function. The one particle distribution function is proportional to the probability of finding a particle in a state with given momentum. This quantity is greater than zero for bosons or classical particles. For fermions it is bounded between zero and one, because, according to the Pauli exclusion principle, no more than one particle can occupy any given quantum state. Therefore for fermions distribution function is *equal* to *probability* of finding fermion in state with given momentum.

Due to nonlinear character of a problem the time evolution of the distribution function depends on another statistical quantity, the two particle distribution function. The evolution of the latter depends on three-particle distribution function, and so on. As a result, one has an infinite hierarchy of coupled, in general operator, equations for N-particle distribution functions.

In quantum mechanics this infinite hierarchy of equations is called BBGKY hierarchy (after Born, Bogoliubov, Green, Kirkwood and Yvon who discovered it). There is no algorithm to solve these equation exactly.

If there is no way to solve the problem, one usually simplifies the problem until there is a simple solution and starts from there. The problem of many noninteracting particles (also known as *ideal gas*) has an exact solution. Next one assumes that interaction of particles is weak (in some sense) and tries to develop a perturbation theory around the noninteracting case.

Gaining a good understanding of the relaxation processes of many particle (or many wave) systems is still a very difficult task. A successful approach requires many ingredients. First, one must make approximations concerning

the relative strength and uniformity (in momentum space) of the nonlinear coupling. Second, one needs to understand how the infinite hierarchy of momentum equations can effectively decouple and give rise to a closed kinetic Boltzmann equation for the redistribution of particles (waves) and energy in momentum space. One of the goals of this manuscript is to show that one can indeed, as one can do for classical systems, derive the quantum kinetic Boltzmann equation in a self consistent manner without resorting to a priori statistical hypotheses or cumulant discard assumptions¹. Third, systems are rarely in isolation and frequently involve sources (some instability or forcing that injects particles and energy often at specific locations in momentum space) and sinks (regions of absorption of particles and energy). Moreover, and in analogy with hydrodynamic turbulence and classical wave systems, the presence of sources and sinks dramatically changes the nature of the equilibria reached by the quantum kinetic equation. A second and major goal of this manuscript is to describe these equilibria and show how they can affect the output of semiconductor lasers.

1.2.2 Brief literature review.

Fermionic quantum systems have been studied intensively for more than five decades. Many theoretical approaches (see, for example, [3]-[16]) have been developed but the common feature of all is the derivation of the quantum mechanical Boltzmann kinetic equation (henceforth referred to as the quantum kinetic equation or QKE) which describes the evolution and relaxation of the particle distribution function, $\langle a_k^\dagger a_k \rangle$, due to collisions. It is the analogue of the classical kinetic equation (KE) of wave turbulence (see, e.g., [2]) and

¹The two-particle distribution function is equal to the product of two one-particle distribution functions plus a correction describing the interaction of particles. We call that correction “the cumulant”. The cumulant is exactly zero for noninteracting particles.

its natural quantum extension to boson gases. The QKE accounts for phase space blocking effects (Pauli exclusion principle) and is equivalent to what one would obtain by treating the scattering cross-section using the second Born approximation. Examples of variations of this equation and its derivation include the Lenard-Balescu equation which accounts for dynamical screening effects (see, e.g., [9]-[10]). Other extensions include generalized scattering cross sections, such as the exchange effects (crossed diagrams), as well as T-matrix effects (see, e.g., [4],[11]). T-matrix approaches are especially important in systems that allow for bound states. Further generalizations of the quantum Boltzmann equation are the various forms of the Kadanoff-Baym equations. The most general Kadanoff-Baym equations are two-time equations which describe charge-carrier correlations consistently with relaxation dynamics. The Markov approximation, which is the lowest-order gradient expansion with respect to macroscopic times, yields the familiar form of the Lenard-Balescu equation, and the additional static screening and small momentum transfer approximation yields the Landau kinetic equation. In contrast to the slow relaxation dynamics for which the Kadanoff-Baym gradient expansion is applicable, recent investigations have addressed the issue of ultrafast relaxation and the related problems of memory effects as contained in the Kadanoff-Baym equations (see, e.g., [13] and all references therein) and in the generalized Kadanoff-Baym equations of Lipavski, Spicka, and Velicky (see, e.g., [14]-[16]).

1.2.3 Weak turbulence as a tool to decouple BBGKY hierarchy.

In all of the derivations of kinetic equations, the principal obstacle to be overcome is the closure problem. Due to the nonlinear character of the quantum mechanical Coulomb interaction Hamiltonian, the time evolution of the

distribution function (expectation value of two operator products) $n_k \equiv \langle a_k^\dagger a_k \rangle$ is determined by four operator expectation values $\langle a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \rangle$. The problem compounds. The time evolution of the N operator product expectation value is determined by $(N+2)$ operator expectation values and one is left with an infinite set of moment operator equations known as the BBGKY hierarchy. The closure problem is to find a self consistent approximation of this infinite hierarchy which reduces the infinite set of coupled equations to an infinite set of equations which are essentially decoupled. To do this, one needs to make approximations and these almost always involve the introduction of small parameters.

In what follows we introduce one such small parameter, the relative strength $\epsilon, 0 < \epsilon \ll 1$, of the coupling coefficient $T_{kk_1, k_2 k_3}$ in the system Hamiltonian ($V = d$ -dimensional system volume, see (2.55))

$$\begin{aligned}
 H = & \frac{V}{(2\pi)^d} \int d\mathbf{k} \hbar \omega_k a_k^\dagger a_k \\
 & + \frac{V^3}{(2\pi)^{3d}} \frac{1}{2} \int d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 d\mathbf{k}_4 T_{kk_1, k_2 k_3} a_k^\dagger a_{k_1}^\dagger a_{k_2} a_{k_3} \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3).
 \end{aligned}
 \tag{1.1}$$

By relative, we mean the ratio of $T_{kk_1, k_2 k_3}$ to ω_k . In other words, the linear response of the Hamiltonian is dominant over short times. This is not a trivial approximation because in order to develop a consistent asymptotic closure we need $T_{kk_1, k_2 k_3}$ to be small compared to ω_k *uniformly* in k . There are many important examples where this is not the case. For instance, for the classical nonlinear Schroedinger system (see, e.g., [17]), which describes the weak turbulence of optical waves of diffraction in a nonlinear medium, $\omega_k \propto k^2$ and $T_{kk_1, k_2 k_3} = 1/(4\pi^2)\alpha$ where α is a positive (negative) constant for the focusing (defocusing) case. It is clear that the ratio of $T_{kk_1, k_2 k_3}$ to ω_k increases dramatically as $k \rightarrow 0$. This has real physical consequences. The

asymptotic closure for the classical case (see, e.g. [18]-[20]), analogous to one we are about to derive for fermions. whose central feature is the classical kinetic equation describing resonant four-wave energy exchange, is only valid when the particles and energy are at finite k values. But the dynamics of the classical kinetic equation are such that most of the energy travels to a sink at large k and most of the particles and some energy travels to low k . Unless there is a strong damping near $\mathbf{k} = 0$, the flow of particles and energy towards $\mathbf{k} = 0$ will trigger collapsing filaments in the focusing case or build condensates in the defocusing case. In either case, unless there is strong damping near $\mathbf{k} = 0$, the weak turbulence theory of four wave interactions breaks down. Likewise in plasmas and highly excited semiconductors, while the frequency ω_k is αk^2 , the bare coupling coefficient T_{kk_1,k_2k_3} behaves as $1/k^2$ reflecting Coulomb interactions. Again, even though the carriers may be initially excited at $\mathbf{k}$ values much greater than zero, the natural dynamics of either the classical or quantum kinetic equations will lead to particle deposit at small $\mathbf{k}$. However, in both of these cases there is another effect which modifies the T_{kk_1,k_2k_3} and brings the theory closer to the Nonlinear Schroedinger case. The physical origin of this effect is screening and it is manifested as a weakened potential at long distances or small $\mathbf{k}$ values. The modification is a renormalization of the coupling coefficient T_{kk_1,k_2k_3} near $\mathbf{k} = 0$ which effectively cancels the singularity, or equivalently replaces k^{-2} by $(k^2 + \kappa^2)^{-1}$, where κ is the inverse screening length. This is the small k limit of the dynamically screened effective interaction in the Lenard-Balescu approach (see, e.g., [9]). In this manuscript, we do not be concerned with the issue ² with the self consistency of this approximation because we will

²The strong analogy with the nonlinear Schroedinger equation would suggest that the question of the self consistency of the quantum weak turbulence theory with out small k damping might be revisited.

be introducing a sink at small k values (greater than κ) which remove the potential danger in the nonuniformity of the ratio of T_{kk_1,k_2k_3} to ω_k . This is not at all artificial. The sink is, in the semiconductor laser context, nothing other than the lasing output. In what follows, then, we assume that in the k regions of interest, the ratio of T_{kk_1,k_2k_3} to ω_k is uniformly small.

There are essentially two reasons for the successful closure of the hierarchy over long times (asymptotic closure). First, to leading order in ϵ , the cumulants (the non Gaussian part) corresponding to the expectation values of products of N operators ($N > 2$) play no role in the long time behavior of cumulants of order $r < N$. This is a consequence of phase mixing and due to the nondegenerate nature of the dispersion relation $\omega_k = \omega(|\mathbf{k}|)$. In fact, we will find that these (zeroth order in ϵ) cumulants slowly decay. The net result is that the initial state (subject to certain smoothness conditions) plays no role in the long time dynamics. Second, and more important, the higher order (in ϵ) contributions to these N -operator cumulants, which are generated directly by the nonlinearities in the system, are dominated by products of lower order cumulants. Some of these dominant terms are supported only on certain well defined low dimensional (resonant) manifolds in momentum space. These are responsible for the redistribution of particle number among the different momentum states and for the slow decay in time of the leading order approximation to the cumulants of order $N > 2$. The other dominant terms are nonlocal and lead to a nonlinear frequency renormalization of ω_k .

As a result, we are led to a very simple and natural asymptotic closure of the BBGKY hierarchy.

1.2.4 Kolmogorov Spectra and Semiconductor Lasers.

We now review the salient features of semiconductor lasers. In many ways, they are like two level lasers in that the coherent light output is associated with the in phase transitions of an electron from a higher to lower energy state. In semiconductors, the lower energy state is the valence band from which sea electrons are removed leaving behind positively charged holes. The higher energy state is the conduction band. The quantum of energy released corresponds to an excited electron in the conduction band combining with a hole in the lower band below the bandgap. Bandgaps, or forbidden energy zones are features of the energy spectrum of an electron in periodic potentials introduced in this case by the periodic nature of the semiconductor lattice.

However, there are two important ways in which the semiconductor laser differs from and is more complicated than the traditional two-level laser model. First, there is a continuum of bandgaps parameterized by the electron momentum $\mathbf{k}$ and the laser output is a weighted sum of contributions from polarizations corresponding to electron-hole pairs at each momentum value. In this feature, the semiconductor laser resembles an inhomogeneously broadened two level laser. Second, electrons and holes interact with each other via Coulomb forces. Although this interaction is screened by the presence of many electrons and holes, it is nonetheless sufficiently strong to lead to a nonlinear coupling between electrons and holes at different momenta. The net effect of these collisions is a redistribution of carriers (the common name for both electrons and holes) across the momentum spectrum. In fact it is the fastest (≈ 100 fs.) process (for electric field pulses of duration greater than picoseconds) and because of this, the gas of carriers essentially relaxes to a distribution corresponding to an equilibrium of this collision process. This equilibrium state is commonly taken to be that of thermodynamic equi-

librium for fermion gases, the Fermi-Dirac distribution characterized by two parameters, the chemical potential μ and temperature T , slightly modified by the presence of broadband pumping and damping.

But the Fermi-Dirac distribution is not the only equilibrium of the collision process. We have found other stationary solutions, called finite flux equilibria, for which there is a finite and constant flux of carriers and energy across a given spectral window. The Fermi-Dirac solution has zero flux of both quantities. It is the aim of this manuscript to suggest that these finite flux equilibria are more relevant to situations in which energy and carriers are added in one region of the spectrum, redistributed via collision processes to another region where they are absorbed. Moreover, it may be advantageous to pump the laser in this way, because finite fluxes deform the distribution in such a way that more carriers are concentrated in the lasing region (see Figure 1.1). Consequently, more carriers contribute to inversion and lasing process and less carriers are lost due to nonradiative recombination processes. In addition such a strategy may partially overcome the effects of Pauli blocking. The Pauli exclusion principle means that two electrons with the same energy and spin cannot occupy the same state at a given momentum. This may lead to inefficiency because the pumping is effectively multiplied by a factor $(1 - n_s(\mathbf{k}))$, $s = e, h$ for electrons and holes respectively, denoting the probability of not finding electron (hole) in a certain $\mathbf{k}$ (used to denote both momentum and spin) state. But, near the momentum value corresponding to the lasing frequency ω_L , $n_s(\mathbf{k})$ is large ($n_e(\mathbf{k}) + n_h(\mathbf{k})$ must exceed unity) and Pauli blocking is significant. Therefore, pumping the laser in a window about $\omega_0 > \omega_L$ in such a way that one balances the savings gained by deforming distribution function “in a good way” and possibly by lessening the Pauli blocking (because the carriers density $n_s(\mathbf{k})$ decreases with $k = |\mathbf{k}|$) with

FIGURE 1.1. “Typical” Fermi-Dirac distribution functions.

This picture presents “typical” Fermi-Dirac distribution functions for electrons n_ω (long-dashed), holes m_ω (short-dashed), inversion $n_\omega + m_\omega - 1$ (solid line) and gain (dotted line) $\sqrt{\omega}(n_\omega + m_\omega - 1)$. $\hbar\omega$ is the reduced mass kinetic energy (4.5). Lasing can occur only in the regions where inversion and gain are positive.

the extra input energy required (because k is larger), and then using the finite flux solution to transport carriers (and energy) back to lasing frequency, seems an option worth considering.

The aim of this manuscript is to demonstrate, using the simplest possible model, that this alternative is viable.

These finite flux equilibria are the analogies of the Kolmogorov spectra associated with fully developed, high Reynolds number hydrodynamic turbulence and the wave turbulence of surface gravity waves on the sea. In the former context, energy is essentially added at large scales (by stirring or some instability mechanism), is dissipated at small (Kolmogorov and smaller) scales of the order of less than the inverse three quarter power of the Reynolds

number. It cascades via nonlinear interactions from the large scales to the small scales through a window of transparency (the inertial range in which neither forcing nor damping is important) by the constant energy flux Kolmogorov solution. Indeed, for hydrodynamic turbulence, the analogue to the Fermi-Dirac distribution, the Rayleigh-Jeans spectrum of equipartitions, is irrelevant altogether. The weak turbulence of surface gravity waves is the classical analogue of the case of weakly interacting fermions. The mechanism for energy and carrier density (particle number) transfer is “energy” and “momentum” conserving binary collisions satisfying the “four wave resonance” conditions

$$\mathbf{k} + \mathbf{k}_1 = \mathbf{k}_2 + \mathbf{k}_3, \quad \omega(\mathbf{k}) + \omega(\mathbf{k}_1) = \omega(\mathbf{k}_2) + \omega(\mathbf{k}_3). \quad (1.2)$$

In the semiconductor context, $\hbar\omega(\mathbf{k}) = \hbar\omega_{\text{gap}} + \epsilon_e(\mathbf{k}) + \epsilon_h(\mathbf{k})$ (which can be well approximated by $\alpha + \beta k^2$) where $\hbar\omega_{\text{gap}} = \epsilon_{\text{gap}}$ corresponds to the minimum bandgap and $\epsilon_e(\mathbf{k})$, $\epsilon_h(\mathbf{k})$ are electron and hole energies. In each case, there is also a simple relation $E(\mathbf{k}) = \omega n(\mathbf{k})^3$ between the spectral energy density $E(\mathbf{k})$ and carrier (particle number) density $n(\mathbf{k})$. As a consequence of conservation of both energy and carriers, it can be argued (schematically shown in Figure (3.1) for one species system and in Figure (4.5) for two-species system and described in their captions), that the flux energy (and some carriers) from intermediate momentum scales (around ω_0 say) at which it is injected, to higher momenta (where it is converted into heat) must be accompanied by the flux of carriers and some energy from ω_0 to lower momenta at which it will be absorbed by the laser. It is the latter solution that we plan to exploit.

³In case of electrons in a conduction band, $E(\mathbf{k}) = (\hbar\omega + \epsilon_{\text{gap}})n(\mathbf{k})$, where ϵ_{gap} is the band gap energy. We will return to this in the Chapter 3.

1.2.5 Main results

Here we list and briefly discuss the main results of this manuscript.

- 1. We systematically derive evolution equations over long times $O(\epsilon^{-2})$, of the order of the inverse square of the coupling strength, for the *leading order* approximations of *all* N^{th} order cumulants $N \geq 2$. The first of these is the QKE, a closed equation for the particle number, and is consistent with what one obtains using the Hartree-Fock approximation⁴ when one takes proper account of the frequency renormalization *to order* ϵ^2 . The remaining equations for the leading order behavior of the higher order cumulants decouple and can be solved by a simple renormalization of the frequency which depends only on particle number density. The first correction is the well known Hartree-Fock self energy correction whereas the second correction is new and complex. The imaginary part of the latter is positive definite as the particle number approaches an equilibrium solution of the QKE. As a result, the leading order contribution to the cumulants of order $N > 2$ (which contain information on the initial state) slowly decays. Not so the higher order corrections. We obtain specific expressions for these and show that they contain terms with cumulants of higher order, products of cumulants of order N with products of particle number and products simply containing particle number alone. Only the latter two types of terms exert a long time influence and it is this fact that leads us to a natural asymptotic closure of the hierarchy (see e.g. [18]-[20] for extensive discussions of asymptotic closure for classical systems).

⁴Here, we use the term Hartree-Fock approximation in the commonly used sense, which is not identical to the strict meaning of a quantum system with Hartree-Fock wave function. In the latter, scattering and correlations are excluded.

- 2. The connections with classical systems and boson systems are discussed. By analogy with results obtained in the case of the classical kinetic equation, we introduce a new four parameter family of steady (equilibrium) solutions for the QKE. The four parameters are temperature T , chemical potential μ , particle number flow rate Q and energy density flow rate P . When $P = Q = 0$, the equilibrium solution is the well known Fermi-Dirac distribution. For either P or Q nonzero, the distributions are the analogues of the Kolmogorov distributions of classical wave turbulence, in which particles (energy) flow from sources at intermediate momentum scales to sinks at low (high) momentum values.

These solutions have not been considered in the fermionic context before. It turns out in fact, in contrast to the pure Kolmogorov solutions (for which $Q = 0$, $P > 0$, or $P = 0$, $Q > 0$) that the relevant equilibrium solutions of the QKE which describe (a) the finite flux of particles and a little energy between intermediate momenta at which the system is pumped and a sink at low momenta and (b) the finite flux of energy and a few particles between the intermediate momenta and the energy dissipation sink at high momenta, involve special relations between Q and P . These solutions are also new for the cases of classical wave turbulence and boson systems.

- 3. Again by analogy with the classical case, we introduce a simple, local approximation to the collision integral in the QKE which gives excellent qualitative results. This is known as the differential approximation (see, e.g., [17],[21]) and is strictly valid only when the principal transfer of energy and particles is between close neighbors in momentum space. Its most important feature, however, is that it allows us explore both

analytically and numerically the behavior of the collision integral and thereby gain a clear qualitative picture about the nature of its steady (equilibrium) solutions.

- 4. We also generalize the differential kinetic equation to the case of system consisting of two kind of particles - electrons and holes. In the two-particle case the total number of electrons and the total number of holes is conserved, so that solution with constant particle (and zero energy) flux may be realized in each of the subsystems. However energy of electrons and energy of holes are not conserved. Only *total* energy of electrons *and* holes is conserved so that for the constant energy flux solution to be realized one has to consider *both* electron and hole subsystems. These *combined* flux solutions has not been considered even in the classical case.
- 5. We examine the relevance of these results in the context of semiconductor lasers using a simplified model which assumes that any relaxation due to carrier-phonon interactions is negligible with respect to carrier-carrier interactions. We suggest that it may be advantageous to pump these lasers in a fairly narrow momentum window whose corresponding frequency is greater than the lasing frequency and allow the finite flux steady (equilibrium) solutions to carry particles and energy back to the lasing frequency via collision processes. Indeed we show that, at least for the model we use, this strategy is more efficient than pumping the system across a wide range of momenta as it is done in practice. In many numerical experiments, for equal amounts of carriers and energy pumping, we find that the laser turns on when the finite flux equilibrium is excited but fails to turn on under broad band pump-

ing. This is to say that lasing threshold is much lower for narrow-band pumping case. When the pumping is increased so that the laser turns on under the latter conditions, the output power is consistently smaller than that emitted when the finite flux solution is operative.

This result persist across quite a big range of parameters - pumping and damping strengthes. different mass ratios of electron and holes. etc.

To conclude, *for the same amount of carriers pumped and approximately same amount of energy pumped the output power in the narrow band pumping case, when a finite flux distribution is excited, is consistently higher than in the broad band case, when carrier distributions have zero or small flux. The lasing threshold is much lower for a laser operating on Kolmogorov-type spectra then on equilibrium spectra.*

1.3 Outline

The semiconductor material interacting with the light may be described by the following Hamiltonian

$$\begin{aligned}
 H = & \hbar \sum_{\mathbf{k}} ((\epsilon_{ek} + \epsilon_{gap}) a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \epsilon_{hk} b_{-\mathbf{k}}^{\dagger} b_{-\mathbf{k}}) \\
 & + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}', \mathbf{q} \neq 0} V_{\mathbf{q}} (a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}'} a_{\mathbf{k}} + b_{\mathbf{k}+\mathbf{q}}^{\dagger} b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{\mathbf{k}'} b_{\mathbf{k}} - 2a_{\mathbf{k}+\mathbf{q}}^{\dagger} b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{\mathbf{k}'} a_{\mathbf{k}}) \\
 & - \sum_{\mathbf{k}} \mathcal{E} (d_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} b_{-\mathbf{k}}^{\dagger} + d_{\mathbf{k}}^* a_{\mathbf{k}} b_{-\mathbf{k}}) \\
 & + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} c_{\mathbf{q}}^{\dagger} c_{\mathbf{q}} + \sum_{\mathbf{k}, \mathbf{q}} \hbar G_{\mathbf{q}} a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}} (c_{\mathbf{q}} + c_{-\mathbf{q}}^{\dagger}) + \sum_{\mathbf{k}, \mathbf{q}} \hbar G_{\mathbf{q}} b_{\mathbf{k}+\mathbf{q}}^{\dagger} b_{\mathbf{k}} (c_{\mathbf{q}} + c_{-\mathbf{q}}^{\dagger}),
 \end{aligned} \tag{1.3}$$

here $a_{\mathbf{k}}^{\dagger}, a_{\mathbf{k}}$ is a creation/annihilation operators for an electron, $b_{\mathbf{k}}^{\dagger}, b_{\mathbf{k}}$ are creation /annihilation operators for a hole, $c_{\mathbf{k}}^{\dagger}, c_{\mathbf{k}}$ are creation /annihilation

operators for phonons. First line in this Hamiltonian represents electron and hole kinetic energies, second line describes the carrier-carrier interaction through the screened Coulomb potential V_q (2.54), third line is carrier-field interaction and last line is phonon kinetic energy and phonon-carrier interaction.

It would be difficult, if not impossible, to study this Hamiltonian all at once. Therefore we break the big problem in smaller parts and study pieces of this Hamiltonian in different Chapters. We hope that by the end of this manuscript the reader would be more comfortable with (1.3).

- Chapter 2 is distilled from Quantum Mechanics (see, e.g.[22] and Solid-state Physics textbooks (see, e.g. [23])). We introduce the concept of a semiconductor, explain the basics of band structure and introduce parabolic band approximation. Then we introduce the notion of indistinguishable particles, bosons and fermions and the second quantization formalism, a convenient tool for description of many-body systems. We also write down a Hamiltonian of interacting electrons and holes. We end the chapter by introducing the Heisenberg picture of quantum mechanics and deriving the Heisenberg Equation of motion for quantum mechanical operators.
- *Chapter 3* is the “heart “ of this thesis. All this Chapter is devoted to (1.1) part of (1.3). We generalize the concept of weak turbulence to include quantum systems and systematically and rigorously rederive the Quantum Boltzmann Kinetic equation. We then state and study its major properties, such as conservation laws and Boltzmann H-theorem. We analyze its stationary solutions and show that this equation indeed has a second (“finite flux”) class of steady (equilibrium) solutions. We introduce a so called differential kinetic equation, a tremendous sim-

plification to the kinetic equation, which nevertheless has the same “global” properties. We study this differential kinetic equation, both analytically and numerically, in detail.

- *Chapter 4* is devoted to first two lines of Hamiltonian (1.3). We derive the 2-particle quantum differential kinetic equation. This equation generalizes the differential kinetic equation for the case of two kinds of particles - electrons and holes. We study this equation both analytically and numerically and show that although it constitutes a tremendous simplification of original kinetic equation, it has “correct” global properties, and thus may be used to study carrier dynamics.
- Chapter 5 is devoted to phonons - last line of (1.3). We are going to assume that phonons are in equilibrium with themselves (concept of heat bath), so that only carrier-phonon interaction will be studied. At a later stages we will model carrier-phonon interaction phenomenologically through pumping-damping terms.
- Chapter 6 is again drawn from textbooks, (see, e.g. [24], [25], [26]) and devoted to the first three lines of Hamiltonian (1.3) (with second line included more or less phenomenologically) describing light-matter interactions. We rederive Maxwell-Bloch equations, used to describe a semiconductor interacting with the light fields.
- *Chapter 7* introduces the notion of a laser and explains the basics of semiconductor laser operation. This chapter is a “crown” of all previous chapters - we “fuse” together the knowledge of all previous chapters. We describe the derivation of the model equations, and perform analyses and numerical simulation of the model.

We show that indeed for the laser operating on “Quantum Kolmogorov Spectra” (as opposed to Fermi Dirac distribution) the output laser intensity is consistently bigger for the same amount of pumping, at least for the model we use.

This is the best we can treat the Hamiltonian (1.3). The last line is included phenomenologically through pumping-damping processes.

- Chapter 8 makes concluding remarks and lists some of the remaining challenges in treating (1.3) and semiconductor lasers.

Chapter 2

SETTING UP THE STAGE

2.1 Conductors, Semiconductors and Insulators

Valence electrons are responsible for binding atoms in a periodic lattice. These electrons can be tightly bound to the ions. Then the resulting material cannot conduct electrical current and therefore is called an insulator. In the opposite extreme, the valence electrons can move freely around the crystal and such materials can conduct electrical current. Then they are said to be conductors.

Semiconductors are intermediate between these two limiting cases. In a ground state, electrons are bound to the ions and cannot conduct current. In this state, semiconductors are insulators. In excited state, electrons are free to move and become similar to a conduction electrons of a metal. The semiconductor then becomes a conductor. The ground state and the lowest excited state are separated by an energy gap. By absorbing a photon, an electron can be excited across the energy gap. The reverse transition is also possible - electron goes from excited to ground state emitting photon. Thus in the spectral range around the bandgap, the semiconductor has interesting optical and electrical properties. Semiconductors are also extremely sensitive to imperfections and impurities. By adding impurities one can “design” semiconductors with desired properties.

2.2 Schroedinger Equation in Periodic potential.

2.2.1 Bravais Lattice.

A fundamental concept in the description of any crystalline solid is that of the *Bravais lattice*, which specifies the periodic array in which the repeated units of the crystal are arranged. The units themselves may be single atoms, groups of atoms, molecules, ions, etc. but the Bravais lattice summarizes only the geometry of the underlying periodic structure, regardless of what the actual units may be. Following [23] we give two equivalent definitions of a Bravais lattice:

1. A Bravais lattice is an infinite array of discrete points with an arrangement and orientation that appears *exactly* the same, from whichever of the points the array is viewed.
2. A (three-dimensional) Bravais lattice consists of all points with position vectors $\mathbf{R}$ of the form

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3,$$

where $\mathbf{a}_i, i = 1, 2, 3$ are any three vectors not all in the same plane. and $n_i, i = 1, 2, 3$ range through all integer values. The vectors $\mathbf{a}_i$ are called *primitive vectors* and are said to *generate* or *span* the lattice.

2.2.2 Bloch Theorem.

Let us derive a Schroedinger equation which takes into account the fact that a semiconductor consists of a periodic lattice of atoms. This periodicity of the lattice implies

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{R}_n), \quad (2.1)$$

where $\mathbf{R}_n$ is the lattice vector $\mathbf{R}_n = \sum_i^d \mathbf{a}_i n_i$, $\mathbf{a}_i$ being the basic lattice vectors, which span the unit cell, n_i are integers, d is the dimension of the space.

Let us introduce the translational operator T_n :

$$T_n f(\mathbf{r}) = f(\mathbf{r} + \mathbf{R}_n), \quad (2.2)$$

where f is an arbitrary function. Applying T to the wave function $\psi(\mathbf{r})$ of an electron in a periodic potential $V(\mathbf{r})$,

$$T_n \psi(\mathbf{r}) = \psi(\mathbf{r} + \mathbf{R}_n) = t_n \psi(\mathbf{r}), \quad (2.3)$$

where t_n is a phase factor, because the probability density $|\psi(\mathbf{r})|^2$ and $|\psi(\mathbf{r} + \mathbf{R}_n)|^2$ have to be identical. Hence $|t_n| = 1$.

2.2.3 Schroedinger Equation.

A complete set set of functions exists, which are simultaneously eigenfunctions of the crystal Hamiltonian $\mathcal{H}$ and T_n :

$$\begin{aligned} \mathcal{H} \psi_n(\mathbf{r}) &= E_n \psi_n(\mathbf{r}), \\ T_n \psi(\mathbf{r}) &= \psi_n(\mathbf{r} + \mathbf{R}_n) = t_n \psi(\mathbf{r}), \end{aligned} \quad (2.4)$$

because $\mathcal{H}$ has full lattice symmetry and $[\mathcal{H}, T_n]_- \equiv \mathcal{H}T_n - T_n\mathcal{H} = 0$. Since $T_{n+m} = T_n T_m$, $t_n t_m = t_{n+m}$.

Therefore, as a manifestation of crystal periodicity (translational symmetry), one has the Bloch theorem

$$e^{i\mathbf{k}\mathbf{R}_n} \psi_n(\mathbf{r}) = \psi_n(\mathbf{r} + \mathbf{R}_n) \quad (2.5)$$

To satisfy this relation, we use an ansatz

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{e^{i\mathbf{k}\mathbf{r}}}{L^{3/2}} u_{n,\mathbf{k}}(\mathbf{r}) \quad (2.6)$$

where L^3 is the volume of the crystal and $\mathbf{k}$ is the quasimomentum. This ansatz fulfills Bloch theorem if the functions $u_{n,\mathbf{k}}$ is periodic with the periodicity of the crystal in a real space

$$u_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r} + \mathbf{R}_n) \quad (2.7)$$

The functions $u_{n,\mathbf{k}}(\mathbf{r})$ are called Bloch functions. Inserting (2.6) into Schroedinger equation $H\Psi = E\Psi$ ¹:

$$\mathcal{H}\psi_{n,\mathbf{k}}(\mathbf{r}) = \left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) \right] \psi_{n,\mathbf{k}} = E_n \psi_{n,\mathbf{k}}. \quad (2.8)$$

We introduced quantum mechanical operator of particle momentum, $\mathbf{p} = -i\hbar\nabla$. We then use the relation

$$\begin{aligned} & \sum_j \frac{\partial^2}{\partial x_j^2} \psi(\mathbf{r}) \\ &= -k^2 u(\mathbf{r}) + 2i \sum_j k_j \frac{e^{i\mathbf{k}\mathbf{r}}}{L^{3/2}} \frac{\partial u}{\partial x_j} + \frac{e^{i\mathbf{k}\mathbf{r}}}{L^{3/2}} \sum_j \frac{\partial^2 u}{\partial x_j^2} \\ &= -\frac{e^{i\mathbf{k}\mathbf{r}}}{L^{3/2}} (\nabla + i\mathbf{k})^2 u_{n,\mathbf{k}}, \end{aligned} \quad (2.9)$$

we obtain

$$\left(-\frac{\hbar^2}{2m} (\nabla + i\mathbf{k})^2 + V(r) \right) u_{n,\mathbf{k}} = E_{n\mathbf{k}} u_{n,\mathbf{k}} \quad (2.10)$$

2.3 Tight-Binding Approximation

Let us consider the situation when the wave functions of electrons are strongly localized around atom. Then there is not much of an overlap between the wave functions of electrons of different atoms, and therefore we will expand

¹As I was told in kindergarten, it is not possible to cancel Ψ from both sides of this equation.

everything in what is called “overlap integrals”. We also assume that, in the vicinity of each lattice point, the full periodic Hamiltonian of a crystal can be approximated by a Hamiltonian of the atom located at this point. If ψ_n is a bound state of the atom Hamiltonian H_{atom} , and

$$H_{atom}\psi_n = E_n\psi_n, \quad (2.11)$$

then we require that $\psi_n(\mathbf{r})$ be very small when $r = |\mathbf{r}|$ exceeds a distance of the order of lattice constant.

Write the Hamiltonian of the crystal as

$$H = H_{atom} + \Delta U(\mathbf{r}), \quad (2.12)$$

where we added a correction needed to produce the full periodic potential out of single atom potential. If $\psi_n(\mathbf{r})$ satisfies the atomic Schroedinger equation (2.11), then it will also satisfy the crystal Schroedinger equation (2.12), provided that $\Delta U(\mathbf{r})$ vanishes whenever $\psi_n(\mathbf{r})$ does not. If this were indeed the case, then each atomic level $\psi_n(\mathbf{r})$ would yield N levels in the periodic potential, with wave functions $\psi_n(\mathbf{r} - \mathbf{R}_n)$, for each of N sites $\mathbf{R}_n$ of the lattice. To preserve the Bloch description we must find N linear combinations of these degenerate wave functions that satisfy the Bloch condition (2.5):

$$\psi_n(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_n(\mathbf{r}). \quad (2.13)$$

The N linear combinations we require are

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \psi_n(\mathbf{r} - \mathbf{R}), \quad (2.14)$$

where $\mathbf{k}$ ranges through the N values in the first Brillouin zone consistent with the Born-von Karman periodic boundary conditions $\exp(iN_i\mathbf{k} \cdot \mathbf{a}_i) = 1$, summation is taken over an infinite Bravais lattice. This sum converges

rapidly because of the short range of the atomic wave functions $\psi_n(\mathbf{r})$. The Bloch condition (2.13) is verified for the (2.14) by

$$\begin{aligned}
 \psi(\mathbf{r} + \mathbf{R}) &= \sum_{\mathbf{R}'} e^{i\mathbf{k} \cdot \mathbf{R}'} \psi(\mathbf{r} + \mathbf{R} - \mathbf{R}') \\
 &= e^{i\mathbf{k} \cdot \mathbf{R}} \left[\sum_{\mathbf{R}'} e^{i\mathbf{k} \cdot (\mathbf{R}' - \mathbf{R})} \psi(\mathbf{r} - (\mathbf{R}' - \mathbf{R})) \right] \\
 &= e^{i\mathbf{k} \cdot \mathbf{R}} \left[\sum_{\bar{\mathbf{R}}} e^{i\mathbf{k} \cdot \bar{\mathbf{R}}} \psi(\mathbf{r} - (\bar{\mathbf{R}})) \right] \\
 &= e^{i\mathbf{k} \cdot \mathbf{R}} \psi(\mathbf{r}). \tag{2.15}
 \end{aligned}$$

Here again the summation is taken over an infinite Bravais lattice. With the sum taken over all sites it is permissible to make the crucial replacement of the summation variable $\mathbf{R}'$ by $\bar{\mathbf{R}} = \mathbf{R}' - \mathbf{R}$ in the second to last line of (2.15). Thus the wave function (2.14) satisfy the Bloch condition but has energy levels of a single atom. Band structure arising in this way $E_n(\mathbf{k})$ is simply the set of atomic levels, independent of value of $\mathbf{k}$. To remove this not very physical result we must recognize that before $\psi_n(\mathbf{r})$ becomes very small, there is some nonzero value of $\Delta U(\mathbf{r})$. Therefore we should try to find solution of the full crystal equation in a more general form suggested by (2.14):

$$\psi(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \phi(\mathbf{r} - \mathbf{R}), \tag{2.16}$$

but with the function $\phi(\mathbf{r})$ not necessarily an exact atomic stationary state wave function, but one will be defined by further consideration. Since we expect that the product $\Delta U(\mathbf{r})\psi_n(\mathbf{r})$ is small but not zero, we expect $\phi(\mathbf{r})$ to be quite close to the atomic wave function $\psi_n(\mathbf{r})$. Therefore it is legitimate to expand $\phi(\mathbf{r})$ in a relatively small number of well localized atomic wave

functions $\psi_n(\mathbf{r})$:

$$\phi(\mathbf{r}) = \sum_n b_n \psi_n(\mathbf{r}). \quad (2.17)$$

Let us multiply the crystal Schroedinger equation

$$H\psi(\mathbf{r}) = (H_{atom} + \Delta U(\mathbf{r}))\psi(\mathbf{r}) = \mathcal{E}(\mathbf{k})\psi(\mathbf{r}) \quad (2.18)$$

by the atomic wave function $\psi_m^*(\mathbf{r})$, integrate by $d\mathbf{r}$, use

$$\int \psi_m^*(\mathbf{r}) H_{atom} \psi(\mathbf{r}) d\mathbf{r} = \int (H_{atom} \psi_m(\mathbf{r}))^* \psi(\mathbf{r}) d\mathbf{r} = E_m \int \psi_m^*(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r}, \quad (2.19)$$

to get

$$(\mathcal{E}(\mathbf{k}) - E_m) \int \psi_m^*(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r} = \int \psi_m^*(\mathbf{r}) \Delta U(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r}. \quad (2.20)$$

Substituting (2.16) and (2.17) into (2.20) and using the fact that the atomic wave functions are orthonormal

$$\int \psi_m^*(\mathbf{r}) \psi_n(\mathbf{r}) d\mathbf{r} = \delta_{nm},$$

we get the eigenvalue equation that determines the coefficients $b_n(\mathbf{k})$ and the energy levels $\mathcal{E}(\mathbf{k})$:

$$\begin{aligned} (\mathcal{E}(\mathbf{k}) - E_m) b_m = & -(\mathcal{E}(\mathbf{k}) - E_m) \sum_n \left(\sum_{\mathbf{R} \neq 0} \int \psi_m^*(\mathbf{r}) \psi_n(\mathbf{r} - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{r} \right) b_n \\ & + \sum_n \left(\int \psi_m^*(\mathbf{r}) \Delta U(\mathbf{r}) \psi_n(\mathbf{r}) d\mathbf{r} \right) b_n \\ & + \sum_n \left(\sum_{\mathbf{R} \neq 0} \int \psi_m^*(\mathbf{r}) \Delta U(\mathbf{r}) \psi_n(\mathbf{r} - \mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}} d\mathbf{r} \right) b_n. \end{aligned} \quad (2.21)$$

The first term on the right of (2.21) contains integrals of the form

$$\int d\mathbf{r} \psi_m^*(\mathbf{r}) \psi_n(\mathbf{r} - \mathbf{R}). \quad (2.22)$$

We interpret our assumption of well-localized atomic levels to mean that (2.22) is small compared to unity. We assume that the integrals in the third term on the right of (2.21) are small, since they also contain the product of two atomic wave functions centered at different sites. Finally, we assume that the second term on the right of (2.21) is small because we expect the atomic wave functions to become small at distance large enough for the periodic potential to deviate strongly from the atomic one.

Consequently, the RHS of (2.21) (and therefore $(\mathcal{E}(\mathbf{k}) - E_m)b_m$) is always small. This is possible if $\mathcal{E}(\mathbf{k}) - E_m$ is small whenever b_m is not (and vice versa). Thus $\mathcal{E}(\mathbf{k})$ must be close to atomic level, say E_0 , and all the b_m except those going with that level and levels degenerate with (or close to) it in energy must be small:

$$\mathcal{E}(\mathbf{k}) \simeq E_0, \quad b_m \simeq 0 \quad \text{unless} \quad E_m \simeq E_0. \quad (2.23)$$

If the estimates in (2.23) were strict equalities, we would be back to the extreme case when the crystal levels were identical to the atomic ones. Now, however, we can determine the levels in the crystal more accurately.

Often the atomic wave functions have so short a range that only nearest-neighbor terms in the sum over $\mathbf{R}$ of infinite Bravais lattice in (2.21) need to be retained.

If all b 's are zero except for a single atomic s level ², then (2.21) gives

²The wave functions for ground state of the Schroedinger equation with Coulomb potential are spherical in shape and often referred as "s" state. First excited state is "p" state and non-isotropic. For the case of hydrogen atom these wave-functions are given by spherical functions $Y_l^m, l = 1, 2, \dots; m = -l, -l+1, \dots, l$. See quantum mechanics textbook, for e.g. [22].

directly the band structure of the corresponding s -band:

$$\begin{aligned}
\mathcal{E}(\mathbf{k}) &= E_s - \frac{\beta + \sum_{\text{Bravais lattice}} \gamma(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}}{1 + \sum_{\text{Bravais lattice}} \alpha(\mathbf{R}) e^{i\mathbf{k} \cdot \mathbf{R}}} \\
\beta &= - \int d\mathbf{r} \Delta U(\mathbf{r}) |\phi(\mathbf{r})|^2, \\
\alpha(\mathbf{R}) &= \int d\mathbf{r} \phi^*(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R}), \\
\gamma(\mathbf{R}) &= - \int d\mathbf{r} \phi^*(\mathbf{r}) \Delta U(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R}), \tag{2.24}
\end{aligned}$$

where E_s is the energy level of the s^{th} state. For the s state $\psi(\mathbf{r})$ is real and spherically symmetric, thus $\alpha(-\mathbf{R}) = \alpha(\mathbf{R})$. Since $\Delta U(-\mathbf{r}) = \Delta U(\mathbf{r})$ it follows that $\gamma(-\mathbf{r}) = \gamma(\mathbf{r})$. Assuming further only nearest neighbors interactions, we get

$$\mathcal{E}(\mathbf{k}) = E_s - \beta - \sum_{\text{nearest neighbors}} \gamma(\mathbf{R}) \cos(\mathbf{k} \cdot \mathbf{R}). \tag{2.25}$$

Let us apply the developed formalism for a simple case of the face-centered cubic crystal. It is easy to see that the twelve nearest neighbors atom have relative coordinates

$$\mathbf{R} = \frac{a}{2}(\pm 1, \pm 1, 0), \frac{a}{2}(\pm 1, 0, \pm 1), \frac{a}{2}(0, \pm 1, \pm 1), \tag{2.26}$$

where a is the lattice constant. Let $(\mathbf{k}) = (k_x, k_y, k_z)$, then

$$\mathbf{k} \cdot \mathbf{R} = \frac{a}{2}(\pm k_i \pm k_j), \quad i, j = x, y; y, z; z, x. \tag{2.27}$$

Since the s -level wave function $\phi(\mathbf{r})$ is spherically symmetric, $\gamma(\mathbf{R})$ is the same for all 12 terms in (2.25): $\gamma(\mathbf{R}) \equiv \gamma$. Therefore, performing the summation in (2.25) we obtain

$$\begin{aligned}
\mathcal{E}(\mathbf{k}) &= E_s - \beta - 4\gamma \left(\cos \frac{1}{2} k_x a \cos \frac{1}{2} k_y a + \cos \frac{1}{2} k_y a \cos \frac{1}{2} k_z a + \right. \\
&\quad \left. \cos \frac{1}{2} k_z a \cos \frac{1}{2} k_x a \right) \tag{2.28}
\end{aligned}$$

where the overlap integral γ is defined by

$$\gamma = - \int d(\mathbf{r}) \phi^*(x, y, z) \Delta U(x, y, z) \phi(x - \frac{a}{2}, y - \frac{a}{2}, z). \quad (2.29)$$

In the limit of small ka this reduces to

$$\mathcal{E}(\mathbf{k}) = E_s - \beta - 12\gamma + \gamma a^2 k^2 \quad (2.30)$$

which is nothing but the **parabolic band approximation**.

Without proof, we mention that for the attractive potential the overlapping integral γ is negative for s-type atomic wave-functions, and is positive for p-type atomic wave-functions (see, e.g. [23]). As a result, there are few bands with positive and negative curvatures separated by band-gaps, i.e. forbidden energy zones.

We now summarize the important points of this section:

1. The discrete atomic energy levels become quasi-continuous energy regions called energy bands.
2. There is an energy band gap between different bands.
3. Depending on the corresponding atomic functions, the bands may have positive or negative curvature around the band extrema.
4. In the vicinity of the band extrema one can often make a parabolic band approximation:

$$\epsilon_{\lambda=c,v} \simeq \epsilon_{\lambda,0} + \frac{\hbar^2 k^2}{2\mu_{\lambda,eff}}, \quad \mu_{\lambda,eff} = \frac{\hbar^2}{\left(\frac{\partial^2 \epsilon_{\lambda}(k)}{\partial k^2}\right)_{k=0}}. \quad (2.31)$$

In the regimes where the parabolic band approximation is valid, the electrons and holes may be considered to be quasi-free particles with their effective masses.

5. The states in the bands are filled starting from the state of lower energy and in accordance to Pauli exclusion principle. The last completely filled state is called the *valence band*. The next higher state is called the *conduction band*.

There are then three possibilities: insulator, metal and semiconductor:

- The conduction band is empty and separated by a large energy gap from the valence band. The electrons cannot be accelerated by an external electric field since no free electrons are available. The resulting material is then called an *insulator*.
- The conduction band is separated by a relatively small energy gap from the valence band. The definition of *small* is somewhat arbitrary. Usually *small* in this context means smaller or of the order of (visible) optical photon energy. Then in the ground state the conduction band is empty, but the electrons can be moved relatively easily from the valence band into the conduction band, by say, absorbing quanta of visible or infrared light. When the electron gets excited and “jumps” from the valence to conduction band, it leaves behind a positively charged quasi-particle called “hole” which contributes to electrical conductivity.

The resulting material is called a *semiconductor*.

- If the conduction band is always partly filled, we have a finite electrical conductivity and then we call the material a “metal”.

2.4 Basics of Band Structure.

We are going to use a very simple model to describe the neighborhood of the semiconductor bandgap of potential. Namely, we use the parabolic bands

FIGURE 2.1. Band structure for 2 parabolic bands.

Here $\epsilon_{e,k} = \hbar^2 k^2 / (2\mu_e)$, $\epsilon_{h,k} = \hbar^2 k^2 / (2\mu_h)$ so that the curvature of the band is proportional to inverse mass of the particle: $\frac{\partial^2 \epsilon_{a,k}}{\partial k^2} \propto \frac{1}{\mu_a}$, $a = e, h$. In a ground state electrons occupy the valence band, but can be excited to the conduction band, leaving behind a positively charged vacancy - a hole. The electron in the conduction band is shown by black circle, the hole in the valence band is shown by white circle.

approximation and write the conduction electron energy as

$$\epsilon_{e,k} = \frac{\hbar^2 k^2}{2\mu_e}. \quad (2.32)$$

and the hole energy as

$$\epsilon_{h,k} = \frac{\hbar^2 k^2}{2\mu_h}, \quad (2.33)$$

where μ_e, μ_h are the effective masses of electron and hole respectively (see figure (2.1)).

For an optical (vertical) transition, the transition energy at the carrier momentum $\mathbf{k}$ is given by

$$\hbar\tilde{\omega}_\kappa = \epsilon_{e,k} + \epsilon_{h,k} + \epsilon_{gap}. \quad (2.34)$$

We also want to note that

1. The actual band structure of semiconductor is much more complicated. There are many conduction and valence bands and the particles are sometime referred as light and heavy electrons and holes. Just as in an atom gas with many energy level differences we are going to focus on one which matches the lasing frequency of interest and that all others included phenomenologically via damping process.
2. When the electron gets excited and leaving the valence band the energy of the valence band is decreasing. The bigger the momentum of leaving electron the bigger is the energy loss. This is why the valence band curvature is negative.

2.5 Description of Semiconductor Media

In this section we are going to introduce a convenient form for describing electrons and holes in the semiconductor. Electrons and holes, being fermions, obey Pauli exclusion principle - no more than one particle can occupy any given quantum state. In addition, according to the Slack determinant rule (see e.g. [22]), the wave function should change its sign once the two fermions are permuted. One can achieve this by properly antisymmetrising each wave function, but it appears to be much easier to use a second quantization formalism.

2.5.1 Bosons and Fermions.

In classical mechanics, identical particles (electrons say,) do not lose their “personality”, despite the identity of their physical properties. We may assign

a name or number to all the particles and can follow, at least in principle, their trajectories. Therefore at any time the particles may be identified.

In a quantum mechanics the situation is different. Due to the uncertainty principle the notion of trajectory loses its meaning. If one knows the exact coordinates of a particle, one does not know its momentum, and its coordinates at any subsequent instant do not have any definite value. Even if we succeed in identifying or numbering particles at some instant of time, we make no progress towards identifying them at any subsequent instant. This brings us to the very important conclusion of *indistinguishability of similar particles* in quantum mechanics. Particles lose their individuality! This is a very fundamental property of quantum systems (see, for example, [22]).

Let us consider a system composed of two identical particles. Let $\psi(\mathbf{x}_1, \mathbf{x}_2)$ be a wave function of the system, $\mathbf{x}_1, \mathbf{x}_2$ being coordinates and spin projections (and any other quantum numbers) of each particle. Since particles are *identical* or *indistinguishable*, the state of the system obtained by merely interchanging of the two particles must be completely equivalent physically to the original state of the system. Thus the wave function $\psi(\mathbf{x}_2, \mathbf{x}_1)$ of system with interchanged particles can only be different by an unimportant (unobservable) phase factor from $\psi(\mathbf{x}_1, \mathbf{x}_2)$, i.e.

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = e^{i\alpha} \psi(\mathbf{x}_2, \mathbf{x}_1), \quad (2.35)$$

where α is some real constant. By repeating the interchange of the particles we return to the original state, while the function ψ is multiplied by $e^{2i\alpha}$. Therefore $e^{2i\alpha} = 1$, and $e^{i\alpha} = \pm 1$. Thus

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \pm \psi(\mathbf{x}_2, \mathbf{x}_1). \quad (2.36)$$

There are only two possibilities: the wave function is either *symmetrical* (i.e. unchanged when particles are interchanged) or *anti symmetrical* (i.e.

change sign when particles are interchanged). Clearly all states of a system of identical particles must have the same symmetry: otherwise, a state which is a superposition of a states of a different symmetry would be neither symmetric nor antisymmetric. This result can be immediately generalized to systems consisting of any number of identical particles.

The property of being described by symmetrical or anti-symmetrical wave functions depends on the nature of the particles. Particles described by *anti-symmetrical* wave functions are said to be fermions and are described by *Fermi-Dirac statistics*, while those described by *symmetrical* wave functions are said to be bosons and are described by *Bose-Einstein statistics*.

2.5.2 Second Quantization of a Fermions.

Creation/Annihilation operators. To make a long story short, we introduce so called *field operators* $\hat{\phi}_s^\dagger(\mathbf{r}), \hat{\phi}_s(\mathbf{r})$ which create or annihilate particle at position $\mathbf{r}$ in space with spin projection s . In the above example (2.35):

$$\psi(\mathbf{x}_1, \mathbf{x}_2) = \hat{\phi}_s^\dagger(\mathbf{x}_1) \cdot \hat{\phi}_s^\dagger(\mathbf{x}_2)|0 >, \quad (2.37)$$

where $|0 >$ is a vacuum state - no particles or fields in a system. These field operators may be expanded in a generalized Fourier series:

$$\begin{aligned} \hat{\phi}_s^\dagger(\mathbf{r}) &= \sum_{\mathbf{k}} a_{\mathbf{k},s}^\dagger \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}} \\ \hat{\phi}_s(\mathbf{r}) &= \sum_{\mathbf{k}} a_{\mathbf{k},s} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}}, \end{aligned} \quad (2.38)$$

where $a_{\mathbf{k},s}^\dagger, a_{\mathbf{k},s}$ are so called creation/annihilation operators we are going to work with (see, for example, [22]).

These operators obey anticommutation relations:

$$a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}, \quad a_i a_j + a_j a_i = 0, \quad a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0. \quad (2.39)$$

Here indexes i and j refer to quantum numbers such as momentum $\mathbf{k}$, spin s and band λ . These anticommutation relations are the manifestation of a Fermi-Dirac statistics of fermions.

Let us define $|1_{\mathbf{k}}\rangle$ to be a quantum state consisting of an electron with momentum $\mathbf{k}$, and $|0_{\mathbf{k}}\rangle$ be a state with no electron with momentum $\mathbf{k}$. Then the action of creation/annihilation operators can be defined as

$$\begin{aligned} a_{\mathbf{k}}^{\dagger}|0_{\mathbf{k}}\rangle &= |1_{\mathbf{k}}\rangle \\ a_{\mathbf{k}}|1_{\mathbf{k}}\rangle &= |0_{\mathbf{k}}\rangle \\ a_{\mathbf{k}}|0_{\mathbf{k}}\rangle &= a_{\mathbf{k}}^{\dagger}|1_{\mathbf{k}}\rangle = 0 \end{aligned} \quad (2.40)$$

The first line states that the action of the creation operator on an empty state creates a particle in that state. The second line states that the action of annihilation operator on a filled state annihilates a particle in that state. The last line states that no more than one particle can occupy any given quantum state (Pauli principle; $a_{\mathbf{k}}^{\dagger}|1_{\mathbf{k}}\rangle = 0$) and that the action of an annihilation operator on an empty state gives the empty (vacuum) state.

The combination $\hat{n}_{\mathbf{k}} \equiv a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$ can be interpreted as the number operator for a state $\mathbf{k}$. $|1_{\mathbf{k}}\rangle$ and $|0_{\mathbf{k}}\rangle$ are eigenstates of this operator. Indeed,

$$\begin{aligned} a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}|1_{\mathbf{k}}\rangle &= |1_{\mathbf{k}}\rangle, \\ a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}|0_{\mathbf{k}}\rangle &= 0 \end{aligned} \quad (2.41)$$

so that $a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$ counts the number of particles in state $\mathbf{k}$.

To complete the description of N -particle system we have to specify a basis set. Let us choose a basis composed of eigenstates of $\hat{n}_{\mathbf{k}} \equiv a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$. Introduce the Hartree-Fock state by

$$\psi_i^{\text{HF}} \equiv a_{\mathbf{k}_{i_1}}^{\dagger} a_{\mathbf{k}_{i_2}}^{\dagger} a_{\mathbf{k}_{i_3}}^{\dagger} \dots a_{\mathbf{k}_{i_N}}^{\dagger} |0\rangle = |1_{\mathbf{k}_{i_1}} 1_{\mathbf{k}_{i_2}} 1_{\mathbf{k}_{i_N}}\rangle, \quad (2.42)$$

which is a state with $\mathbf{k}_{i_1}, \mathbf{k}_{i_2} \dots \mathbf{k}_{i_N}$ states occupied, and all other states empty. Then

$$\hat{n}_{\mathbf{k}}|\psi_i^{\text{HF}}\rangle = \begin{cases} 1, & \text{if } \mathbf{k} = \mathbf{k}_{i_j} \\ 0, & \text{otherwise.} \end{cases} \quad (2.43)$$

These states form a complete set of states of the system (see proof in any textbook). Thus any state of a system may be represented as

$$|\phi\rangle = \sum_i c_i |\psi_i^{\text{HF}}\rangle, \quad (2.44)$$

where $c_i = \langle \phi | \psi_i^{\text{HF}} \rangle$.

Different types of fermions. In principle, one may have several types of particles in the system, for example, electrons and holes in a semiconductor. Therefore one may have several types of annihilation/creation operators, each correspond to different types of particle. Let us complement the wave vector index $\mathbf{k}$ by a particle-type index. For the case of semiconductors this index will denote the band: “c” for conduction and “v” for the valence band.

We will often use the so called electron-hole representation. In this representation we then use $a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger$ to designate electrons in the conduction band. When the electron gets excited to conduction band it leaves a positively charged vacancy in the valence band. This vacancy is called hole. This is positively charged quasi-particle which can move freely around the crystal and contribute to electrical conductivity. We introduce the hole creation operator as

$$b_{\mathbf{k}}^\dagger = a_{c, -\mathbf{k}}$$

where the subscript “c” refers to electron in the conduction band. This equation states that creation of a hole with momentum $\mathbf{k}$ corresponds to annihilation of a valence band electron with opposite momentum (and spin) values. Momentum and spin of hole is equal to opposite of electron momenta

and spin, as transition of electron from valence to conduction band and thus creating of electron-hole pair or recombination of these two particles should not change the total momentum (or spin) of the system ³. It is this recombination which will be responsible for lasing in later chapters. Likewise we introduce hole annihilation operator as

$$b_{\mathbf{k}} = a_{v, -\mathbf{k}}^{\dagger},$$

where subscript “v” refers to valence band electron. This equation states that annihilation of a hole with momentum $\mathbf{k}$ corresponds to creation a valence band electron with opposite momentum (and spin) values.

The second quantized operators $\mathcal{O}^{(2)}$ are linked to first quantized operators $\mathcal{O}^{(1)}$ through

$$\mathcal{O}^{(2)} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \dots \int d\mathbf{r}_N \hat{\phi}^{\dagger}(\mathbf{r}_N) \dots \hat{\phi}^{\dagger}(\mathbf{r}_2) \hat{\phi}^{\dagger}(\mathbf{r}_1) \mathcal{O}^{(1)} \hat{\phi}(\mathbf{r}_1) \hat{\phi}(\mathbf{r}_2) \dots \hat{\phi}(\mathbf{r}_N) \quad (2.45)$$

where the $\hat{\phi}(\mathbf{r})$, $\hat{\phi}^{\dagger}(\mathbf{r})$ are given by (2.38). In particular, the kinetic energy of N-interacting electrons is given by

$$\begin{aligned} \mathcal{K}^{(2)} &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 \dots \int d\mathbf{r}_N \hat{\phi}^{\dagger}(\mathbf{r}_N) \dots \hat{\phi}^{\dagger}(\mathbf{r}_2) \hat{\phi}^{\dagger}(\mathbf{r}_1) \\ &\quad \times \sum_{i=1}^N \frac{\hat{\mathbf{p}}^2}{2m^e} \hat{\phi}(\mathbf{r}_1) \hat{\phi}(\mathbf{r}_2) \dots \hat{\phi}(\mathbf{r}_N) \end{aligned} \quad (2.46)$$

where $\hat{\mathbf{p}} = i\hbar \frac{\partial}{\partial \mathbf{r}}$ is the momentum operator. The momentum operator has plane waves (free particles) as eigenfunctions. Assuming that the particles are, in some sense, interacting weakly, use (2.38) to write

$$\mathcal{K} = \sum_{\mathbf{k}} \sum_{\lambda} \epsilon_{\lambda \mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}, \quad (2.47)$$

³Emitted photon has negligible small momenta and zero spin.

where λ is the band index. Since we are using the two-band model,

$$\mathcal{K} = \sum_{\mathbf{k}} [\epsilon_{c\mathbf{k}} a_{c\mathbf{k}}^\dagger a_{c\mathbf{k}} + \epsilon_{v\mathbf{k}} a_{v\mathbf{k}}^\dagger a_{v\mathbf{k}}]. \quad (2.48)$$

In the electron-hole representation, (2.48) becomes

$$\mathcal{K} = \sum_{\mathbf{k}} [\epsilon_{c\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \epsilon_{v\mathbf{k}} [1 - b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}]]. \quad (2.49)$$

The origin of energy is arbitrary, so

$$\mathcal{K} = \sum_{\mathbf{k}} [(\epsilon_{gap} + \epsilon_{e\mathbf{k}}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \epsilon_{h\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}]. \quad (2.50)$$

The potential energy of electron-hole interaction is given by

$$\begin{aligned} \mathcal{P} = & \int d\mathbf{r}_1 \int d\mathbf{r}_2 \dots \int d\mathbf{r}_N \hat{\phi}^\dagger(\mathbf{r}_N) \dots \hat{\phi}^\dagger(\mathbf{r}_2) \hat{\phi}^\dagger(\mathbf{r}_1) \\ & \times \sum_{i,j,i \neq j} \frac{e^2}{\epsilon_b |\mathbf{r}_i - \mathbf{r}_j|} \hat{\phi}(\mathbf{r}_1) \hat{\phi}(\mathbf{r}_2) \dots \hat{\phi}(\mathbf{r}_N), \end{aligned} \quad (2.51)$$

or in the second quantization (we skip some tedious operator algebra, see. e.g. [24])

$$\mathcal{P} = \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q} \neq 0} V_q (a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}} + b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}'-\mathbf{q}}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}} - 2a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}}). \quad (2.52)$$

with

$$V_q = \frac{1}{V} \int d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} \cdot V(r) = \frac{4\pi e^2}{\epsilon_b V q^2} \quad (2.53)$$

We see that the potential is *singular*. This create some problems in the derivation of Quantum Kinetic equation in the Chapter 3, as we are going to assume that interaction potential to be small compared to $\omega_{\mathbf{k}}$ *uniformly* in $\mathbf{k}$. Therefore we are going to assume that our potential is *screened* by

the presence of many other electrons and holes. Screening weakens potential at long distances or small $\mathbf{k}$ values. The modification is a renormalization of the coupling coefficient T_{kk_1,k_2k_3} near $\mathbf{k} = 0$ which effectively cancels the singularity, or equivalently replaces k^{-2} by $(k^2 + \kappa^2)^{-1}$, where κ is the inverse screening length. In what follows we assume

$$V_q = V_q^{\text{screened}} \equiv \frac{4\pi e^2}{\epsilon_b V(q^2 + \kappa^2)} \quad (2.54)$$

To conclude, the Hamiltonian of interacting electrons and holes are $\mathcal{H} = \mathcal{K} + \mathcal{P}$, or

$$\begin{aligned} \mathcal{H} = & \sum_{\mathbf{k}} [(\epsilon_{gap} + \epsilon_{e\mathbf{k}}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \epsilon_{h\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}] + \\ & \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q} \neq 0} V_q (a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}} + b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}'-\mathbf{q}}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}} - 2a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}'-\mathbf{q}}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}}). \end{aligned} \quad (2.55)$$

This is the Hamiltonian used in the Introduction (1.1) and for derivation on one-particle Quantum Kinetic Equation in the Chapter 3. To express interaction matrix element T_{kk_1,k_2k_3} through V_q use

$$\begin{aligned} \tilde{T}_{kk_1,k_2k_3} &= V_{k_1-k_3} \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \\ T_{kk_1,k_2k_3} &= \frac{1}{8} \left(\tilde{T}_{kk_1,k_2k_3} - \tilde{T}_{k_1k,k_2k_3} - \tilde{T}_{kk_1,k_3k_2} + \tilde{T}_{k_1k,k_3k_2} \right. \\ &\quad \left. + \tilde{T}_{k_3k_2,k_1k}^* - \tilde{T}_{k_2k_3,k_1k}^* - \tilde{T}_{k_3k_2,kk_1}^* + \tilde{T}_{k_2k_3,kk_1}^* \right). \end{aligned} \quad (2.56)$$

so that (3.2) is satisfied.

2.5.3 Heisenberg Equation of Motion

Non-relativistic quantum mechanics may be formulated in two equivalent ways - in the Schroedinger or in the Heisenberg pictures.

In the Schroedinger picture, the operators are functions of coordinates only and usually are independent on time. The time dependence of mean values of physical quantities is due only to the time dependence of the wave function of the state:

$$\bar{f}(t) = \int \Psi^*(q, t) \hat{f} \Psi(q, t) dq, \quad (2.57)$$

where $\Psi(q, t)$ is a wave function of a state, $\hat{f}$ is an operator which corresponds to some physical quantity, q is coordinate, and $\bar{f}(t)$ is a time dependence of the mean value of a physical quantity.

In the Heisenberg picture used in this manuscript, the time dependence is transferred from wave functions to operators so that operators become time dependent and wave functions are time independent.

Let us define the operator

$$\hat{S} = \exp(-i/\hbar \hat{H}t), \quad (2.58)$$

where $\hat{H}$ is the Hamiltonian of the system. By definition, the eigenvalues of $\hat{S}$ are the same as those of the operator $\hat{H}$, i.e. the stationary wave functions $\psi_n(q)$, where

$$\hat{S} \psi_n(q) = e^{-\frac{i}{\hbar} E_n t} \psi_n(q), \quad (2.59)$$

where E_n are eigenvalues of $\hat{H}$: $\hat{H} \psi_n(q) = E_n \psi_n(q)$. Hence it follows that an arbitrary wave function $\Psi(q, t)$ can be expanded in terms of stationary wave functions in the operator form

$$\Psi(q, t) = \hat{S} \Psi(q, 0). \quad (2.60)$$

Let us calculate Hermitian conjugate of the operator $\hat{S}$:

$$\hat{S}^\dagger = \exp\left(\frac{i}{\hbar} \hat{H}^* t\right) = \exp\left(\frac{i}{\hbar} \hat{H} t\right) = \hat{S}^{-1}, \quad (2.61)$$

here $\bar{\cdot}$ denotes the complex conjugate operator. Hence the operator $\hat{S}$ is a unitary operator. Defining the time dependent operator $\hat{f}(t)$ as

$$f(t) = \hat{S}^{-1} \hat{f} \hat{S}. \quad (2.62)$$

we have

$$\bar{f}(t) = \int \Psi^*(q, 0) \hat{f}(t) \Psi(q, 0). \quad (2.63)$$

Now we have a formula which is analogous to (2.57) but with time dependence transferred from wave functions to operators.

Differentiating (2.62) with respect to time and assuming that operators $\hat{H}$ and $\hat{f}$ do not themselves involve time dependence we get

$$\frac{\partial}{\partial t} \hat{f}(t) = \frac{i}{\hbar} \left(\hat{H} \hat{f} - \hat{f} \hat{H} \right), \quad (2.64)$$

which is the so called Heisenberg equation of motion for operators. This equation will be heavily used in this manuscript.

Chapter 3

QUANTUM BOLZMANN KINETIC EQUATION

3.1 Systematic Derivation of the Kinetic Equation and Evolution equations for Higher Order Cumulants

3.1.1 Basic Definitions and Evolution Equation

We start from the Hamiltonian (1.1) of a spatially homogeneous system of particles with binary interactions. Here, $e_k = \hbar\omega_k$ is the energy level of momentum state $\mathbf{k}$ ¹ where $\mathbf{k}$ is a d-dimensional wave vector, and $a_k^\dagger, a_k$ are fermionic creation/annihilation operators fulfilling the anticommutation relations.

$$a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij} \quad a_i a_j + a_j a_i = 0. \quad (3.1)$$

We include the size of the system in the definition of the interaction matrix element $T_{12,34}$. We introduce for convenience the short hand notation: $\mathbf{k}_1 \equiv 1$, $\frac{V}{(2\pi)^d} d\mathbf{k}_1 \equiv d1$, and $\frac{(2\pi)^d}{V} \delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) \equiv \delta_{34}^{12}$, $\hbar = 1$ ². The Hamiltonian now reads

$$H = \int d1 \omega_1 a_1^\dagger a_1 + \frac{1}{2} \int d1234 T_{12,34} a_1^\dagger a_2^\dagger a_3 a_4 \delta_{34}^{12}.$$

¹In the semiconductor context, the energy available on an electron transfer consist of three parts (see Figure (2.1) and (2.34)), $\epsilon_{e,k} = \frac{\hbar^2 k^2}{2m_e}$, ϵ_{gap} and $\frac{\hbar^2 k^2}{2m_h}$ and the energy density ϵ_k to leading order in amplitude is $(\epsilon_{gap} + \epsilon_{e,k})n_k^e + \epsilon_{h,k}n_k^h$ where n_k^e (n_k^h) is the probability of finding an electron (hole) of momentum $\mathbf{k}$ in the conduction (valence) band. The single species model presented in this chapter is equivalent to redefining the energy density as $\epsilon_k - \epsilon_{gap} \int n_k d\mathbf{k}$, unifying electrons and holes and defining

$$\epsilon_k = \hbar\omega_k = \frac{\hbar^2 k^2}{2m}, \quad 1/m = 1/m_e + 1/m_h.$$

² $\hbar = 1$ through Chapters 3 and 4.

If one interchanges the indices 1 and 2 or 3 and 4 in the above expression and uses the fact that the Hamiltonian is Hermitian, the following properties can be derived:

$$T_{12,34} = -T_{21,34} = T_{21,43} = T_{43,21}^* \quad (3.2)$$

In the Heisenberg picture, the equations of motion are

$$\dot{a}_k = i[H, a]_- \equiv iHa - iaH \quad (3.3)$$

which give

$$\begin{aligned} \dot{a}_k^\dagger &= i\omega_k a_k^\dagger + i \int T_{32,10} a_3^\dagger a_2^\dagger a_1 \delta_{32}^{10} d123 \\ \dot{a}_k &= -i\omega_k a_k - i \int T_{01,23} a_1^\dagger a_2 a_3 \delta_{32}^{10} d123. \end{aligned} \quad (3.4)$$

From the Heisenberg equations of motion, one can now derive the BBGKY hierarchy of equations for the normal ordered expectations values. The first three are,

$$\frac{d}{dt} \rho_k = 2\text{Im} \int T_{01,23} N_{0123} \delta_{32}^{10} d123. \quad (3.5)$$

$$\begin{aligned} \frac{d}{dt} N_{1'2'3'4'} &= i\Delta_{3'4'}^{1'2'} N_{1'2'3'4'} + i \int d123 (T_{32,11'} (N_{323'4'} \delta_{2'}^1 - N_{322'13'4'}) \delta_{11'}^{32} + \\ &\quad T_{32,12'} N_{1'3213'4'} \delta_{12'}^{32} - \\ &\quad T_{3'1,23} N_{1'2'1234'} \delta_{13'}^{32} - T_{4'1,23} (N_{1'2'23} \delta_1^{3'} - N_{1'2'13'23}) \delta_{14'}^{32}) , \\ &\quad \mathbf{k}'_1 + \mathbf{k}'_2 - \mathbf{k}'_3 - \mathbf{k}'_4 = 0, \end{aligned} \quad (3.6)$$

$$\begin{aligned} \frac{d}{dt} N_{1'2'3'4'5'6'} &= i\Delta_{4'5'6'}^{1'2'3'} N_{1'2'3'4'5'6'} \\ &+ i \int d123 [T_{32,11'} (\delta_{2'}^1 N_{323'4'5'6'} - \delta_{3'}^1 N_{322'4'5'6'} + N_{322'3'14'5'6'}) \delta_{11'}^{32} \\ &\quad + T_{32,12'} (\delta_{3'}^1 N_{1'324'5'6'} - N_{1'323'14'5'6'}) \delta_{12'}^{32} \\ &\quad + T_{32,13'} N_{1'2'3214'5'6'} \delta_{13'}^{32} - T_{4'1,23} N_{1'2'3'1235'6'} \delta_{23}^{4'1} \end{aligned}$$

$$\begin{aligned}
& -T_{5'1,23} \left(\delta_{4'}^1 \cdot N_{1'2'3'236'} - N_{1'2'3'14'236'} \right) \delta_{23}^{5'1} \\
& -T_{6'1,23} \left(\delta_{5'}^1 \cdot N_{1'2'3'4'23} - \delta_{4'}^1 \cdot N_{1'2'3'5'23} + N_{1'2'3'14'5'23} \right) \delta_{23}^{6'1} \Big], \\
& \mathbf{k}'_1 + \mathbf{k}'_2 + \mathbf{k}'_3 - \mathbf{k}'_4 - \mathbf{k}'_5 + \mathbf{k}'_6 = 0.
\end{aligned} \tag{3.7}$$

where

$$\begin{aligned}
\Delta_{34}^{12} & \equiv (\omega_{k_1} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4}), \\
\Delta_{456}^{123} & \equiv (\omega_{k_1} + \omega_{k_2} + \omega_{k_3} - \omega_{k_4} - \omega_{k_5} - \omega_{k_6}).
\end{aligned} \tag{3.8}$$

Here, the expectation value is taken with respect to an arbitrary initial state Φ , i.e.,

$$\begin{aligned}
\rho(k_1) \delta_2^1 & = \langle \Phi | a_1^\dagger a_2 | \Phi \rangle \\
.N_{1234} & = \langle \Phi | a_1^\dagger a_2^\dagger a_3 a_4 | \Phi \rangle \\
.N_{123456} & = \langle \Phi | a_1^\dagger a_2^\dagger a_3^\dagger a_4 a_5 a_6 | \Phi \rangle \\
.N_{12345678} & = \langle \Phi | a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger a_5 a_6 a_7 a_8 | \Phi \rangle
\end{aligned} \tag{3.9}$$

In the definitions of these $2m$ ($m = 1, 2, \dots$) order expectation values, the first m indices correspond to creation operators and the last m indices correspond to annihilation operators. The number of creation and number of annihilation operators are equal to each other because the Hamiltonian (1.1) conserves number of particles. The fact that the right hand sides of (3.9) are zero on $\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4 = 0$, $\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4 - \mathbf{k}_5 - \mathbf{k}_6 = 0$ respectively is a direct consequence of the spatial homogeneity of the system. This means that the N^{th} order moment of the spatially dependent field operators (2.38) $\psi^\dagger(\mathbf{x}_j), \psi(\mathbf{x}_j)$, the generalized Fourier transforms of the creation and annihilation operators $a^\dagger(\mathbf{k}_j), a(\mathbf{k}_j)$, depends only on the relative spacing; i.e. on the differences of the coordinates $\mathbf{x}_j$, $j = 1 \dots N$.

3.1.2 Cumulants and their evolution.

Definitions of lower order cumulants. Let us define the cumulant of the N product of spatially dependent field operators $\psi(\mathbf{x}_j)$, $j = 1, 2, \dots, N$ to be the moment of order N from which the appropriate combinations of products of lower order moments are subtracted so that the resulting expression has the property that it decays to zero as the separations $\mathbf{x}_j - \mathbf{x}_i$ become large. The Fourier transforms of these cumulants are therefore well defined ordinary (as opposed to generalized) functions and these are the objects $\rho(k)$, $\mathcal{P}_{1234}$, ... with which we deal. Moreover, if the statistics are exactly Gaussian (namely, Hartree-Fock like), then all cumulants of order N , $N > 2$, are zero. Because these weakly interacting fermionic systems relax to a near Gaussian state, the cumulants are the most convenient dependent variables (for classical systems, see e.g., [18],[19],[20]).

For the two and three particle functions we define the fourth and sixth order cumulants $\mathcal{P}_{1234}$ and $\mathcal{Q}_{123456}$ respectively by

$$N_{1234} = \rho_1 \rho_2 (\delta_3^2 \delta_4^1 - \delta_4^2 \delta_3^1) + \mathcal{P}_{1234} \delta_{34}^{12} \quad (3.10)$$

and

$$\begin{aligned} N_{123456} = & \rho_1 \rho_2 \rho_3 \cdot (\delta_4^3 (\delta_5^2 \delta_6^1 - \delta_5^1 \delta_6^2) + \delta_5^3 (\delta_6^2 \delta_4^1 - \delta_4^2 \delta_6^1) + \delta_6^3 (\delta_5^1 \delta_4^2 - \delta_4^1 \delta_5^2)) + \\ & \rho_3 [+ \mathcal{P}_{1256} \delta_4^3 \delta_{56}^{12} - \mathcal{P}_{1246} \delta_5^3 \delta_{46}^{12} + \mathcal{P}_{1245} \delta_6^3 \delta_{45}^{12}] + \\ & \rho_2 [- \mathcal{P}_{1356} \delta_4^2 \delta_{56}^{13} + \mathcal{P}_{1346} \delta_5^2 \delta_{46}^{13} - \mathcal{P}_{1345} \delta_6^2 \delta_{45}^{13}] + \\ & \rho_1 [+ \mathcal{P}_{2356} \delta_4^1 \delta_{56}^{23} - \mathcal{P}_{2346} \delta_5^1 \delta_{46}^{23} + \mathcal{P}_{2345} \delta_6^1 \delta_{45}^{23}] \\ & + \mathcal{Q}_{123456} \delta_{456}^{123} \end{aligned} \quad (3.11)$$

The expressions are analogues to what one would obtain in the classical case. There, the symbols $a^\dagger$ and a are complex numbers (as opposed to operators

in the quantum case) and one defines the cumulants by expanding the fourth order moments into all possible decompositions; namely

$$\langle a_1^* a_2^* a_3 a_4 \rangle = \{a_1^* a_3\} \{a_2^* a_4\} \delta_3^1 \delta_4^2 + \{a_1^* a_4\} \{a_2^* a_3\} \delta_4^1 \delta_3^2 + \{a_1^* a_2^* a_3 a_4\} \delta_{34}^{12} \quad (3.12)$$

where angle brackets denote moments and curly brackets denote the corresponding cumulants. In the classical case, it is consistent, but not necessary (one can keep the other terms and discover they play no essential role), to set all correlations such as $\{a_1^* a_2^*\}$ and $\{a_3 a_4\}$ equal to zero. In the quantum case, one also decomposes $\langle \Phi | a_1^\dagger a_2^\dagger a_3 a_4 | \Phi \rangle$ into products of all possible decompositions. Again, it is consistent, but not necessary, to set terms such as $\{a_1^\dagger a_2^\dagger\}$ and $\{a_3 a_4\}$ equal to zero. The resulting decomposition should be consistent with the anticommutation relations (3.1), from which follows that $.N_{1234} = -.N_{2134}$. Therefore, certain terms (for example, $\rho_1 \rho_2 \delta_4^2 \delta_3^1$) are negative in (3.10-3.11).

A general algorithm for the decomposition of the $.N^{\text{th}}$ order expectation value is given below.

Definitions of higher order cumulants. Diagrams. In this section we present simple diagrams which can help one to visualize the definition of cumulants. These diagrams are only meant as an aid to visualize the correlation contribution and should not be confused with other diagrams such as Feymann diagrams. The following pictures are intended to illustrate the ways to factorized $.N_{1234}$, $.N_{123456}$ and $.N_{12345678}$. Let us denote by square boxes operator averages according to (3.9), so that two connected arrows present ρ (2 operator expectation value), and

$$.N_{1234} = \begin{array}{c} \xrightarrow{4} \\ \xrightarrow{3} \end{array} \boxed{} \begin{array}{c} \xrightarrow{1} \\ \xrightarrow{2} \end{array}$$

Let us present cumulants in the form of vertices, with incoming arrows representing the arguments of annihilation operators, and the outgoing the arguments of creation operators. Then the second order cumulant (which is the same as the two operator average) is represented by two arrows:

$$\rho_1 \delta_2^1 = \begin{array}{c} \nearrow 1 \\ \searrow 2 \end{array}$$

The fourth order cumulant is represented by four arrows:

$$\mathcal{P}_{1234} = \begin{array}{c} \nearrow 1 \\ \searrow 4 \\ \nearrow 2 \\ \searrow 3 \end{array}$$

so that the definition of fourth order cumulant $\mathcal{P}_{1234}$ is

$$N_{1234} = \rho_1 \rho_2 (\delta_3^2 \delta_4^1 - \delta_4^2 \delta_3^1) + \mathcal{P}_{1234} \delta_{34}^{12}. \quad (3.13)$$

This partition can be represented graphically as

$$\begin{array}{c} \xrightarrow{2} \\ \xrightarrow{1} \end{array} \boxed{} \begin{array}{c} \xrightarrow{3} \\ \xrightarrow{4} \end{array} = - \begin{array}{c} \nearrow 3 \\ \searrow 4 \\ \nearrow 4 \\ \searrow 3 \end{array} + \begin{array}{c} \nearrow 4 \\ \searrow 3 \\ \nearrow 3 \\ \searrow 4 \end{array} + \begin{array}{c} \nearrow 3 \\ \searrow 4 \\ \nearrow 4 \\ \searrow 3 \end{array}$$

Because of the commutation relations (3.1), if we interchange two indices

corresponding to two creation or two annihilation operators, the average should change its sign, for example: $N_{1234} = -N_{2134}$. The definitions of cumulants should not contradict this property, so each product of lower order cumulants should be either positive or negative, depending upon whether it corresponds to an odd or even permutation. This explains the negative sign in from of $\rho_1 \rho_2 \delta_4^2 \delta_3^1$ term in (3.13). Similarly, the definition of the sixth order cumulant Q_{123456} is

$$\begin{aligned}
 N_{123456} = & \rho_1 \rho_2 \rho_3 \cdot (\delta_4^3 (\delta_5^2 \delta_6^1 - \delta_5^1 \delta_6^2) + \delta_5^3 (\delta_6^2 \delta_4^1 - \delta_4^2 \delta_6^1) + \delta_6^3 (\delta_5^1 \delta_4^2 - \delta_4^1 \delta_5^2)) + \\
 & \rho_3 [+ \mathcal{P}_{1256} \delta_4^3 \delta_{56}^{12} - \mathcal{P}_{1246} \delta_5^3 \delta_{46}^{12} + \mathcal{P}_{1245} \delta_6^3 \delta_{45}^{12}] + \\
 & \rho_2 [- \mathcal{P}_{1356} \delta_4^2 \delta_{56}^{13} + \mathcal{P}_{1346} \delta_5^2 \delta_{46}^{13} - \mathcal{P}_{1345} \delta_6^2 \delta_{45}^{13}] + \\
 & \rho_1 [+ \mathcal{P}_{2356} \delta_4^1 \delta_{56}^{23} - \mathcal{P}_{2346} \delta_5^1 \delta_{46}^{23} + \mathcal{P}_{2345} \delta_6^1 \delta_{45}^{23}] \\
 & + Q_{123456} \delta_{456}^{123}.
 \end{aligned} \tag{3.14}$$

This partition can be represented as

$$\begin{array}{c}
 \begin{array}{c} 3 \\ 2 \\ 1 \end{array} \begin{array}{|c|} \hline \\ \hline \end{array} \begin{array}{c} 4 \\ 5 \\ 6 \end{array} = \\
 \\
 \begin{array}{cccccc}
 \begin{array}{c} 1 \nearrow 4 \\ 2 \rightarrow 5 \\ 3 \nearrow 6 \end{array} & \begin{array}{c} 1 \nearrow 4 \\ 2 \rightarrow 6 \\ 3 \nearrow 5 \end{array} & \begin{array}{c} 1 \nearrow 5 \\ 2 \rightarrow 4 \\ 3 \nearrow 6 \end{array} & \begin{array}{c} 1 \nearrow 5 \\ 2 \rightarrow 6 \\ 3 \nearrow 4 \end{array} & \begin{array}{c} 1 \nearrow 6 \\ 2 \rightarrow 4 \\ 3 \nearrow 5 \end{array} & \begin{array}{c} 1 \nearrow 6 \\ 2 \rightarrow 5 \\ 3 \nearrow 4 \end{array} \\
 - & + & + & - & - & +
 \end{array} \\
 \\
 \begin{array}{ccccc}
 \begin{array}{c} 1 \nearrow 4 \\ 2 \nearrow 5 \\ 3 \nearrow 6 \end{array} & \begin{array}{c} 1 \nearrow 5 \\ 2 \nearrow 4 \\ 3 \nearrow 6 \end{array} & \begin{array}{c} 1 \nearrow 6 \\ 2 \nearrow 4 \\ 3 \nearrow 5 \end{array} & \begin{array}{c} 2 \nearrow 4 \\ 1 \nearrow 5 \\ 3 \nearrow 6 \end{array} & \begin{array}{c} 2 \nearrow 5 \\ 1 \nearrow 4 \\ 3 \nearrow 6 \end{array} \\
 + & - & + & - & +
 \end{array} \\
 \\
 \begin{array}{ccccc}
 \begin{array}{c} 2 \nearrow 6 \\ 1 \nearrow 4 \\ 3 \nearrow 5 \end{array} & \begin{array}{c} 3 \nearrow 4 \\ 1 \nearrow 5 \\ 2 \nearrow 6 \end{array} & \begin{array}{c} 3 \nearrow 5 \\ 1 \nearrow 4 \\ 2 \nearrow 6 \end{array} & \begin{array}{c} 3 \nearrow 6 \\ 1 \nearrow 4 \\ 2 \nearrow 5 \end{array} & \begin{array}{c} 3 \nearrow 6 \\ 1 \nearrow 5 \\ 2 \nearrow 4 \end{array} \\
 - & + & - & + & +
 \end{array} \\
 \\
 \begin{array}{c} \begin{array}{c} 3 \nearrow 6 \\ 1 \nearrow 4 \\ 2 \nearrow 5 \end{array} \end{array}
 \end{array}$$

Again, because of the commutation relations (3.1), if we interchange two indices corresponding to two creation or two annihilation operators, the average should change its sign, for example: $N_{123456} = -N_{213456}$. The picture below illustrates a simple algorithm of counting the parity of permutation by counting the number of crossing between lines connecting different arguments. In the example below, one sees that the parity of $n_1 \delta_5^1 \mathcal{P}_{2346}$ term in the expansion of N_{123456} is odd (because of the odd number of crossings), so the product is negative.

In the same manner, the definition of $\mathcal{Q}_{12345678}$

$$\begin{aligned}
 \mathcal{N}_{12345678} = & \rho_1 \rho_2 \rho_3 \rho_4 (\delta_5^4 \delta_6^3 \delta_7^2 \delta_8^1 + \dots) \\
 & \rho_4 \mathcal{Q}_{123678} \delta_5^4 + \dots + \rho_1 \rho_2 \mathcal{P}_{3456} \delta_8^1 \delta_7^2 + \dots + \mathcal{P}_{3456} \mathcal{P}_{1278} + \dots \\
 & + \mathcal{R}_{12345678}
 \end{aligned} \tag{3.15}$$

can be presented as

Because of the large number of terms in this case, we show only schematically the factorization of $\mathcal{N}_{1'2'3'4'5'6'7'8'}$. One has to choose *all* possible permutations of indices, corresponding to different topologies putting “annihila-

tion” arguments to the incoming and “creation” arguments to the outgoing arrows.

Cumulants evolution equations. Having defined the higher order cumulants, we can now write down the evolution equations for the cumulant hierarchy. For the purpose of deriving the QKE, it is sufficient to consider only the equations for ρ_k and $\mathcal{P}_{1234}$. To obtain the frequency corrections to order ϵ^2 ($\epsilon, 0 < \epsilon \ll 1$, is a measure of the strength of the coupling coefficient), we need to consider contributions coming from the equation for $\mathcal{Q}_{123456}$. In carrying out the analysis on ρ_k , $\mathcal{P}_{1234}$ and $\mathcal{Q}_{123456}$, one finds, just as in the classical case, that certain patterns emerge which allow one to identify the terms in the equations for the cumulants of arbitrary high order that gives rise to long time effects. Taking account of these terms gives the expansion (3.20,3.21) which will be discussed in the next section. In this section we only write down equations for ρ_k and $\mathcal{P}_{1234}$. They are

$$\frac{d}{dt}\rho_{k_0} = 2\text{Im} \int T_{01,23}\mathcal{P}_{0123}\delta_{23}^{01}d123. \quad (3.16)$$

where Im denotes the imaginary part and the symbol zero denotes $\mathbf{k}$, and ³

$$\begin{aligned} \frac{d}{dt}\mathcal{P}_{1'2'3'4'} &= i\tilde{\Delta}_{3'4'}^{1'2'}\mathcal{P}_{1'2'3'4'} - (\dot{\rho}_{1'}\rho_{2'} + \rho_{1'}\dot{\rho}_{2'}) (\delta_{3'}^{2'}\delta_{4'}^{1'} - \delta_{3'}^{1'}\delta_{4'}^{2'}) \\ &+ \frac{2iT_{4'3',2'1'}\rho_{3'}\rho_{4'}(1 - \rho_{2'} - \rho_{1'}) + 2iT_{4'3',2'1'}\rho_{1'}\rho_{2'}(\rho_{3'} + \rho_{4'} - 1)}{1} \\ + i \int d123 [& T_{32,11'}\mathcal{P}_{323'4'}\delta_{2'}^1\delta_{11'}^{32} - T_{4'1,23}\mathcal{P}_{1'2'23}\delta_3^1\delta_{14'}^{32} \\ - T_{32,11'} \cdot (& \rho_2'(+\mathcal{P}_{323'4'}\delta_1^{2'} - \mathcal{P}_{3214'}\delta_3^{2'} + \mathcal{P}_{3213'}\delta_4^{2'}) + \\ & \rho_2(\mathcal{P}_{32'14'}\delta_{3'}^2 - \mathcal{P}_{32'13'}\delta_{4'}^2) + \\ & \rho_3(-\mathcal{P}_{22'14'}\delta_{3'}^3 + \mathcal{P}_{22'13'}\delta_{4'}^3) + \underline{\underline{\mathcal{Q}_{322'13'4'}}} \delta_{11'}^{32} \\ + T_{32,12'} \cdot (& \rho_2(-\mathcal{P}_{1'314'}\delta_{3'}^2 + \mathcal{P}_{1'313'}\delta_{4'}^2) + \\ & \rho_3(+\mathcal{P}_{1'214'}\delta_{3'}^3 - \mathcal{P}_{1'213'}\delta_{4'}^3) + \end{aligned}$$

³We underline terms which will be especially important for further analyses.

$$\begin{aligned}
& \rho'_1(+\mathcal{P}_{323'4'}\delta_1^{1'} - \mathcal{P}_{3214'}\delta_3^{1'} + \mathcal{P}_{3213'}\delta_{4'}^{1'}) + \underline{\underline{\mathcal{Q}_{1'3213'4'}}} \delta_{12'}^{32} \\
-T_{3'1,23} (& \rho_1(+\mathcal{P}_{1'2'23}\delta_{4'}^1) + \\
& \rho'_2(-\mathcal{P}_{1'134'}\delta_2^{2'} + \mathcal{P}_{1'124'}\delta_3^{2'} - \mathcal{P}_{1'123}\delta_{4'}^{2'}) + \\
& \rho'_1(+\mathcal{P}_{2'134'}\delta_2^{1'} - \mathcal{P}_{2'124'}\delta_3^{1'} + \mathcal{P}_{2'123}\delta_{4'}^{1'}) + \underline{\underline{\mathcal{Q}_{1'2'1234'}}} \delta_{13'}^{32} + \\
T_{4'1,23} (& \rho_1(+\mathcal{P}_{1'2'23}\delta_3^1) + \\
& \rho'_2(-\mathcal{P}_{1'123}\delta_{3'}^{2'} + \mathcal{P}_{1'13'3}\delta_2^{2'} - \mathcal{P}_{1'13'2}\delta_3^{2'}) + \\
& \rho'_1(+\mathcal{P}_{2'123}\delta_{3'}^{1'} - \mathcal{P}_{2'13'3}\delta_2^{1'} + \mathcal{P}_{2'13'2}\delta_3^{1'}) + \underline{\underline{\mathcal{Q}_{1'2'13'23}}} \delta_{14'}^{32}] ,
\end{aligned} \tag{3.17}$$

on $\mathbf{k}_{1'} + \mathbf{k}_{2'} = \mathbf{k}_{3'} + \mathbf{k}_{4'}$, and the Hartree Fock self-energy is

$$\begin{aligned}
& \tilde{\Delta}_{3'4'}^{1'2'} = \\
& \omega_{1'} + \omega_{2'} - \omega_{3'} - \omega_{4'} + 2 \int d1 ((T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1) .
\end{aligned} \tag{3.18}$$

At this stage, it is worthwhile pointing out precisely those terms, (underlined in (3.17)) that give rise to the various long terms effects:

1. The terms that gives rise to particle number transfer in the QKE are

$$2iT_{4'3',2'1'}\rho_{3'}\rho_{4'}(1 - \rho_{2'} - \rho_{1'}) + 2iT_{4'3',2'1'}\rho_{1'}\rho_{2'}(\rho_{3'} + \rho_{4'} - 1).$$

The reason is that when one solves for $\mathcal{P}_{1234}$, one obtains an expression which contains this term multiplied by

$$A_t(\Delta_{3'4'}^{1'2'}) = \int_0^t d\tau \exp[i\Delta_{3'4'}^{1'2'}t] = (i\Delta_{3'4'}^{1'2'})^{-1}(\exp(\Delta_{3'4'}^{1'2'}t) - 1).$$

In the long time limit,

$$\lim_{t \rightarrow \infty} A_t(x) = \pi \text{sgn} t \cdot \delta(x) + iP\left(\frac{1}{x}\right).$$

Under the operator Im in (3.16), the delta-function is counted twice, and the principal value term cancels. The observant reader will notice that the QKE can be effectively derived by simply ignoring all terms in the equation for $\mathcal{P}_{1'2'3'4'}$ (except $i\Delta_{3'4'}^{1'2'}\mathcal{P}_{1'2'3'4'}$) proportional to cumulants of order greater than two. In the literature, this is called the Hartree-Fock approximation. What we show in this manuscript is that, for the magnitude ϵ of the coupling coefficient uniformly (in $\mathbf{k}$) small, the Hartree-Fock approximation is indeed self consistent when one takes proper account of the frequency renormalization *to order* ϵ^2 .

2. The order ϵ renormalizations to the frequency comes from the decomposition of sixth order moments such as $N_{1'2'13'23}\delta_{11'}^{23}$ in (3.7). These give rise to terms in the equation for $\mathcal{P}_{1'2'3'4'}$ which are proportional to $\mathcal{P}_{1'2'3'4'}$ itself. Indeed one obtains one such contributions from each of the sixth order moments in (3.7) leading to an expressions in the equation for $\mathcal{P}_{1'2'3'4'}$ equal to

$$2i \int d1 (T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) \rho_1.$$

When added to the frequency factor $i(\omega_{1'} + \omega_{2'} - \omega_3 - \omega_4)$, we obtain the term denoted by $\tilde{\Delta}_{3'4'}^{1'2'}$ in (3.17). It is not too difficult to see that, in the equation for every cumulant Q_N , there is a term proportional to

$$iQ_N \sum_{i=1}^N (\omega_j + 2 \int T_{j1,1j} \rho_1 d1)$$

and this gives rise to the first contribution in the renormalization of the frequency (3.41). In the literature, $\tilde{\Delta}_{3'4'}^{1'2'}$ is called Hartree-Fock self energy for fourth order averages.

3. The order ϵ^2 terms in the renormalization to the frequency arise from

the terms

$$i \int (T_{32,11'} Q_{322'13'4'} \delta_{11'}^{32} + T_{32,12'} Q_{1'3213'4'} \delta_{12'}^{32} + T_{3',23} Q_{1'2'1234'} + T_{3'1,23} Q_{1'2'13'23} \delta_{13'}^{32}) d123 \quad (3.19)$$

containing the sixth order cumulants in (3.17). The equations for the sixth order cumulant contains, in addition to terms proportional to a product of lower order particle number densities, terms proportional to $\mathcal{P}_{1'2'3'4'}$ with a factor containing $\rho_k(1 - \rho_k)$.

4. All other terms are integrals which contain highly oscillatory factors which, because of the Riemann-Lebesgue lemma, contribute nothing in the long time limit.

3.1.3 Asymptotic Expansions and Closure

We take advantage of the small parameter, the strength ϵ of the coupling coefficient and make the formal substitution $T_{12,34} \rightarrow \epsilon T_{12,34}$. We expand all cumulants Q_N in an asymptotic expansion

$$Q_2 \equiv \rho_k = n_k + \epsilon Q_2^{(1)} + \epsilon^2 Q_2^{(2)} + \dots \quad (3.20)$$

and

$$Q_N(k_1, k_2, k_3 \dots k_N; t) = Q_N^{(0)} + \epsilon Q_N^{(1)} + \epsilon^2 Q_N^{(2)} + \dots \quad N > 2 \quad (3.21)$$

Because of resonant interactions, these asymptotic expansions will be nonuniform in time. Namely, terms proportional to ϵt , $\epsilon^2 t$, etc., will appear in Q_N . These terms are removed and the asymptotic expansions (3.20,3.21) rendered well ordered by allowing corrections to the time dependence of the

leading order cumulants n_k , $Q_N^{(0)}$, $N > 2$. We make the ansatz

$$\frac{\partial n_k}{\partial t} = \epsilon^2 F_2^{(2)} + \dots \quad (3.22)$$

$$\frac{\partial Q_{1,2,\dots,N}^{(0)}}{\partial t} = i(\omega_1 + \omega_2 + \dots - \omega_N) Q_{1,2,\dots,N}^{(0)} + \epsilon F_{1,2,\dots,N}^{(1)} + \epsilon^2 F_{1,2,\dots,N}^{(2)} + \dots \quad (3.23)$$

and choose $F_2^{(2)}$, $F_N^{(1)}$, $F_N^{(2)}$... $N > 2$ in order to keep (3.20,3.21) asymptotically uniform for times $\omega_{k_0} t = O(\epsilon^{-2})$. Equations (3.22) and (3.23) describe the long time behavior of the system.

This method goes by many names, averaging, multiple time scales etc., familiar to nonlinear physicists (see, e.g., [5],[18]-[20]). It will turn out that $F_2^{(2)}$ depends only on n_k itself leading to a closed equation for the particle number, the QKE. It will also turn out that $F_N^{(1)}$, $F_N^{(2)}$, $N > 2$ are simply products of $Q_N^{(0)}$ with a function of n_k , which is the symmetric sum of N components. This means that the resulting equations (3.23) are easily solved by simply renormalizing the frequency.

Now we can use these rules of factorization and get a system of evolution equations for ρ and $\mathcal{P}_{1234}$:

$$\frac{d}{dt} \rho_{k_0} = 2\text{Im} \int T_{01,23} \mathcal{P}_{0123} \delta_{23}^{01} d123$$

Since ρ is real, the contribution from the factorized terms

$$4\text{Im} \rho_0 \int d1n_1 \text{Re} T_{01,10}$$

is equal to zero.

$$\begin{aligned} \frac{d}{dt} \mathcal{P}_{1'2'3'4'} &= i\Delta_{3'4'}^{1'2'} \mathcal{P}_{1'2'3'4'} - (\dot{\rho}_{1'} \rho_{2'} + \rho_{1'} \dot{\rho}_{2'}) (\delta_{3'}^{2'} \delta_{4'}^{1'} - \delta_{3'}^{1'} \delta_{4'}^{2'}) \\ &+ \frac{2iT_{4'3',2'1'} \rho_{3'} \rho_{4'} (1 - \rho_{2'} - \rho_{1'}) + 2iT_{4'3',2'1'} \rho_{1'} \rho_{2'} (\rho_{3'} + \rho_{4'} - 1)}{T_{32,11'} \mathcal{P}_{323'4'} \delta_2^1 \delta_{11'}^{32} - T_{4'1,23} \mathcal{P}_{1'2'23} \delta_3^1 \delta_{14'}^{32}} \\ + i \int d123 [& \end{aligned}$$

$$\begin{aligned}
& -T_{32,11'} \cdot (\quad \rho_2'(+\mathcal{P}_{323'4'}\delta_1^{2'} - \mathcal{P}_{3214'}\delta_{3'}^{2'} + \mathcal{P}_{3213'}\delta_{4'}^{2'}) + \\
& \quad \rho_2(-\underline{\mathcal{P}_{32'3'4'}}\delta_1^2 + \mathcal{P}_{32'14'}\delta_{3'}^2 - \mathcal{P}_{32'13'}\delta_{4'}^2) + \\
& \quad \rho_3(+\underline{\mathcal{P}_{22'3'4'}}\delta_1^3 - \mathcal{P}_{22'14'}\delta_{3'}^3 + \mathcal{P}_{22'13'}\delta_{4'}^3) + \underline{\underline{\mathcal{Q}_{322'13'4'}}}) \delta_{11'}^{32}, \\
& +T_{32,12'} \cdot (\quad \rho_2(+\underline{\mathcal{P}_{1'33'4'}}\delta_1^3 - \mathcal{P}_{1'314'}\delta_{3'}^2 + \mathcal{P}_{1'313'}\delta_{4'}^2) + \\
& \quad \rho_3(-\underline{\mathcal{P}_{1'23'4'}}\delta_1^2 + \mathcal{P}_{1'214'}\delta_{3'}^3 - \mathcal{P}_{1'213'}\delta_{4'}^3) + \\
& \quad \rho_1'(+\mathcal{P}_{323'4'}\delta_1^{1'} - \mathcal{P}_{3214'}\delta_{3'}^{1'} + \mathcal{P}_{3213'}\delta_{4'}^{1'}) + \underline{\underline{\mathcal{Q}_{1'3213'4'}}}) \delta_{12'}^{32} \\
& -T_{3'1,23} (\quad \rho_1(+\underline{\mathcal{P}_{1'2'34'}}\delta_2^1 - \mathcal{P}_{1'2'24'}\delta_3^1 + \mathcal{P}_{1'2'23}\delta_{4'}^1) + \\
& \quad \rho_2'(-\mathcal{P}_{1'134'}\delta_2^{2'} + \mathcal{P}_{1'124'}\delta_3^{2'} - \mathcal{P}_{1'123}\delta_{4'}^{2'}) + \\
& \quad \rho_1'(+\mathcal{P}_{2'134'}\delta_2^{1'} - \mathcal{P}_{2'124'}\delta_3^{1'} + \mathcal{P}_{2'123}\delta_{4'}^{1'}) + \underline{\underline{\mathcal{Q}_{1'2'1234'}}}) \delta_{13'}^{32} + \\
& T_{4'1,23} (\quad \rho_1(+\mathcal{P}_{1'2'23}\delta_3^1 - \underline{\mathcal{P}_{1'2'3'3}}\delta_2^1 + \mathcal{P}_{1'2'3'2}\delta_3^1) + \\
& \quad \rho_2'(-\mathcal{P}_{1'123}\delta_{3'}^{2'} + \mathcal{P}_{1'13'3}\delta_2^{2'} - \mathcal{P}_{1'13'2}\delta_3^{2'}) + \\
& \quad \rho_1'(+\mathcal{P}_{2'123}\delta_{3'}^{1'} - \mathcal{P}_{2'13'3}\delta_2^{1'} + \mathcal{P}_{2'13'2}\delta_3^{1'}) + \underline{\underline{\mathcal{Q}_{1'2'13'23}}}) \delta_{14'}^{32}] \\
\end{aligned} \tag{3.24}$$

We rewrite the last equation in the more compact form:

$$\begin{aligned}
& \frac{d}{dt}\mathcal{P}_{1'2'3'4'} = i\tilde{\Delta}_{3'4'}^{1'2'}\mathcal{P}_{1'2'3'4'} - (\dot{\rho}_{1'}\rho_{2'} + \rho_{1'}\dot{\rho}_{2'}) (\delta_{3'}^{2'}\delta_{4'}^{1'} - \delta_{3'}^{1'}\delta_{4'}^{2'}) \\
& + \frac{2iT_{4'3'2'1'}\rho_3\rho_{4'}(1 - \rho_{2'} - \rho_{1'}) + 2iT_{4'3'2'1'}\rho_{1'}\rho_{2'}(\rho_{3'} + \rho_{4'} - 1)}{1} \\
& + i \int d123 [T_{32,11'}\mathcal{P}_{323'4'}\delta_2^1\delta_{11'}^{32} - T_{4'1,23}\mathcal{P}_{1'2'23}\delta_3^1\delta_{14'}^{32} \\
& -T_{32,11'} \cdot (\quad \rho_2'(+\mathcal{P}_{323'4'}\delta_1^{2'} - \mathcal{P}_{3214'}\delta_{3'}^{2'} + \mathcal{P}_{3213'}\delta_{4'}^{2'}) + \\
& \quad \rho_2(\mathcal{P}_{32'14'}\delta_{3'}^2 - \mathcal{P}_{32'13'}\delta_{4'}^2) + \\
& \quad \rho_3(-\mathcal{P}_{22'14'}\delta_{3'}^3 + \mathcal{P}_{22'13'}\delta_{4'}^3) + \underline{\underline{\mathcal{Q}_{322'13'4'}}}) \delta_{11'}^{32}, \\
& +T_{32,12'} \cdot (\quad \rho_2(-\mathcal{P}_{1'314'}\delta_{3'}^2 + \mathcal{P}_{1'313'}\delta_{4'}^2) + \\
& \quad \rho_3(+\mathcal{P}_{1'214'}\delta_{3'}^3 - \mathcal{P}_{1'213'}\delta_{4'}^3) + \\
& \quad \rho_1'(+\mathcal{P}_{323'4'}\delta_1^{1'} - \mathcal{P}_{3214'}\delta_{3'}^{1'} + \mathcal{P}_{3213'}\delta_{4'}^{1'}) + \underline{\underline{\mathcal{Q}_{1'3213'4'}}}) \delta_{12'}^{32} \\
& -T_{3'1,23} (\quad \rho_1(+\mathcal{P}_{1'2'23}\delta_4^1) + \\
& \quad \rho_2'(-\mathcal{P}_{1'134'}\delta_2^{2'} + \mathcal{P}_{1'124'}\delta_3^{2'} - \mathcal{P}_{1'123}\delta_{4'}^{2'}) + \\
& \quad \rho_1'(+\mathcal{P}_{2'134'}\delta_2^{1'} - \mathcal{P}_{2'124'}\delta_3^{1'} + \mathcal{P}_{2'123}\delta_{4'}^{1'}) + \underline{\underline{\mathcal{Q}_{1'2'1234'}}}) \delta_{13'}^{32} + \\
& T_{4'1,23} (\quad \rho_1(+\mathcal{P}_{1'2'23}\delta_3^1) +
\end{aligned}$$

$$\begin{aligned} & \rho'_2(-\mathcal{P}_{1'123}\delta_{3'}^{2'} + \mathcal{P}_{1'13'3}\delta_2^{2'} - \mathcal{P}_{1'13'2}\delta_3^{2'}) + \\ & \rho'_1(+\mathcal{P}_{2'123}\delta_{3'}^{1'} - \mathcal{P}_{2'13'3}\delta_2^{1'} + \mathcal{P}_{2'13'2}\delta_3^{1'}) + \underline{\underline{\mathcal{Q}_{1'2'13'23}}})\delta_{14'}^{32}] \end{aligned} \quad (3.25)$$

where the Hartree-Fock exchange self energy is defined by

$$\tilde{\Delta}_{3'4'}^{1'2'} = \omega_{1'} + \omega_{2'} - \omega_{3'} - \omega_{4'} + 2 \int d1 ((T_{1'1.11'} + T_{2'1.12'} - T_{3'1.13'} - T_{4'1.14'})\rho_1) \quad (3.26)$$

We have underlined the terms in (3.25) which will play the dominant role in the following analyses. Although all the terms are of the same order initially, the effects of the underlined terms will persist and lead to long time cumulative effects. Then underlined terms in the second line of (3.25) will lead to QKE (3.39). The Hartree-Fock self energy will contribute to the frequency renormalization (3.41). The underlined twice terms give the coupling with high order moments leading to (3.41).

The equation for $\mathcal{Q}_{1'2'3'4'5'6'}$ is very long, so that we will show only its structure, which is similar to the structure of (3.24):

$$\begin{aligned} \frac{d}{dt}\mathcal{Q}_{1'2'3'4'5'6'} &= \underline{i\tilde{\Delta}_{4'5'6'}^{1'2'3'}\mathcal{Q}_{1'2'3'4'5'6'}} - \dot{\rho} \cdot \rho \cdot \rho - (\dot{\rho} \cdot \mathcal{P} + \rho \dot{\mathcal{P}}) \\ &+ i\Delta_{4'5'6'}^{1'2'3'} \cdot \delta \cdot \rho \mathcal{P} \\ &+ i \int \left(T\delta \left(\rho\rho\rho + \underline{\delta\rho\mathcal{P}} + \delta\mathcal{Q} \right. \right. \\ &\left. \left. + \rho\rho\rho\rho + \delta\rho\mathcal{Q} + \delta\mathcal{P}\mathcal{P} + \underline{\underline{\delta\delta\rho\rho\mathcal{P}}} + \mathcal{R} \right) \right) \end{aligned} \quad (3.27)$$

where the most important terms are underlined, and where we introduce

the Hartree-Fock exchange self energy for six operators cumulants as

$$\begin{aligned} \tilde{\Delta}_{4'5'6'}^{1'2'3'} &= \Delta_{4'5'6'}^{1'2'3'} \\ &+ 2 \int d1 n_1 (T_{1'1,11'} + T_{2'1,12'} + T_{3'1,13'} - T_{4'1,14'} - T_{5'1,15'} - T_{6'1,16'}) \end{aligned} \quad (3.28)$$

So the Hartree-Fock self energy for the six operator cumulant will give the frequency renormalization to order ϵ for $\mathcal{Q}_{1'2'3'4'5'6'}$. The underlined terms under integral sign will give resonant growth, which will lead to (3.41).

3.1.4 Long Formulas.

We recommend the reader to skip this section at first reading and go directly to section (3.1.5). Section (3.1.4) contains technical details of derivations.

Formulation of the method We represent solutions to second order in ϵ in the form

$$\begin{aligned} \rho(t) &= n(t, t_2) + \epsilon n^{(1)}(t) + \epsilon^2 n^{(2)}(t) \\ \mathcal{P}_{1234}(t) &= \mathcal{P}_{1234}^{(0)}(t, t_1, t_2) + \epsilon \mathcal{P}_{1234}^{(1)}(t, t_1) + \epsilon^2 \mathcal{P}_{1234}^{(2)}(t) \\ \mathcal{Q}_{123456}(t) &= \mathcal{Q}_{123456}^{(0)}(t, t_1, t_2) + \epsilon \mathcal{Q}_{123456}^{(1)}(t, t_1) + \epsilon^2 \mathcal{Q}_{123456}^{(2)}(t) \end{aligned}$$

where $t_1 = \epsilon t$, $t_2 = \epsilon^2 < t$. So that

$$\frac{d\rho}{dt} = \frac{\partial n}{\partial t} + \epsilon \frac{\partial n^{(1)}}{\partial t} + \epsilon^2 \left(\frac{\partial}{\partial t} n^{(2)} + \frac{\partial n}{\partial t_2} \right)$$

and

$$\begin{aligned} \frac{d\mathcal{P}_{1234}}{dt} &= \frac{\partial \mathcal{P}_{1234}^{(0)}}{\partial t} + \epsilon \left(\frac{\partial \mathcal{P}_{1234}^{(1)}}{\partial t} + \frac{\partial \mathcal{P}_{1234}^{(0)}}{\partial t_1} \right) \\ &+ \epsilon^2 \left(\frac{\partial}{\partial t} \mathcal{P}_{1234}^{(2)} + \frac{\partial}{\partial t_1} \mathcal{P}_{1234}^{(1)} + \frac{\partial}{\partial t_2} \mathcal{P}_{1234}^{(0)} \right), \end{aligned} \quad (3.29)$$

And we can look for solutions in the perturbative manner, order by order. If at some order we get "secular divergence" (linear growth with time) of some

terms, we can choose slower time evolution in such a way, that it removes the secular divergence, if we treat t , t_1 and t_2 as independent variables.

The equations below are somewhat long, and we use short hand notation where possible. By accurately doing all calculations, we know in advance which terms would give secular divergence. We try to emphasize it along the way, so one can distinguish between resonant terms which *are* important and between those, which “are just there”. We try to accurately list all former ones and give the structure of latter ones, by putting dots instead of indices.

Zeroth order

$$\begin{aligned}\frac{d}{dt}n_{k_0} &= 0 \\ \frac{d}{dt}\mathcal{P}_{1'2'3'4'}^{(0)} &= i\Delta_{3'4'}^{1'2'}\mathcal{P}_{1'2'3'4'}^{(0)} \\ \frac{d}{dt}\mathcal{Q}_{1'2'3'4'5'6'}^{(0)} &= i\Delta_{4'5'6'}^{1'2'3'}\delta\mathcal{N}_{1'2'3'4'5'6'}^{(0)}\end{aligned}$$

with the solution

$$\begin{aligned}n_{k_0}(t) &= \text{const} \\ \mathcal{P}_{1'2'3'4'}^{(0)}(t) &= \tilde{\mathcal{P}}_{1'2'3'4'}e^{i\Delta_{3'4'}^{1'2'}t} \\ \mathcal{Q}_{1'2'3'4'5'6'}^{(0)}(t) &= \tilde{\mathcal{Q}}_{1'2'3'4'5'6'}e^{i\Delta_{4'5'6'}^{1'2'3'}t}\end{aligned}\tag{3.30}$$

where $\tilde{\mathcal{P}}_{1'2'3'4'}$, $\tilde{\mathcal{Q}}_{1'2'3'4'5'6'}$ are the initial values of the nonfactorized 2 and 3 particle correlations function.

We got the very natural result - if one neglects the interaction completely, then n_k is a time independent constant, and $\mathcal{P}$, $\mathcal{Q}$'s simply oscillate.

First order Let us write down equations for first order contributions to n_k and $\mathcal{P}$, $\mathcal{Q}$. On the left hand side we have time derivatives from first order

contributions, while to the right hand side we should substitute zeroth order expressions with known time dependence.

$$\begin{aligned}
\frac{d}{dt}n_{k_0}^{(1)} &= 2\text{Im} \int T_{01,23} \mathcal{P}_{0123}^{(0)}(t) \delta_{23}^{01} d123 \\
&= 2\text{Im} \int T_{01,23} \tilde{\mathcal{P}}_{0123}^{(0)} e^{i\Delta_{23}^{01}t} \delta_{23}^{01} d123 \\
\frac{d}{dt}\mathcal{P}_{1'2'3'4'}^{(1)} &= i\Delta_{3'4'}^{1'2'} \mathcal{P}_{1'2'3'4'}^{(1)} \\
&+ 2i\mathcal{P}_{1'2'3'4'}^{(0)} \int d1 (T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1 \\
&- (n_{1'}^{(0)} 2\text{Im} \int d123 T_{2'1,23} \tilde{\mathcal{P}}_{2'123}^{(0)} e^{i\Delta_{23}^{2'1}t} \delta_{23}^{2'1} \\
&+ n_{2'}^{(0)} 2\text{Im} \int d123 T_{1'1,23} \tilde{\mathcal{P}}_{1'123}^{(0)} e^{i\Delta_{23}^{1'1}t} \delta_{23}^{1'1}) \times (\delta_{3'}^{2'} \delta_{4'}^{1'} - \delta_{3'}^{1'} \delta_{4'}^{2'}) + \\
&+ 2iT_{4'3',2'1'} n_3 n_{4'} (1 - n_{2'} - n_{1'}) + 2iT_{4'3',2'1'} n_1 n_{2'} (n_{3'} + n_{4'} - 1) \\
&+ i \int d123 (T_{32,11'} \tilde{\mathcal{P}}_{323'4'}^{(0)} e^{it\Delta_{3'4'}^{32}} \delta_{2'}^1 \delta_{11'}^{32} - T_{4'1,23} \tilde{\mathcal{P}}_{1'2'23}^{(0)} e^{it\Delta_{23}^{1'2'}} \delta_{3'}^1 \delta_{14'}^{32}) \\
&+ i \int (Tn\tilde{\mathcal{P}}e^{it\Delta_{23}^{1'2'}} \delta_{23}^{1'2'}) \\
&+ i \int d123 \left(-T_{32,11'} \tilde{\mathcal{Q}}_{322'13'4'} e^{it\Delta_{13'4'}^{322'}} \delta_{1'}^{321} + T_{32,12'}^* \tilde{\mathcal{Q}}_{1'3213'4'} e^{it\Delta_{13'4'}^{1'32}} \delta_{12'}^{32} \right. \\
&\quad \left. - T_{3'1,23} \tilde{\mathcal{Q}}_{1'2'1234'} e^{it\Delta_{234'}^{1'2'1}} \delta_{13'}^{32} - T_{4'1,23} \tilde{\mathcal{Q}}_{1'2'13'23} e^{it\Delta_{3'23}^{1'2'1}} \right)
\end{aligned} \tag{3.31}$$

Let us integrate these equations over time. Introduce

$$A_t(x) = \int_0^t d\tau \exp[ix\tau]$$

then

$$n_{k_0}^{(1)} = 2\text{Im} \int T_{01,23} \tilde{\mathcal{P}}_{0123}^{(0)} \cdot A_t(\Delta_{23}^{01}) \delta_{23}^{01} d123$$

We already run into problem here - if we integrate (3.31) "as it is" we would have linearly growing terms, coming from its first line. Let us then introduce in $\mathcal{P}^{(0)}$ dependence on $t_1 = \epsilon t$ to remove the linear growth by choosing:

$$\frac{\partial \mathcal{P}_{1'2'3'4'}^{(0)}}{\partial t_1} = \mathcal{P}_{1'2'3'4'}^{(0)} 2i \int d1 ((T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1)$$

with the solution

$$\mathcal{P}_{1'2'3'4'}^{(0)} = \tilde{\mathcal{P}}_{1'2'3'4'}^{(0)} * \exp \left(2i \int d1 ((T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1) t_1 \right) \quad (3.32)$$

which is the frequency shift for $\mathcal{P}_{1'2'3'4'}^{(0)}$. So frequency shift leads to self-consistent change of (3.30) - we know have $\tilde{\Delta}$'s instead of Δ 's with former defined by (3.26,3.28). In a similar way writing equation for second order in ϵ will modify frequency of oscillations in 1st order and, generally, n -th order equations will lead to frequency shift in $n - 1$ order. This is very important observation because we may self-consistently put tilde's everywhere. Integrating (3.31) with respect to t we get

$$\begin{aligned} \mathcal{P}_{1'2'3'4'}^{(1)}(t) &= \mathcal{P}_{1'2'3'4'} e^{it\tilde{\Delta}_{3'4'}^{1'2'}} + \\ &\quad - e^{it\Delta_{3'4'}^{1'2'}} [n_{1'}^{(0)} 2\text{Im} \int d123 T_{2'1,23} \tilde{\mathcal{P}}_{2'123}^{(0)} \mathcal{A}_t(\Delta_{23}^{2'1} - \Delta_{3'4'}^{1'2'}) \delta_{23}^{2'1} \\ &\quad + n_{2'}^{(0)} 2\text{Im} \int d123 T_{1'1,23} \tilde{\mathcal{P}}_{1'123}^{(0)} \mathcal{A}_t(\Delta_{23}^{1'1} - \Delta_{3'4'}^{1'2'}) \delta_{23}^{2'1}] \\ &\quad \cdot (\delta_{3'}^{2'} \delta_{4'}^{1'} - \delta_{3'}^{1'} \delta_{4'}^{2'}) + \\ &\quad + e^{it\tilde{\Delta}_{3'4'}^{1'2'}} (2iT_{4'3',2'1'} n_{3'} n_{4'} (1 - n_{2'} - n_{1'}) \\ &\quad + 2iT_{4'3',2'1'} n_{1'} n_{2'} (n_{3'} + n_{4'} - 1)) \\ &\quad \times \mathcal{A}_t(-\tilde{\Delta}_{3'4'}^{1'2'}) \\ &\quad + ie^{it\Delta_{3'4'}^{1'2'}} \int d123 (T_{32,11'} \tilde{\mathcal{P}}_{323'4'}^{(0)} \mathcal{A}_t(\Delta_{1'2'}^{32}) \delta_{2'}^1 \delta_{11'}^{32} \\ &\quad - T_{4'1,23} \tilde{\mathcal{P}}_{1'2',23}^{(0)} \mathcal{A}_t(\Delta_{23}^{3'4'}) \delta_{3'}^1 \delta_{14'}^{32}) \\ &+ ie^{it\tilde{\Delta}_{3'4'}^{1'2'}} \int d123 \left(-T_{32,11'} \tilde{\mathcal{Q}}_{322'13'4'} \mathcal{A}_t(\Delta_{13'4'}^{322'}) \delta_{11'}^{32} \right. \\ &\quad + T_{32,12'}^* \tilde{\mathcal{Q}}_{1'3213'4'} \mathcal{A}_t(\Delta_{13'4'}^{1'32}) \delta_{12'}^{32} \\ &\quad \left. - T_{3'1,23} \tilde{\mathcal{Q}}_{1'2'1234'} \mathcal{A}_t(\Delta_{234'}^{1'2'1}) \delta_{13'}^{32} - T_{4'1,23} \tilde{\mathcal{Q}}_{1'2'13'23} \mathcal{A}_t(\Delta_{3'23}^{1'2'1}) \right) \\ &\quad + ie^{it\Delta_{3'4'}^{1'2'}} \int d123 (T n \tilde{\mathcal{P}} \mathcal{A}_t(\Delta_{\dots}^{1'2'} - \Delta_{3'4'}^{1'2'}) \delta) \end{aligned} \quad (3.33)$$

The Equation for $\mathcal{Q}_{123456}$ at first order is too long to be shown here, but in complete analogy we get a frequency shift for $\mathcal{Q}_{1'2'3'4'5'6'}^{(0)}$.

Second Order The equation for $n^{(2)}(k)$ is

$$\frac{d}{dt}n_{k_0}^{(2)} = 2\text{Im} \int T_{01,23} \mathcal{P}_{0123}^{(1)}(t) \delta_{23}^{01} d123$$

with $\mathcal{P}_{0123}^{(1)}(t)$ from previous section. To integrate it over time we introduce

$$E(x, y) = \int_0^t A_\tau(x - y) e^{iy\tau} d\tau$$

Then

$$\begin{aligned} n_0^{(2)}(t) = & 2\text{Im} \int T_{01',2'3'} \delta_{2'3'}^{01'} d1'2'3' \times \\ & [\tilde{\mathcal{P}}_{01',2'3'} A_t(\tilde{\Delta}_{2',4'}^{01'}) \\ & - [n_0^{(0)} 2\text{Im} \int T_{1',1,23} \tilde{\mathcal{P}}_{1',123}^{(0)} E_t(\Delta_{23}^{1'1}, \Delta_{2'3'}^{01'}) \delta_{23}^{1'1} \\ & + n_{1'}^{(0)} 2\text{Im} \int T_{01,23} \tilde{\mathcal{P}}_{0123}^{(0)} E_t(\Delta_{23}^{01}, \Delta_{2'3'}^{01'}) \delta_{23}^{1'1}] \cdot (\delta_{2'}^{1'} \delta_{3'}^0 - \delta_{2'}^0 \delta_{3'}^{1'}) + \\ & + E_t(\tilde{\Delta}_{2'3'}^{01'}, 0) (2iT_{3'2',1'0} n_{2'} n_{3'} (1 - n_{1'} - n_0)) \\ & + 2iT_{3'2',1'0} n_0 n_{1'} (n_{2'} + n_{3'} - 1)) \\ & i \int d123 (T_{32,10} \tilde{\mathcal{P}}_{322'3'}^{(0)} E_t(\Delta_{2'3'}^{32}, \Delta_{2'3'}^{01'}) \delta_{1'}^1 \delta_{10}^{32} \\ & - T_{3'1,23} \tilde{\mathcal{P}}_{01'23}^{(0)} E_t(\Delta_{23}^{01'}, \Delta_{1'2'}^{32}) \delta_{2'}^1 \delta_{13'}^{32}) \\ & + i \int d123 (T \tilde{\mathcal{Q}}^{(0)} E_t(\Delta_{\cdot}, \tilde{\Delta}_{2'3'}^{01'}) \delta_{\cdot}) \\ & + i \int d123 (T n \tilde{\mathcal{P}}_{\dots}^{(0)} E_t(\Delta_{\cdot}, \Delta_{2'3'}^{01'}) \delta_{\cdot})] \end{aligned} \quad (3.34)$$

Consider the long time behavior of the above equation. It turns out, that $A_t(x)$ and $E_t(x, y)$ are bounded in the limit of $t \rightarrow \infty$, while

$$E_t(x, 0) \rightarrow^{\rightarrow \infty} (\pi \text{sgn}(t) \delta(x) + iP(\frac{1}{x}))(t - i \frac{\partial}{\partial x})$$

which means that underline terms of (3.34) are unbounded in time. (In the limit $t \rightarrow \infty$ the following is true $E(x, 0) = E(0, x)$.) To remove this unphysical result we introduce $\epsilon^2 t$ dependence in n_{k_0} .

At the limit of the time going to infinity, we have

$$n_{k_0}^{(2)}(t) = (2\text{Im} \int T_{01',2'3'} \delta_{2'3'}^{01'} d1'2'3' \times (\pi \text{sgn}(t) \delta(\Delta_{2'3'}^{01'}) + iP(\frac{1}{\Delta_{2'3'}^{01'}}))(t - i \frac{\partial}{\partial \Delta_{2'3'}^{01'}}) \\ (2iT_{3'2',1'0} n_{2'} n_{3'} (1 - n_{1'} - n_0) + 2iT_{3'2',1'0} n_0 n_{1'} (n_{2'} + n_{3'} - 1))) - \frac{\partial}{\partial t_2} n_{k_0} t$$

Requiring, that these two parts cancel each other, one gets the Kinetic Equation (3.39).

$$\frac{\partial}{\partial t_2} n_0 = (4 \int |T_{01',2'3'}|^2 \delta_{2'3'}^{01'} d1'2'3' \times (\pi \text{sgn}(t) \delta(\Delta_{2'3'}^{01'})) \\ (n_{2'} n_{3'} (1 - n_{1'} - n_0) + n_0 n_{1'} (n_{2'} + n_{3'} - 1)))$$

The equation for $\mathcal{P}^{(2)}$ appears to be quite long:

$$\begin{aligned} \frac{d}{dt_2} \mathcal{P}_{1'2'3'4'}^{(2)} &= i \Delta_{3'4'}^{1'2'} \mathcal{P}_{1'2'3'4'}^{(2)} + \\ &+ 2\mathcal{P}_{1'2'3'4'}^{(1)} \int d1 \left((T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1^{(0)} \right) \\ &+ 2\mathcal{P}_{1'2'3'4'}^{(0)} \int d1 \left((T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1^{(1)} \right) \\ &- [n_{1'}^{(1)} 2\text{Im} \int T_{2'1,23} \tilde{\mathcal{P}}_{2'123}^{(0)} e^{i\Delta_{23}^{2'1} t} \delta_{23}^{2'1} + n_{1'}^{(0)} 2\text{Im} \int T_{2'1,23} \mathcal{P}_{2'123}^{(1)} \delta_{23}^{2'1} \\ &+ n_{2'}^{(1)} 2\text{Im} \int T_{1'1,23} \tilde{\mathcal{P}}_{1'123}^{(0)} e^{i\Delta_{23}^{2'1} t} \delta_{23}^{1'1} + n_{2'}^{(0)} 2\text{Im} \int T_{1'1,23} \mathcal{P}_{1'123}^{(1)} \delta_{23}^{1'1}] \\ &\times (\delta_{3'}^{2'} \delta_{4'}^{1'} - \delta_{3'}^{1'} \delta_{4'}^{2'}) + \\ &+ \left[2iT_{4'3',2'1'} n_{3'}^{(1)} n_{4'} (1 - n_{2'} - n_{1'}) + 2iT_{4'3',2'1'} n_{1'}^{(1)} n_{2'} (n_{3'} + n_{4'} - 1) \right] \\ &+ \left[2iT_{4'3',2'1'} n_{3'} n_{4'}^{(1)} (1 - n_{2'} - n_{1'}) + 2iT_{4'3',2'1'} n_{1'} n_{2'}^{(1)} (n_{3'} + n_{4'} - 1) \right] \\ &+ \left[2iT_{4'3',2'1'} n_{3'} n_{4'} (1 - n_{2'}^{(1)} - n_{1'}^{(1)}) + 2iT_{4'3',2'1'} n_{1'} n_{2'} (n_{3'}^{(1)} + n_{4'}^{(1)} - 1) \right] \\ &+ i \int d123 (T n \tilde{\mathcal{P}}^{(1)} \delta) + \\ &+ i \int d123 (T n^{(1)} \tilde{\mathcal{P}}^{(0)} e^{it\Delta_{123}} \delta) + \\ &+ i \int d123 (T_{32,11'} \tilde{\mathcal{P}}_{323'4'}^{(1)} \delta_{2'}^1 \delta_{11'}^{32} - T_{4'1,23} \tilde{\mathcal{P}}_{1'2'23}^{(1)} \delta_{3'}^1 \delta_{14'}^{32}) \end{aligned}$$

$$\begin{aligned}
& +i \int d123 \left(\underline{\underline{-T_{1'1.23}\delta_{23}^{1'1}Q_{322'13'4'}^{(1)} + T_{2'1.23}\delta_{23}^{2'1}Q_{1'3213'4'}^{(1)}}} \right. \\
& \quad \left. \underline{\underline{-T_{3'1.23}\delta_{23}^{3'1}Q_{1'2'1234'}^{(1)} + T_{4'1.23}\delta_{23}^{4'1}Q_{1'2'13'23}^{(1)}}} \right)
\end{aligned} \tag{3.35}$$

In order to analyze the long-time behavior of the $\mathcal{P}_{1234}^{(2)}$ we have to substitute in RHS of the above equation equations for n , $n^{(1)}$, $\mathcal{P}^{(1)}$ and $\mathcal{Q}^{(1)}$ from previous section. These are rather long but straight-forward calculations. The most difficult is the term, which is underlined twice, because it is the sum of 36 terms, each of them contain equation for $\mathcal{P}^{(1)}$, which is itself term 36 terms long, so that the underlined twice term has 36×36 expressions. By studying their structure, we found that all of them are nonresonant.

By analyzing (3.35) we found that it has some resonant contributions in the first line, giving renormalization of frequency of $\mathcal{P}_{1'2'3'4'}^{(1)}$, so that renormalized frequencies enters the QKE. In addition there are divergences, coming from terms, which are underlined three times. Indeed, if one looks into (3.27) then when factorizing the 8-operator's averages one gets terms like $n, \mathcal{P}, \dots$ and $n, n, \mathcal{P}, \dots$, and some of them will give linear divergence with time. Since we can not write down the equation for $\mathcal{Q}^{(1)}$ because of its huge length, we will write down the equation for $N_{1'3213'4'}^{(1)}$, from which one can reconstruct the equation for $\mathcal{Q}_{1'3213'4'}^{(1)}$ by making appropriate factorizations. Note, that $\mathcal{Q}_{1'3213'4'}^{(1)}$ is the last term on the last line of previous equation.

$$\begin{aligned}
\frac{d}{dt} N_{1'3213'4'}^{(1)} &= i \Delta_{13'4'}^{1'32} N_{1'3213'4'}^{(1)} \\
&+ i \int [\quad T_{jh,g1'} \left(\delta_{g3} N_{jh213'4'}^{(0)} - \delta_{g2} N_{jh313'4'}^{(0)} + N_{jh32g13'4'} \right) \delta_{jh g1'} \\
&\quad + T_{jh,g3} \left(\delta_{g2} N_{1'jh13'4'}^{(0)} - N_{1'jh2g13'4'}^{(0)} \right) \delta_{jh g3} \\
&\quad + T_{jh,g2} \frac{N_{1'3jh g13'4'}^{(0)}}{\delta_{jh g2}} - T_{1g,hj} \frac{N_{1'32g h j3'4'}^{(0)}}{\delta_{1g h j}} \\
&\quad - T_{3'g,hj} \left(\delta_{g1} N_{1'32h j4'}^{(0)} - N_{1'32g1 h j4'}^{(0)} \right) \delta_{3'g h j}]
\end{aligned}$$

$$-T_{4'g,hj} \left(\delta_{g3'} V_{1'321hj}^{(0)} - \delta_{g1} V_{1'323'hj}^{(0)} + V_{1'32g13'hj}^{(0)} \right) \delta_{4'ghj}]$$

Now, if one factorizes the underlined terms in the above equation, one will have, among others, terms like $n\mathcal{P}_{1'2'3'4'}^{(0)}$ and $nn\mathcal{P}_{1'2'3'4'}^{(0)}$. Such terms are resonant, and by correcting these divergences one gets

$$\begin{aligned} \frac{\partial \mathcal{P}_{1'2'3'4'}^{(0)}}{\partial t_2} = & -2\mathcal{P}_{1'2'3'4'}^{(0)} \cdot \int d123 \cdot (n_1 + n_2 n_3 - n_1 n_3 - n_1 n_2) \cdot \\ & \left[|T_{1'1,23}|^2 \delta_{23}^{1'1} F(\tilde{\Delta}_{1'1}^{23}) + |T_{2'1,23}|^2 \delta_{23}^{2'1} F(\tilde{\Delta}_{12'}^{23}) + \right. \\ & \left. |T_{3'1,23}|^2 \delta_{23}^{3'1} F(\tilde{\Delta}_{23}^{3'1}) + |T_{4'1,23}|^2 \delta_{23}^{4'1} F(\tilde{\Delta}_{23}^{4'1}) \right] \end{aligned} \quad (3.36)$$

where we defined

$$F(x) = \left(\pi \delta(x) + iP\left(\frac{1}{x}\right) \right)$$

This is the equation which describes evolution of $\mathcal{P}_{1'2'3'4'}^{(0)}$ on the t_2 time scale (on the t_1 time scale it has a frequency shift (3.32)) and has “quantum” (n) and “classical” (nn) parts. Note, that $\mathcal{Q}_{123456}^{(0)}$ does not enter in QKE (3.39) or in (3.41), therefore our hierarchy is *decoupled*. This is the equation which describes evolution of $\mathcal{P}_{1'2'3'4'}^{(0)}$ on t_2 time scale (on t_1 time scale it has frequency shift (3.32)) In fact, by analogy with classical case (see e.g., [18],[19],[20]) we can assume, that in general, long time evolution of higher order cumulants are defined by the same kind of frequency renormalization.

So the results are given by

$$\begin{aligned}
\frac{\partial \mathcal{P}_{1'2' \dots N}^{(0)}}{\partial t_2} &= i \mathcal{P}_{1'2'3'4'}^{(0)} \cdot \left(\Omega_{1'}^{(2)} + \Omega_{2'}^{(2)} - \Omega_{3'}^{(2)*} - \Omega_{4'}^{(2)*} \right) \\
\frac{\partial \mathcal{Q}_{1'2'3'4'5'6'}^{(0)}}{\partial t_2} &= i \mathcal{Q}_{1'2'3'4'5'6'}^{(0)} \cdot \left(\Omega_{1'}^{(2)} + \Omega_{2'}^{(2)} + \Omega_{3'}^{(2)} - \Omega_{4'}^{(2)*} - \Omega_{5'}^{(2)*} - \Omega_{6'}^{(2)*} \right) \\
\frac{\partial \mathcal{R}_{1'2'3'4'5'6'7'8'}^{(0)}}{\partial t_2} &= i \mathcal{R}_{1'2'3'4'5'6'7'8'}^{(0)} \cdot \\
&\quad \times \left(\Omega_{1'}^{(2)} + \Omega_{2'}^{(2)} + \Omega_{3'}^{(2)} + \Omega_{4'}^{(2)} \right. \\
&\quad \left. - \Omega_{5'}^{(2)*} - \Omega_{6'}^{(2)*} - \Omega_{7'}^{(2)*} - \Omega_{8'}^{(2)*} \right)
\end{aligned} \tag{3.37}$$

where

$$\begin{aligned}
\Omega_{k'}^{(2)} &= 2 \int d123 (n_1 + n_2 n_3 - n_1 n_3 - n_1 n_2) T_{k'123}^2 \delta_{23}^{k'1} \\
&\quad \times \left(P\left(\frac{1}{\tilde{\Delta}_{23}^{k'1}}\right) + i\pi \text{sgn}(t) \delta(\tilde{\Delta}_{23}^{k'1}) \right).
\end{aligned} \tag{3.38}$$

3.1.5 Results.

Let us summarize the results: The quantum kinetic equation is given by

$$\begin{aligned}
\frac{\partial}{\partial t} n_k &\equiv \epsilon^2 F_2^{(2)} = (4\epsilon^2 \int |T_{01',2'3'}|^2 \delta_{2'3'}^{01'} d1'2'3' \times (\pi \text{sgn}(t) \delta(\tilde{\Delta}_{2'3'}^{01'})) \\
&\quad \times (n_{2'} n_{3'} (1 - n_{1'} - n_k) + n_k n_{1'} (n_{2'} + n_{3'} - 1))).
\end{aligned} \tag{3.39}$$

where the Hartree Fock self-energy is

$$\tilde{\Delta}_{3'4'}^{1'2'} = \omega_{1'} + \omega_{2'} - \omega_{3'} - \omega_{4'} + 2 \int d1 ((T_{1'1,11'} + T_{2'1,12'} - T_{3'1,13'} - T_{4'1,14'}) n_1).$$

From the form of (3.39), it is clear that number density is redistributed by binary particle collisions which satisfy momentum and energy conservation. In particular, exchange of particle number (momenta, energy) is associated with particles whose momenta and energies lie on the resonant manifold defined to a good approximation by

$$\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4 = 0, \quad \omega_{k_1} + \omega_{k_2} - \omega_{k_3} - \omega_{k_4} = 0. \quad (3.40)$$

The evolution equation for $Q_{1'2'\dots N}^{(0)}$ can be written

$$\begin{aligned} \frac{\partial \ln Q_{12\dots N}^{(0)}}{\partial t} &= i \left(\sum_{i=1}^{N/2} \Omega_i - \sum_{i=N/2+1}^N \Omega_i^* \right), \\ \Omega_{k'} &= \omega_{k'} + 2\epsilon \int d1 n_1 T_{1'1,11'} \\ &\quad + 2\epsilon^2 \int d123 (n_1 + n_2 n_3 - n_1 n_3 - n_1 n_2) T_{k'123}^2 \delta_{23}^{k'1} \\ &\quad \times \left(P\left(\frac{1}{\tilde{\Delta}_{23}^{k'1}}\right) + i\pi \text{sgn}(t) \delta(\tilde{\Delta}_{23}^{k'1}) \right) \end{aligned} \quad (3.41)$$

which can be interpreted as a complex frequency renormalization.

We can calculate the sign of $\text{Im}\Omega$ once n_k reaches its steady (equilibrium) state. For steady state $\dot{n}_k = 0$ we rewrite the QKE (3.39) as

$$\begin{aligned} &\int |T_{01',2'3'}|^2 \delta_{2'3'}^{01'} d1'2'3' \times (\pi \text{sgn}(t) \delta(\tilde{\Delta}_{2'3'}^{01'})) \\ &\quad \times (n_{2'} n_{3'} - n_{1'} n_{2'} - n_{1'} n_{3'} + n_{1'}) \\ &= \\ &\frac{1}{n_k} \int |T_{01',2'3'}|^2 \delta_{2'3'}^{01'} d1'2'3' \times (\pi \text{sgn}(t) \delta(\tilde{\Delta}_{2'3'}^{01'})) \\ &\quad \times (n_{2'} n_{3'} (1 - n_{1'})) \geq 0. \end{aligned} \quad (3.42)$$

The LHS of the above equation is the imaginary part of Ω_k . Observe that, because $\text{Im}\Omega_k \geq 0$, the leading order approximations to the N^{th} ($N \geq 2$)

order cumulant decays with time. This means that the memory of (smooth) initial states is gradually forgotten.

Time irreversibility. We want to make two very important points which are often overlooked. While the leading order contributions (which at $t = 0$ is the initial state multiplied by an oscillatory factor) to the N^{th} order cumulants for $N > 2$ play no role in the long time behavior of the system and indeed slowly decay, higher order (in ϵ) contributions do not disappear in the long time limit. The system retains a weakly non Gaussian character which is responsible for and essential for particle number and energy transfer. For example, in the long time limit, the order ϵ fourth order cumulant has a quasi stationary contribution (the terms with higher order cumulants asymptote to zero by means of phase mixing and the Riemann-Lebesgue lemma)

$$\begin{aligned} & \mathcal{P}_{1'2'3'4'}^{(1)}(t) \\ &= 2iT_{4'3',2'1'}(n_{3'}n_{4'}(1 - n_{2'} - n_{1'}) + n_{1'}n_{2'}(n_{3'} + n_{4'} - 1)) \times A_t(\tilde{\Delta}_{3'4'}^{1'2'}) \end{aligned}$$

where

$$A_t(x) = \int_0^t d\tau \exp[ix\tau].$$

Because $\lim_{t \rightarrow \infty} A_t(x) = \pi \text{sgn} t \cdot \delta(x) + iP(\frac{1}{x})$, in the limit $t \rightarrow \infty$,

$$\begin{aligned} \mathcal{P}_{1'2'3'4'}^{(1)}(t) \rightarrow & 2iT_{4'3',2'1'}(n_{3'}n_{4'}(1 - n_{2'} - n_{1'}) + n_{1'}n_{2'}(n_{3'} + n_{4'} - 1)) \\ & \times \left(\pi \text{sgn} t \cdot \delta(\tilde{\Delta}_{3'4'}^{1'2'}) + iP(\frac{1}{\tilde{\Delta}_{3'4'}^{1'2'}}) \right). \end{aligned}$$

Thus, in the long time limit, the order ϵ contribution $\mathcal{P}_{1234}^{(1)}$ to the fourth order cumulant is not smooth but is given by a sum of generalized functions represented by the Dirac delta function and the Cauchy Principal value.

We may therefore legitimately ask: in what sense is the asymptotic series (3.20,3.21) well ordered if it contains terms which are products of powers of ϵ with generalized functions? The answer is that to analyze properly the asymptotic behavior of the system, we must always revert to physical space and look at the corresponding asymptotic expansion for the cumulants $\{\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}'')\psi(\mathbf{r}''')\}$ connected with fourth order expectation values of the field operators. These objects, which decay to zero as the separations $\mathbf{r}' - \mathbf{r}$, $\mathbf{r}'' - \mathbf{r}$, $\mathbf{r}''' - \mathbf{r}$ tend to infinity, are simply the Fourier transform of $\mathcal{P}_{kk'k''k'''}.$ We can also show that no terms worse than single delta functions occur (or products of delta functions which have their support on different resonant submanifolds) at later powers of ϵ so that the resulting asymptotic expansion for the spatial cumulants is indeed well ordered.

The second important point concerns the reversibility or rather the retraceability of solutions of (3.39,3.41). In the derivation of (3.39,3.41), we assumed that the initial cumulants were sufficiently smooth so that integrals over momentum space of multiplications of the initial values of Q_N by $\exp(-i(\omega_1 + \dots - \omega_N)t)$ tend to zero in the asymptotic limit. However, it is clear from (3.41) that the regenerated cumulants have terms of higher order in ϵ which are not smooth and indeed have their (singular) support precisely on the resonant manifold which is the exponent of the oscillatory exponential. What would happen, then, if one were to redo the initial value problem from a later time $t_1 = O(\epsilon^{-2})$, either positive or negative, after which the fourth order cumulant had developed a nonsmooth part? On the surface, it would seem that the sgn term in (3.41) would be $\text{sgn}(t - t_1)$ so that, at every time t_1 , there would be a discontinuity in the slope of $n_k(t)$. But that is not the case. If one accounts for the nonsmooth behavior (3.41) in the new initial value for $\mathcal{P}_{1234}^{(1)}$, then one gets additional terms in (3.41) which give exactly

the same collision integral but with the factor $(\text{sgn} t - \text{sgn}(t - t_1))$. Adding the two contributions, we find the QKE is exactly the same as the one derived beginning at $t = 0$. It is not that the point $t = 0$ is so special. Rather, there is a range of times t , $-\epsilon^{-2} \ll \omega_{k_0} t \ll \epsilon^{-2}$ such that, if one begins anywhere within this range, an initially smooth distribution stays smooth. But once the limit $t \rightarrow \infty$, $\epsilon^2 t$ finite, is taken, an irreversibility and nonsmoothness in the cumulants is introduced.

In a very real sense, then, the infinite dimensional Hamiltonian system acts as if there is an attracting manifold (an inertial or generalized center manifold in the modern vernacular) in its phase space to which the system relaxes as $\omega_{k_0} t \rightarrow O(\epsilon^{-2})$ (in either time direction) on which the slow dynamics is given by the closure equations (3.39),(3.41). On this attracting manifold, the higher order cumulants are essentially slaved to the particle number density and their frequencies are renormalized by contributions which also depends on particle number density. The attenuation in this case is due to losses to the heat bath consisting of all momenta which do not lie on a resonance manifold associated with $\mathbf{k}$.

3.2 Analysis of the Kinetic Equation.

3.2.1 Conservation Laws, Thermodynamic and Finite-Flux solutions of the Kinetic Equation.

The collision integral in (3.39) has the following constants of motion

$$\mathcal{N} = \frac{V}{(2\pi)^d} \int d\mathbf{k} n_{\mathbf{k}}, \quad \mathbf{P} = \frac{V}{(2\pi)^d} \int \hbar \mathbf{k} d\mathbf{k} n_{\mathbf{k}}, \quad \mathcal{E} = \frac{V}{(2\pi)^d} \int \frac{\hbar^2 |\vec{k}|^2}{2m} d\mathbf{k} n_{\mathbf{k}}, \quad (3.43)$$

which can be identified as number of particles, momentum and kinetic energy. In a spatially homogeneous systems, $\mathbf{P} = 0$ so that the only relevant

constants of motion are $\mathcal{N}$ and $\mathcal{E}$.

In this article we will be dealing with the isotropic case only, and, for simplicity, neglect the spin degree of freedom. Therefore we simplify the collision integral by averaging it over all angles. First, we change variables from particles momentum $\mathbf{k}$ to the particle kinetic energy

$$\epsilon_k = \hbar\omega_k = \frac{\hbar^2 k^2}{2m}, \quad (3.44)$$

where m is the coefficient of proportionality between ω_k and $\hbar k^2/2$, and can be associated with (effective) mass of the interacting particles.

We introduce $n_\omega = n(\mathbf{k}(\omega))$ and rewrite the kinetic equation as

$$\begin{aligned} \dot{n}_\omega = \frac{1}{\Omega_0 k^{d-1} (dk/d\omega)} \times & \int_{\omega_i > 0, i=1,2,3} \int \int \mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) S_{\omega\omega_1\omega_2\omega_3} \\ & \times \delta(\omega + \omega_1 - \omega_2 - \omega_3) d\omega_1 d\omega_2 d\omega_3 \end{aligned} \quad (3.45)$$

where $S_{\omega\omega_1\omega_2\omega_3}$ is the angle-averaged potential,

$$\begin{aligned} S_{\omega\omega_1\omega_2\omega_3} &= 4\pi\Omega_0 (kk_1k_2k_3)^{(d-1)} \frac{dk}{d\omega} \frac{dk_1}{d\omega_1} \frac{dk_2}{d\omega_2} \frac{dk_3}{d\omega_3} \\ &\times \langle |T_{k k_1, k_2 k_3}|^2 \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \rangle. \end{aligned} \quad (3.46)$$

The brackets $\langle .. \rangle$ denote averages over unit spheres (including the $\frac{V}{(2\pi)^d}$ factors) in $\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$ space (i.e., we have integrated over all angular contributions) and Ω_0 is the surface area of the unit sphere in d dimensions. Although in our case $d = 3$, we want to stress with the above notation the results can easily be extended to other dimensions, for example to $d = 2$ which is appropriate for the description of semiconductor quantum wells. $\mathcal{K}$ is the kernel of the kinetic equation, which for the quantum (fermionic),

quantum (bosonic) and classical cases is given respectively by (see (3.39) for fermionic case):

$$\begin{aligned}
\mathcal{K}^{\text{fermionic}}(\omega, \omega_1, \omega_2, \omega_3) &= n_{\omega_2} n_{\omega_3} (1 - n_{\omega_1}) (1 - n_{\omega}) - n_{\omega} n_{\omega_1} (1 - n_{\omega_2}) (1 - n_{\omega_3}), \\
\mathcal{K}^{\text{bosonic}}(\omega, \omega_1, \omega_2, \omega_3) &= (n_{\omega_2} n_{\omega_3} (n_{\omega} + n_{\omega_1} + 1) - n_{\omega} n_{\omega_1} (n_{\omega_2} + n_{\omega_3} + 1)), \\
\mathcal{K}^{\text{classical}}(\omega, \omega_1, \omega_2, \omega_3) &= (n_{\omega_2} n_{\omega_3} (n_{\omega} + n_{\omega_1}) - n_{\omega} n_{\omega_1} (n_{\omega_2} + n_{\omega_3})).
\end{aligned}
\tag{3.47}$$

We then introduce the particle density per frequency

$$\dot{N}_{\omega} = \Omega_0 k^{d-1} (dk/d\omega) n_{\omega}$$

so that $\int \dot{N}_{\omega} d\omega = \int n_k d\mathbf{k}$ and

$$\dot{N}_{\omega} = \int_{\omega_1, \omega_2, \omega_3 > 0} \int \int \mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) \times S_{\omega\omega_1\omega_2\omega_3} \delta(\omega + \omega_1 - \omega_2 - \omega_3) d\omega_1 d\omega_2 d\omega_3.
\tag{3.48}$$

One class of steady (equilibrium) solutions of the KE corresponds to the thermal equilibrium. For fermionic systems, it is given by the Fermi Dirac (FD) distribution, and for bosonic systems it is given by the Bose-Einstein distribution.

$$n_k = \frac{1}{\exp(\beta(\epsilon_k - \mu)) \pm 1}
\tag{3.49}$$

where the plus sign corresponds to the fermion case and the minus sign to the bosonic case. μ is the chemical potential and β is the inverse temperature in energy units. The classical analogue of the quantum thermal equilibrium distribution is given by the Rayleigh-Jeans distribution

$$n(k) = T/(\mu + \epsilon_k).
\tag{3.50}$$

It is easy to check that the solutions (3.49,3.50) make the integrand in (3.45,3.48) exactly zero in all three cases.

However, the thermodynamic equilibrium is not the most general steady (equilibrium) solution of the kinetic equation and indeed in some cases has little relevance. The solutions we are most interested in are those which describe the steady state reached *between* ranges of frequencies where particles and energy are added to or removed from the system (these regions, where there is no pumping or damping, are called "windows of transparency" or "inertial ranges"). In particular, we have in mind the following situation. Particles and energy are added to the system in a narrow range of intermediate frequencies about ω_0 . Particles and energy are drained from the system in a ranges of frequencies about $\omega < \omega_L < \omega_0$ and for $\omega > \omega_R > \omega_0$. Because of conservation of energy and particles in the inertial ranges between ω_L and ω_0 and between ω_0 and ω_R where there is no pumping or damping and because the relations between particle number N_ω and energy density $E_\omega = \omega N_\omega$, we will find that a net flux of energy to the higher frequencies must be accompanied by a net flux of particles to lower frequencies as it might be expected by analogy with classical wave turbulence (see e.g. [2]). The presence of sources and sinks drives the system away from the thermodynamic equilibrium. Therefore, in the windows of transparency, $\omega_L < \omega < \omega_0$ and $\omega_0 < \omega < \omega_R$, the system can also relax to equilibrium distributions corresponding to a finite flux of particles and energy flowing through these windows from the sources to the sinks. These are the new solutions of the QKE. The number of such finite flux solutions corresponds to the number of conserved densities (here two, n_k and $\omega_k n_k$, or N_ω and ωN_ω) of the QKE.

To demonstrate the existence of such solutions, we rewrite the KE in the

following form:

$$\begin{aligned}\dot{N}_\omega &= \frac{\partial^2}{\partial \omega^2} \mathcal{W}[n_\omega], \\ \mathcal{W}[n_\omega] &= \int \int \int_{\Omega} (\omega + \omega_1 - \omega_2 - \omega_3) \\ &\quad \times K_{\omega_2 + \omega_3 - \omega, \omega_2, \omega_3} S_{\omega_2 + \omega_3 - \omega, \omega_2, \omega_3} d\omega_1 d\omega_2 d\omega_3,\end{aligned}\tag{3.51}$$

where the integration is over the region $\Omega\{\omega_1, \omega_2, \omega_3 > 0 \mid \omega_1 < \omega_2 + \omega_3 < \omega + \omega_1\}$. This expression can be checked by direct differentiation.

The relevant kinetic equation, which includes the presence of sources and sinks is

$$\frac{\partial N_\omega}{\partial t} = \frac{\partial^2}{\partial \omega^2} \mathcal{W}[n_\omega] + F_\omega - D_\omega,\tag{3.52}$$

where we think of F_ω as having its support near $\omega = \omega_0$ and D_ω its support below ω_L and above ω_R . We ask if (3.52) leads to a steady (equilibrium) solutions in the transparency regions $\omega_L < \omega < \omega_0$ and $\omega_0 < \omega < \omega_R$ where $F_\omega = D_\omega = 0$ corresponding to a finite flux of particles and energy across these windows. One can readily associate the quantities ⁴:

$$Q = \frac{\partial \mathcal{W}}{\partial \omega}, \quad \frac{\partial N_\omega}{\partial t} = \frac{\partial Q}{\partial \omega},$$

and

$$P = \mathcal{W} - \omega \frac{\partial \mathcal{W}}{\partial \omega}, \quad \frac{\partial \omega N_\omega}{\partial t} = -\frac{\partial P}{\partial \omega},\tag{3.53}$$

with the fluxes P and Q of particles N_ω and energy $E_\omega = \omega N_\omega$. Q and P are taken positive if leftward and rightward flowing respectively. In the windows

⁴If, as in the case of semiconductor laser, we take $\frac{E}{\hbar} = (\epsilon_{gap} + \omega)N_\omega$, then the energy flux becomes

$$P = \mathcal{W} - \omega \frac{\partial \mathcal{W}}{\partial \omega} - \frac{\epsilon_{gap}}{\hbar} \frac{\partial \mathcal{W}}{\partial \omega} = \mathcal{W} - \omega \frac{\partial \mathcal{W}}{\partial \omega} - \frac{\epsilon_{gap}}{\hbar} Q.$$

See section (4.5) for more details.

of transparency, we look for solutions for which N_ω is constant in time and then (3.51) integrates to

$$\mathcal{W} = Q\omega + P \quad (3.54)$$

where Q and P are constants. The two parameter family of thermodynamic solutions, parametrized by T and μ is given by solving the homogeneous equation $\mathcal{W} = 0$ for which $P = Q = 0$. Therefore, the thermodynamic solutions carry no fluxes of particles or energy. A more general⁵ steady (equilibrium) solution to (3.51) therefore is the four-parameter family

$$n_\omega = n_\omega(T, \mu, P, Q). \quad (3.55)$$

We are particularly interested in the solutions for which Q_0 particles per unit time and $\omega_0 Q_0$ units of energy per unit time are fed to the system in a narrow frequency window about $\omega = \omega_0$. We will assume that the flux of particles passing through the left (right) window $\omega_L < \omega < \omega_0$ ($\omega_0 < \omega < \omega_R$) is Q_L (Q_R) and the flux of energy through the right (left) window is P_R (P_L). We will also assume that the sinks consume all the particles and energy that reach them. Then (see Figure 3.1)⁶

⁵We purposely do not say "the most general solutions", as there may be some hidden symmetries of the QKE which generate more conserved quantities and thus more general solutions, corresponding to fluxes of those quantities. The statement that the general KE with M conserved quantities has "a most general solution" depending on $2M$ parameters, is also not proven yet for the general collision integral. Remember also that we are considering the isotropic case. This is, of course, an idealization, and generally "drift" solutions may be of equal importance.

⁶For the case of semiconductors, P_L , P_0 and P_R will have certain contributions coming from the fact that the conduction band is separated by an energy gap from the valence band. On purpose we do not include ϵ_{gap} into consideration in this Chapter. See section (4.5) for more details. There (4.37) generalizes (3.56) for semiconductors.

$$\begin{aligned}
Q_L - Q_R &= Q_0 \\
P_R - P_L &= \omega_0 Q_0 \\
P_L &= -\omega_L Q_L \\
Q_R &= -\frac{1}{\omega_R} P_R.
\end{aligned}
\tag{3.56}$$

The first two relations in (3.56) express conservation of particles and energy. The second two express the fact that, in order to maintain equilibrium, the rate of particle destruction at ω_R is the rate of energy destroyed there divided by the energy per particle. Likewise the amount of energy destroyed at ω_L (which absorption, in the context of application discussed in the section 5, will be due to semiconductor lasing) must be ω_L times the number of particles absorbed there. Solving (3.56) we obtain

$$\begin{aligned}
Q_L &= Q_0(\omega_R - \omega_0)/(\omega_R - \omega_L), \\
Q_R &= -Q_0(\omega_0 - \omega_L)/(\omega_R - \omega_L), \\
P_R &= Q_0\omega_R(\omega_0 - \omega_L)/(\omega_R - \omega_L) \\
P_L &= -\omega_L Q_0(\omega_R - \omega_0)/(\omega_R - \omega_L).
\end{aligned}
\tag{3.57}$$

This is very important result - the magnitude of the left/right fluxes depend only on the amount of particles being put in and on the geometry of the problem (i.e. values of ω_L , ω_0 , ω_R). We verify this important result numerically in section (3.3.5) after introducing the differential approximation to the collision integral.

FIGURE 3.1. Setup for input-output fluxes.

Carriers and energy are added at ω_0 at rates Q_0 and $P_0 = \omega_0 Q_0$ respectively. Energy and some carriers are dissipated at $\omega_R > \omega_0$ (an idealization) and carriers and some energy are absorbed by the laser at ω_L . Finite flux stationary solutions are realized in the windows (ω_L, ω_0) and (ω_0, ω_R) although in practice there will be some losses through both of these regions. Energy flux P is defined to be positive if flowing rightwards, so $P_L < 0$ and $P_R > 0$. Particle flux is defined to be positive if flowing leftwards, so $Q_L > 0$ and $Q_R < 0$.

We see from (3.57) that for $\omega_L \ll \omega_0 \ll \omega_R$, $|Q_R| \ll Q_L \simeq Q_0$, $|P_L| \ll P_R \simeq \omega_0 Q_0$ so that the solutions are almost pure Kolmogorov in the sense that almost all energy flows to ω_R and almost all particles flow to ω_L . However, it is important to stress that in the left window, (3.54) becomes

$$\mathcal{W} = Q_L(\omega - \omega_L) \quad (3.58)$$

and in the right window

$$\mathcal{W} = P_R(1 - \frac{\omega}{\omega_R}) \quad (3.59)$$

so that the right hand sides vanish if the frequency approaches the sink value. This aids convergence in these windows.

Solutions to (3.58), (3.59) have not been investigated even in the classical case. In the classical case, Zakharov (see, e.g., [27],[28]) has found the pure Kolmogorov solutions $T = \mu = P = 0$, $T = \mu = Q = 0$ which turns out to have power law behavior $n_\omega = c\omega^{-x}$. Likewise, in the bosonic case, several authors have attempted to find power law solutions which essentially balance the quadratic terms in $\mathcal{W}^{\text{bosonic}}$ with a finite energy flux. However, in the differential approximation, there are no power law solutions.

In many cases it may be that whenever $\omega_R \gg \omega_0$, ω_L may not be all that much smaller than ω_0 . In particular, in order to exploit these solutions in the context of semiconductor lasers, it is advantageous to have ω_0 close enough to ω_L to minimize energy losses (the ratio $P_R/|P_L| = \omega_R(\omega_0 - \omega_L)/(\omega_L(\omega_R - \omega_0))$) but far enough away to force all part of the spectrum to take part in laser action and to facilitate possible pumping decrease due to Pauli blocking. We return to this application after introducing an enormous simplification for $\mathcal{W}$ which gives a very good qualitative description of the collision integral.

3.2.2 Time Flow Theorem - QKE

Assume, that $n_{\mathbf{k},t=t_0}$ is given for time $t = t_0$ and that $0 \leq n_{\mathbf{k},t=t_0} \leq 1$ - i.e. the values which function n can have "physically". Then, if time evolution of $n_{\mathbf{k}}$ is given by (3.39) then $0 \leq n_{\mathbf{k},t} \leq 1$ for all later times.

Proof. Note that KE equation (3.39) is invariant under the following transformation $n_{\mathbf{k}} \rightarrow 1 - n_{\mathbf{k}}$.

Let us assume the "worst case scenario" - that distribution function $n_{\mathbf{k}}$ simultaneously hits values 0 in a number of points, which belongs to set

$$A = \{\vec{k}_j, n_{\vec{k}_j} = 0, j = 1 \dots N\}$$

and hit value 1 in a number of points which belongs to set

$$B = \{\vec{k}_i, n_{\vec{k}_i} = 1, i = 1 \dots M\}.$$

Then for any of the point from set A the following is true (see (3.39))

$$\begin{aligned} \frac{\partial}{\partial t} n_{\vec{k}_j} = & (\epsilon^2 4 \int |T_{\mathbf{k}_j, 1' 2' 3'}|^2 \delta_{2' 3'}^{\vec{k}_j 1'} d1' 2' 3' \times (\pi \text{sgn}(t) \delta(\vec{\Delta}_{2' 3'}^{\vec{k}_j 1'})) \\ & \times (n_{2'} n_{3'} (1 - n_{1'}))) \geq 0, \end{aligned} \quad (3.60)$$

because $0 \leq n_{\vec{k},t} \leq 1$ for all $\vec{k}$. Therefore $n_{\mathbf{k},j}$ can only grow or stay the same at $k \in A$, so that $n_{\vec{k}}$ can not acquire negative values. For any point from set B following the same kind of arguments we get

$$\frac{\partial}{\partial t} n_{\mathbf{k},j \in B} \leq 0,$$

so that $n_{\mathbf{k}}$ can not go above one. Instead of the second part of the proof, we may make $\tilde{n}_{\vec{k}} = 1 - n_{\vec{k}}$ transformation and use first part of the proof.

3.2.3 Entropy, Entropy Production and h-Theorem

The entropy of non-equilibrium Fermionic system may be defined as (see. e.g. [29])

$$\mathcal{S} = - \int d\mathbf{k} (n_{\mathbf{k}} \log n_{\mathbf{k}} + (1 - n_{\mathbf{k}}) \log(1 - n_{\mathbf{k}})) \quad (3.61)$$

which is simply the entropy of an ideal fermion gas. This quantity is well defined for FD distribution function. The rate of change of this quantity is

$$\dot{\mathcal{S}} = \int d\mathbf{k} \dot{n}_{\mathbf{k}} \log\left(\frac{1 - n_{\mathbf{k}}}{n_{\mathbf{k}}}\right) \quad (3.62)$$

and is always well defined. Let us change variables to ω

$$\dot{\mathcal{S}} = \int d\omega \Omega_0 k^{d-1} \frac{dk}{d\omega} \dot{n}_{\omega} \log\left(\frac{1 - n_{\omega}}{n_{\omega}}\right) \quad (3.63)$$

Substituting for $\dot{n}_{\mathbf{k}}$ (3.52) with collision integral given by (3.45) and denoting pumping/damping terms by $\Gamma(n_{\omega})$ we get

$$\begin{aligned} \dot{\mathcal{S}} = \frac{1}{4} \int d\omega_1 d\omega_2 d\omega_3 d\omega_4 \delta(\omega + \omega_1 - \omega_2 - \omega_3) S_{\omega\omega_1\omega_2\omega_3} & \left((x - y) \log\left(\frac{x}{y}\right) \right) \\ & + \int d\omega \Gamma(n_{\omega}) \log\left(\frac{1 - n_{\omega}}{n_{\omega}}\right), \end{aligned} \quad (3.64)$$

where we used a shortcut $x = n_0 n_1 (1 - n_2)(1 - n_3)$ and $y = n_2 n_3 (1 - n_0)(1 - n_1)$ and we symmetrise the integrand. Keeping in mind, that $(x - y) \log(\frac{x}{y}) \geq 0$ one gets the Boltzmann H-theorem.

3.2.4 Summary of QKE properties.

Below we summarize the properties of the quantum kinetic equations, which are important for our discussion:

- Total number of particles and kinetic energy are conserved quantities,

- There exist a thermodynamics solution given by a Fermi-Dirac distribution function
- Any distribution reaches thermodynamic equilibrium distribution, if there is no forcing to the system;
- The Boltzmann H-theorem is satisfied - the value of the entropy is increasing or stays the same. Note that the maximum of the entropy corresponds to thermodynamical equilibrium (proof is too simple to include here, see e.g. [29]).
- If there is a "forcing" to the system, than finite flux solutions are realized. Furthermore, if the forcing is local in k space then the values of the fluxes are *constant* in the inertial regions:
- The distribution function "physically" must be between zero and one. Then, if time evolution of $n_{\mathbf{k}}$ is given by (3.39) then $0 \leq n_{\mathbf{k},t} \leq 1$ for all times:
- The equation are symmetric with respect to $n_{\omega} \rightarrow 1 - n_{\omega}$ transformation.

3.3 Differential Kinetic Equation

3.3.1 Derivation of Differential Kinetic Equation

To simplify our analysis, we use an approximation to the kinetic equation known as the differential approximation (see, e.g., [17], [21], [30]). The differential quantum kinetic equation (DQKE) gives qualitatively correct behavior in general, but is strictly valid only when the particle and energy transfer

happens primarily between neighbors in momentum space. It is easy to verify that it has a four-parameter-family of a steady (equilibrium) solutions and it is easy to identify two of these parameters as fluxes of energy and particle number density and the other two as temperature and chemical potential. The analytical expressions for the fluxes can be calculated so that, for any given distribution, the corresponding fluxes may be easily computed numerically. The steady (equilibrium) solutions can be found analytically in various limits. The DQKE is much more suitable for numerical experiments than the full collision integral, simply because it is easier and faster to compute derivatives than integrals of the collision type.

We now demonstrate the derivation of the differential approximation in the fermion case. This result is new. The results for the cases of classical waves and bosonic systems are discussed in (3.78). Assume that $S_{\omega\omega_1\omega_2\omega_3}$ is dominated by its contribution from the region $\omega \simeq \omega_1 \simeq \omega_2 \simeq \omega_3$. For example we may take

$$\begin{aligned}
 S_{\omega,\omega_1,\omega_2,\omega_3} &= \tilde{\omega}^\gamma \exp \left(((\omega - \omega_1)^2 + (\omega - \omega_2)^2 + (\omega - \omega_3)^2 + (\omega_1 - \omega_2)^2 \right. \\
 &\quad \left. + (\omega_1 - \omega_3)^2 + (\omega_2 - \omega_3)^2) / \tilde{\omega}^2 \right) \\
 \tilde{\omega} &\equiv (\omega\omega_1\omega_2\omega_3)^{\frac{1}{4}}.
 \end{aligned} \tag{3.65}$$

We call such a coupling coefficient “strongly diagonal”. Then obviously the integrand of the QKE deviates significantly from zero in the same region. The first derivation of the differential kinetic equation proceeds as follows (see, e.g., [30]). Multiply both sides of (3.48) a by sufficiently smooth function $\Phi(\omega)$ and integrate with respect to ω :

$$\begin{aligned}
 \int \dot{N}_\omega \Phi(\omega) d\omega &= \int \int \int \mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) \\
 &\quad \times S_{\omega,\omega_1,\omega_2,\omega_3} \delta(\omega + \omega_1 - \omega_2 - \omega_3) \Phi(\omega) d\omega d\omega_1 d\omega_2 d\omega_3
 \end{aligned} \tag{3.66}$$

Symmetrise the RHS of Eqs. (3.66) to get

$$\begin{aligned} \int \dot{N}_\omega \Phi(\omega) d\omega &= \int \int \int \mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) \times S_{\omega, \omega_1, \omega_2, \omega_3} \delta(\omega + \omega_1 - \omega_2 - \omega_3) \\ &\quad \times \frac{1}{4} (\Phi(\omega) + \Phi(\omega_1) - \Phi(\omega_2) - \Phi(\omega_3)) d\omega d\omega_1 d\omega_2 d\omega_3 \end{aligned} \quad (3.67)$$

To do this we use the symmetries of the kernel of the collision integral responsible for particle number and energy conservation⁷. Now make a change of variables $\omega_i = \omega + \Delta_i$, $i = 1, 2, 3$ and expand Φ in the Taylor series with respect to Δ_i around ω . The first nonzero term in the expansion contains the second derivative $\Phi''(\omega)$:

$$\begin{aligned} \Phi(\omega) + \Phi(\omega + \Delta_1) - \Phi(\omega + \Delta_2) &- \Phi(\omega + \Delta_1 - \Delta_2) \\ &= (\Delta_1 - \Delta_2) \Delta_2 \Phi''(\omega) + O(\Delta^2) \end{aligned} \quad (3.68)$$

We also expand $n_{\omega_i} = n_\omega + \Delta_i n'_\omega + \Delta_i^2 / 2 n''_\omega$ in the kernel $\mathcal{K}^{\text{fermionic}}(\omega, \omega_1, \omega_2, \omega_3)$ of the kinetic equation,

$$\begin{aligned} \mathcal{K}^{\text{fermionic}}(\omega, \omega + \Delta_1, \omega + \Delta_2, \omega + \Delta_1 - \Delta_2) \\ = (\Delta_1 - \Delta_2) \Delta_2 (n_\omega'^2 (1 - 2n_\omega) + n_\omega n_\omega'' (n_\omega - 1)) \end{aligned} \quad (3.69)$$

We then substitute (3.68) and (3.69) to (3.67), integrate by parts the $\Phi''(\omega)$ term to get

$$\begin{aligned} \int d\omega \Phi(\omega) \left[\dot{N}_\omega - \frac{\partial^2}{\partial \omega^2} (n_\omega'^2 (1 - 2n_\omega) + n_\omega n_\omega'' (n_\omega - 1)) \right. \\ \left. \times \int d\Delta_1 d\Delta_2 S_{\omega, \omega + \Delta_1, \omega + \Delta_2, \omega + \Delta_1 - \Delta_2} (\Delta_2 (\Delta_1 - \Delta_2))^2 \right] = 0 \end{aligned} \quad (3.70)$$

⁷It is vital to perform this symmetrization. Without it the resulting differential kinetic equation would not conserve particle number and energy.

Using the arbitrariness of Φ we finally get

$$\dot{n}_\omega = -\frac{1}{\Omega_0 k^{d-1}(dk/d\omega)} \frac{1}{4} \frac{\partial^2}{\partial \omega^2} \left[\left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times \int d\Delta_1 d\Delta_2 S_{\omega, \omega+\Delta_1, \omega+\Delta_2, \omega+\Delta_1-\Delta_2} (\Delta_2 (\Delta_1 - \Delta_2))^2 \right].$$

Finally, we assume that $S_{\omega\omega_1\omega_2\omega_3}$ is a homogeneous function of its arguments of degree γ :

$$S_{\epsilon\omega, \epsilon\omega_1, \epsilon\omega_2, \epsilon\omega_3} = \epsilon^\gamma S_{\omega\omega_1\omega_2\omega_3}. \quad (3.71)$$

We define $\omega\delta_i = \Delta_i$, and rewrite the DQKE as

$$\dot{n}_\omega = -\frac{1}{\Omega_0 k^{d-1}(dk/d\omega)} \frac{\partial^2}{\partial \omega^2} \left[\left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times I \times \omega^s \right] \quad (3.72)$$

where I is the interaction strength

$$I = \frac{1}{4} \int d\delta_1 d\delta_2 S_{1, 1+\delta_1, 1+\delta_2, 1+\delta_1-\delta_2} (\delta_2 (\delta_1 - \delta_2))^2,$$

and $s = \gamma + 6$.

An alternative derivation of the DQKE can be given by applying the Zakharov transformation (see, e.g., [28]) directly to the QKE. The Zakharov transformation is a conformal change of variables which reveals the symmetry of original collision integral. It transforms certain regions of the integration domain and, in the classical case, makes the transformed collision integral have a zero integrand for certain power law distributions. The Zakharov-transformed KE takes the form

$$\begin{aligned} \dot{n}_\omega = \frac{1}{\Omega_0 k^{d-1}(dk/d\omega)} \times \frac{1}{4} \times \int_{\Delta_1} \int (\mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) + \left(\frac{\omega}{\omega_2}\right)^{\gamma+3} \mathcal{K}(\omega, \frac{\omega\omega_3}{\omega_2}, \frac{\omega^2}{\omega_2}, \frac{\omega\omega_1}{\omega_2}) \\ + \left(\frac{\omega}{\omega_1}\right)^{\gamma+3} \mathcal{K}(\omega, \frac{\omega}{\omega_1}, \frac{\omega\omega_2}{\omega_1}, \frac{\omega\omega_3}{\omega_1}) + \left(\frac{\omega}{\omega_3}\right)^{\gamma+3} \mathcal{K}(\omega, \frac{\omega\omega_2}{\omega_3}, \frac{\omega\omega_1}{\omega_3}, \frac{\omega^2}{\omega_3})) \\ \times S_{\omega\omega_1\omega_2\omega_3} \delta(\omega + \omega_1 - \omega_2 - \omega_3) d\omega_1 d\omega_2 d\omega_3 \end{aligned} \quad (3.73)$$

We then expand the RHS of the above equation in powers of Δ' 's. The first nonvanishing term is of order Δ^4 and can be represented as second order derivative with respect to ω of

$$\left[\left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times I \times \omega^s \right].$$

The resulting DQKE is given in (3.72).

Kolmogorov solution of the classical KE. Let us find for a power-law steady solution of classical kinetic equation (see, e.g. [27],[28],[2]). We include this here for references and completeness. Assume, that

$$n_\omega = c\omega^{-x}, \quad (3.74)$$

then $\mathcal{K}^{\text{classical}}$ is homogeneous function of its arguments:

$$\mathcal{K}^{\text{classical}}(\alpha\omega_1, \alpha\omega_2, \alpha\omega_3, \alpha\omega_4) = \alpha^{-3x} \mathcal{K}^{\text{classical}}(\omega_1, \omega_2, \omega_3, \omega_4). \quad (3.75)$$

Using (3.75) we rewrite (3.73) as

$$\begin{aligned} \dot{n}_\omega = \frac{1}{\Omega_0 k^{d-1} (dk/d\omega)} \times \frac{1}{4} \times \int_{\Delta_1} \int (\mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) \omega^\xi \times [\omega^{-\xi} + \omega_1^{-\xi} - \omega_2^{-\xi} - \omega_3^{-\xi}] \\ \times S_{\omega\omega_1\omega_2\omega_3} \delta(\omega + \omega_1 - \omega_2 - \omega_3) d\omega_1 d\omega_2 d\omega_3, \end{aligned} \quad (3.76)$$

where $\xi = \gamma + 3 - 3x$. The product of $[]$ brackets in the (3.76) with $\delta(\omega + \omega_1 - \omega_2 - \omega_3)$ are equal to zero, if $\xi = 0$ or $\xi = 1$. This gives the Kolmogorov solution of classical KE:

$$\begin{aligned} n_\omega &= c\omega^{-x}, \\ x &= \gamma/3 + 1 \quad \text{or} \quad x = (\gamma + 2)/3. \end{aligned} \quad (3.77)$$

3.3.2 Solutions and properties of the DQKE

Let us now rewrite the DQKE in the form:

$$\begin{aligned}
 \dot{N}_\omega &= \frac{\partial^2}{\partial \omega^2} \mathcal{W}[n_\omega], \\
 \mathcal{W}^{\text{fermionic}}[n_\omega] &= -I \left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times \omega^s, \\
 \mathcal{W}^{\text{bosonic}}[n_\omega] &= I \left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) - n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times \omega^s, \\
 \mathcal{W}^{\text{classical}}[n_\omega] &= I \left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) \right) \times \omega^s.
 \end{aligned} \tag{3.78}$$

We can now use (3.53) to calculate the fluxes P and Q in terms of n_ω and its derivatives. We concentrate on the fermionic case. There,

$$\begin{aligned}
 Q = \frac{\partial \mathcal{W}}{\partial \omega} &= I s \omega^{s-1} \left(-n'^2 (2n - 1) - n n'' (1 - n) \right) \\
 &\quad + I \omega^s \left(-2n'^3 + n' n'' (1 - 2n) + n n''' (n - 1) \right) \\
 P = \left(\mathcal{W} - \omega \frac{\partial \mathcal{W}}{\partial \omega} \right) &= I \omega^s (1 - s) \left(-n'^2 (2n - 1) - n n'' (1 - n) \right) \\
 &\quad - I \omega^{s+1} \left(-2n'^3 + n' n'' (1 - 2n) + n n''' (n - 1) \right).
 \end{aligned} \tag{3.79}$$

Let us make a change of variables $n = 1/(G+1)$ and $n = 1/(e^m+1)$. n, G, m are functions of ω and t , “dot” is used to denote differentiation with respect to time, and “prime” with respect to ω . Then

$$\dot{G} = (1 + G)^2 \frac{I}{\Omega_0 k^{d-1} (dk/d\omega)} \frac{\partial^2}{\partial \omega^2} \left(\omega^s \frac{G'^2 - G G''}{(1 + G)^4} \right)$$

or

$$\dot{m}_\omega = - \frac{I}{\Omega_0 k^{d-1} (dk/d\omega)} \cosh^2 \left(\frac{m}{2} \right) \frac{\partial^2}{\partial \omega^2} \omega^s \frac{m''}{4 \cosh^4 \left(\frac{m}{2} \right)} \tag{3.80}$$

Since the stationary DQKE is a fourth order ODE, its solutions will have four free parameters. Indeed, assume a steady (equilibrium) state and integrate

(3.78,3.80) twice to get

$$\mathcal{W}[n_\omega] = Q\omega + P.$$

or

$$G = \exp\left(-\frac{\partial^{-2}}{\partial\omega^2} \frac{(Q\omega + P)(G+1)^4}{I\omega^s G^2}\right),$$

or

$$m'' = \frac{Q\omega + P}{I\omega^s} \cosh^4\left(\frac{m}{2}\right), \quad (3.81)$$

where Q and P are fluxes of particle number and energy. For $P = Q = 0$, (3.81) trivially gives

$$n(\omega) = \frac{1}{e^{\frac{1}{T}(\omega-\mu)} + 1},$$

the Fermi-Dirac distribution function. Therefore we observe that the Fermi-Dirac distribution function corresponds to a zero flux solution of the kinetic equation, consistent with our findings of the previous section.

Boltzmann H-theorem. DQKE supports Boltzmann H-theorem. Indeed,

$$\begin{aligned} \dot{S} &= \int d\omega \frac{dk}{d\omega} \dot{n}_\omega \log\left(\frac{1-n_\omega}{n_\omega}\right) \\ &= \int d\omega \log\left(\frac{1-n_\omega}{n_\omega}\right) \frac{\partial^2}{\partial\omega^2} I\omega^s (-1) ((-1+2n)n'^2 + (1-n)nn'') \\ &= \int d\omega \frac{(1-2n)n'^2 + nn''(-1+n)}{(1-n)^2 n^2} \\ &\times I\omega^s (-1) ((-1+2n)n'^2 + (1-n)nn'') \geq 0 \end{aligned} \quad (3.82)$$

we integrated by parts twice⁸ and used the fact

$$\left(\log\left(\frac{1-n}{n}\right)\right)'' = \frac{(1-2n)n'^2 + nn''(-1+n)}{(1-n)^2 n^2} \quad (3.83)$$

⁸Out of integral contributions are zero on any reasonably fast decaying distributions.

Time Flow Theorem - DQKE Here we proof the “Time Flow Theorem” for the DQKE. Assume, that $n_{\vec{k}, t=t_0}$ is given for time $t = t_0$ and that $0 \leq n_{\vec{k}, t=t_0} \leq 1$ - i.e. the values which function n can have “physically”. Then, if time evolution of $n_{\vec{k}}$ is given by (3.39) then $0 \leq n_{\vec{k}, t} \leq 1$ for all times.

Proof As in KE case define sets A and B , for any point from set A $n_{\vec{\omega}_j, \omega_j \in A} = 0$ and since its minimum, then $(\partial n_{\omega} / \partial \omega)|_{\omega=\omega_j \in A} = 0$. From DKE it follows $(\partial / \partial t) n_{\vec{\omega}_j, \omega_j \in A} \geq 0$ on set A . Same arguments lead to $(\partial / \partial t) n_{\vec{\omega}_j, \omega_j \in B} \leq 0$, so that n_{ω} can not acquire values outside of 0..1 region.

3.3.3 Summary of DQKE properties.

We suggest the reader to reread section 3.2.4, i.e. the QDKE has the same global properties as QKE.

3.3.4 DKE - Numerical scheme and boundary conditions.

In this section we explain how to deal numerically with boundary conditions for DQKE. The DQKE looks like

$$\begin{aligned} \dot{N}_{\omega} &= \frac{\partial^2}{\partial \omega^2} \mathcal{W}[n_{\omega}], \\ \mathcal{W}[n_{\omega}] &= -I \left(n_{\omega}^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_{\omega}} \right) + n_{\omega}^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_{\omega})) \right) \times \omega^s = \mathcal{K} \omega^s. \end{aligned} \quad (3.84)$$

where we defined $\mathcal{K} = (-n'^2(2n - 1) - nn''(1 - n))$. Then we identified fluxes of particles and energy as

$$\begin{aligned}
 Q = \frac{\partial \mathcal{W}}{\partial \omega} &= s\omega^{s-1}\mathcal{K} + \omega^s \frac{\partial}{\partial \omega} \mathcal{K} \\
 &= Is\omega^{s-1}(-n'^2(2n - 1) - nn''(1 - n)) \\
 &\quad + I\omega^s(-2n'^3 + n'n''(1 - 2n) + nn'''(n - 1)), \\
 P = \left(\mathcal{W} - \omega \frac{\partial \mathcal{W}}{\partial \omega} \right) &= \omega^s \mathcal{K}(1 - s) - \omega^{s+1} \frac{\partial \mathcal{K}}{\partial \omega} \\
 &= I\omega^s(1 - s)(-n'^2(2n - 1) - nn''(1 - n)) \\
 &\quad - I\omega^{s+1}(-2n'^3 + n'n''(1 - 2n) + nn'''(n - 1)).
 \end{aligned} \tag{3.85}$$

Numerical Scheme We discretize the values of n_ω on a grid with N points and with minimum and maximum values of ω to be $\omega_{min}, \omega_{max}$. Then $n_\omega = n_i, i = 1 \dots N$ and up to $O(\Delta^2)$ terms:

$$\begin{aligned}
 n'_k &= \frac{n_{k+1} - n_{k-1}}{2\Delta}, \\
 n''_k &= \frac{n_{k-1} - 2n_k + n_{k+1}}{\Delta^2}, \\
 n_k^{(3)} &= \frac{1}{2\Delta^3}(-n_{k-2} + 2n_{k-1} - 2n_{k+1} + n_{k+2}), \\
 n_k^{(4)} &= \frac{1}{\Delta^4}(n_{k-2} - 4n_{k-1} + 6n_k - 4n_{k+1} + n_{k+2}).
 \end{aligned} \tag{3.86}$$

We then rewrite a DQKE (3.72) in a form (we also add to it “laser” terms in preparation for subsequent chapters):

$$\begin{aligned}
\dot{n}_\omega &= \frac{n(t + \Delta t) - n(t)}{\Delta t} \\
&= \frac{1}{\text{factor}} (f_\omega \partial^4 n(t + \Delta t) + g_\omega \partial^3 n(t + \Delta t) + h(n(t))) + \text{laser}. \\
\text{factor} &= \Omega k^{d-1} \frac{dk}{d\omega}, \\
f_\omega &= -I \omega^{\frac{(2-D)}{2}} \omega^s n_\omega (1 - n_\omega), \\
g_\omega &= -2I s \omega^{\frac{(2-D)}{2}} \omega^{s-1} n_\omega (1 - n_\omega), \\
h(n_\omega) &= - \left(\omega^{-2+s} \left(4 s \omega n_\omega'^3 + 2 s \omega (-1 + 2 n_\omega) n_\omega' n_\omega'' + n_\omega'^2 \right. \right. \\
&\quad + (s - s^2 + 2 (-1 + s) s n_\omega + 8 \omega^2 n_\omega'') \\
&\quad + n_\omega'' (-((-1 + s) s n_\omega^2) - \omega^2 n_\omega'' + n_\omega ((-1 + s) s + 2 \omega^2 n_\omega'')) \left. \right) \\
\text{laser} &= \text{Pumping and Damping terms, terms describing laser.}
\end{aligned} \tag{3.87}$$

Now we represent (3.87) as a matrix equation for the $n(t + \Delta t)$:

$$\begin{aligned}
Ln(t + \Delta t) &= B. \\
L &= \mathbf{1} - \frac{\Delta t}{\text{factor}} f_\omega \partial^4 - \frac{\Delta t}{\text{factor}} g_\omega \partial^3. \\
B &= n(t) + \frac{\Delta t}{\text{factor}} h(n(t)) + \text{laser} \Delta t.
\end{aligned} \tag{3.88}$$

where $n(t + \Delta t)$, $n(t)$, B are columns, L is a matrix, $\mathbf{1}$ is unity matrix.

At each time step one solves (3.88) for $n(t + \Delta t)$.

Boundary conditions. At left boundary $\omega = \omega_{min}$ and at right boundary $\omega = \omega_{max}$ we specify the values of fluxes $Q = Q_L$ and $P = P_L$ at left and $Q = Q_R$ and $P = P_R$ at right boundary. Then solve the system of equations

(3.85) to calculate K and $\frac{\partial \mathcal{K}}{\partial \omega}$ in terms of P and Q at the boundaries:

$$\begin{aligned} K &= \omega^{-s}(Q\omega + P), \\ \frac{\partial \mathcal{K}}{\partial \omega} &= \omega^{-s-1}[(1-s)\omega Q - sP]. \end{aligned} \quad (3.89)$$

Now we have two boundary conditions at each boundary:

$$\mathcal{K}_{Boundary} = \omega_B^{-s}(Q_B\omega_B + P_B) = (-n'^2(2n-1) - nn''(1-n)) \Big|_{Boundary}, \quad (3.90)$$

$$\begin{aligned} \frac{\partial \mathcal{K}_{Boundary}}{\partial \omega} &= \omega_B^{-s-1}[(1-s)\omega_B Q_B - sP_B] \\ &= (-2n'^3 + n'n''(1-2n) + nn'''(n-1)) \Big|_{Boundary}, \end{aligned} \quad (3.91)$$

where subscript B refers to boundary, left or right ($B = L$ or $B = R$). So given any values of P_R and Q_R we are able to compute n''_{ω_R} and n'''_{ω_R} in terms of n_{ω_R} , P_R , Q_R and ω_R . Indeed, in the difference scheme we use we can relate n' and n'' :

$$\begin{aligned} n'_1 &= \frac{n_2 - n_1}{\Delta} - \frac{n''_1 \Delta}{2}, \\ n'_N &= \frac{n_N - n_{N-1}}{\Delta} + \frac{n''_N \Delta}{2}. \end{aligned} \quad (3.92)$$

where Δ is grid spacing n_1, n_2, n_{N-1}, n_N are values of the grid at first, second, $N^{th}-1$ and N^{th} points. Substituting (3.92) into (3.90) one gets a quadratic

equation for n'' :

$$an''^2 + bn'' + c = 0.$$

Left side :

$$\begin{aligned} a &= \frac{\Delta^2(1 - 2n_1)}{4.0}, \\ b &= (n_1 - n_2)(1 - 2n_1) + n_1(n_1 - 1), \\ c &= \frac{1}{\Delta^2}(n_2 - n_1)^2(1.0 - 2n_1) - \frac{\omega_{min}^{-s}(Q_L\omega_{min} + P_L)}{I}. \end{aligned}$$

Right side :

$$\begin{aligned} a &= \frac{\Delta^2(1 - 2n_N)}{4}, \\ b &= ((n_N - n_{N-1})(1 - 2n_N) + n_N(n_N - 1)), \\ c &= \frac{1}{\Delta^2}(n_N - n_{N-1})^2(1 - 2n_N) - \frac{\omega_{max}^{-s}(Q\omega_{max} + P)}{I}. \end{aligned} \tag{3.93}$$

Since a is small in these equations, we choose

$$n'' = \frac{-b + \text{Sign}(b)\sqrt{b^2 - 4ac}}{2a}. \tag{3.94}$$

where $\text{Sign}(b)$ is sign of b .

After calculating n'' for the boundary we calculate n''' at the boundary from (3.91).

We call (3.90.3.91) *nonlinear boundary conditions*. We specify the Q, P pair at each boundary and thus have two boundary conditions at each side of computational domain.

3.3.5 Numerical Results.

We now numerically investigate the DQKE to gain an intuitive understanding of its properties.

FIGURE 3.2. Numerical solution of DKE in the left transparency window. Numerical solution of (3.95) is presented. Initial conditions are $n_{\omega=0.1} = f_{\omega=0.1}$, $n'_{\omega=0.1} = f'_{\omega=0.1}$, where $f_{\omega} = 1/(\exp(7\omega - 4) + 1)$. The results are shown for $10^6 Q_L = 0, 3, 6, 9$. The dot size indicates the value of the flux, with larger dots corresponding to larger flux.

DQKE in the left transparency window. We begin by studying the time independent solutions of (3.78) and solve (3.58) as an initial value problem with $\mathcal{W}$ given by $\mathcal{W}^{\text{fermionic}}$ (see (3.78)),

$$\begin{aligned} Q_L(\omega - \omega_L) &= \mathcal{W}^{\text{fermionic}} \\ &\equiv -I \left(n_{\omega}^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_{\omega}} \right) + n_{\omega}^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_{\omega})) \right) \times \omega^s. \end{aligned} \quad (3.95)$$

We start from $\omega = 0.1$ and take the initial conditions to be $n_{\omega=0.1} = f_{\omega=0.1}$, $n'_{\omega=0.1} = f'_{\omega=0.1}$, where f_{ω} is a conveniently chosen Fermi-Dirac distribution function $f_{\omega} = 1/(\exp(7\omega - 4) + 1)$. The results are shown on Figure (3.2) for the range of $10^6 Q_L = 0, 3, 6, 9$.

For $Q_L = 0$ we recover the Fermi-Dirac distribution function f_{ω} . However, for nonzero Q the distribution deviates from the Fermi-Dirac function, and

the bigger the flux, the bigger the deviation. For the same initial conditions, the graph of the number density n_ω for the positive finite flux distribution lies below that for the Fermi-Dirac distribution. Further, observe that, for the Fermi-Dirac solution, the chemical potential μ is simply the distance to the point of the inflection of n_ω and the temperature is the width of the exponential decay region. For finite positive fluxes, the distance to the point of inflection (which we call μ_Q) is less than $\mu_{Q=0} = \mu$. Likewise, T_Q , the width of the n_ω distribution for a finite flux is less than $T_0 = T$. As fluxes become larger, the finite flux equilibrium distribution becomes more and more like a Heavy side function with rapidly decreasing μ_Q . This means that n_ω is very small for all $\omega > \mu_Q$ and thus the system can be pumped in this region without possible losses due to the Pauli blocking. We exploit this in the Chapter 7 where the application to semiconductor lasers is considered.

In semiconductor lasers, it is the finite temperature effect of broadening the Fermi-Dirac distribution that contributes to inefficiency. If one could operate at $T = 0$, then one could simply choose the chemical potential, related to the total carrier number (see, e.g., [24]), so that the distribution cuts off immediately after the lasing frequency. However, the finite temperature broadens the distribution and means that one has to pump momentum values which play no role in the lasing process. The effect of the finite flux is to make T effectively smaller.

DQKE in the right transparency window. We next solve (3.59) for steady state solutions in the larger momentum region with $\mathcal{W}^{\text{fermionic}}$:

$$\begin{aligned} \mathcal{W} = P_R(1 - \omega/\omega_R) &= \mathcal{W}^{\text{fermionic}} \\ &\equiv -I \left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times \omega^s \end{aligned} \quad (3.96)$$

FIGURE 3.3. Numerical solution of DKE in the right transparency window. Numerical solution of (3.96) with $n_{\omega=0.3} = f_{\omega=0.3}$, $n'_{\omega=0.3} = f'_{\omega=0.3}$, as Figure (3.2). The results are shown for $10^4 P_R = 0, 3, 6, 9$.

We start from $\omega = 0.3$ with initial conditions $n_{\omega=0.3} = f_{\omega=0.3}$, $n'_{\omega=0.3} = f'_{\omega=0.3}$. The results are shown on Figure (3.3) for the range of $10^4 P_R = 0, 3, 6, 9$.

Again, we recover the Fermi-Dirac function for zero flux, and observe a similar deviation from thermodynamical equilibrium for nonzero fluxes, namely the effective chemical potential and temperature diminishes with increasing of the flux value P_R .

Time evolution of distribution function as given by the DQKE. We then consider the time evolution of the distribution function as given by the DQKE. The fundamental property of the kinetic equation that any distribution function relaxes to its thermodynamical equilibrium value in the absence of forcing (pumping/damping) is also true for the DQKE, as illustrated on Figure (3.4). There an initial distribution function, shown by a thin solid line, relaxes to the FD function, shown by a thick solid line, through several in-

Relaxation to Fermi-Dirac distribution

FIGURE 3.4. Time evolution of the distribution function as described by DKE (3.78), with boundary conditions $P = Q = 0$ at both ends. The initial distribution (thin line) relaxes to a Fermi-Dirac state (thick line). Several intermediate states are shown by long-dashed and short-dashed lines.

intermediate states shown by dashed lines. Since there is no forcing to the system, we take “fluxless” boundary conditions $P = Q = 0$ in (3.79) on the boundaries, so that no particles or energy cross the boundaries. The distribution relaxes to the FD distribution roughly by the time τ_{relax} , which can be estimated as $\omega_{\text{max}}^{(2-s)}/(I(n + n^2))$, where ω_{max} is the frequency where distribution approaches zero value. To check that the final distribution is indeed FD, we calculate $\ln(1/n_\omega - 1)$ and verify that it is a linear function. The total particle number N and energy E are conserved in our numerical runs to an accuracy of 10^{-5} .

We then address the question of what is the steady (equilibrium) solution when the system has some external forcing. To model the forcing, we specify some positive flux of Q on the boundaries, and wait for the distribution to reach a new equilibrium, a hybrid state with a constant flux of Q , a zero P flux, energy E and particle number N (see Figure (3.5)).

The more the flux of number of particles is, the more the final distribution is bent in the manner of Figures (3.2-3.3) and according to (3.81). The total

FIGURE 3.5. Same as in Figure (3.4), but for $P = 0, Q = Q_1 > Q_0$ at both ends.

The initial distribution function (thick line) relaxes to finite- Q -equilibria as shown by the long-dashed line (only the final steady state is shown). Also shown are the results for the boundary conditions $P = 0, Q = Q_1 > Q_0$ at both ends (short-dashed line) and for $P = 0, Q = Q_2 > Q_1$ at both ends (dotted line).

particle number N and energy E are the same for all curves on Figure (3.5).

Verification of the formula for values of Left/Right fluxes. We conclude this section by verifying numerically (3.57). For this purpose we numerically solve (3.52)

$$\frac{\partial N_\omega}{\partial t} = \frac{\partial^2}{\partial \omega^2} \mathcal{W}[n_\omega] + F_\omega - D_\omega, \quad (3.97)$$

with $\mathcal{W}$ given by $\mathcal{W}^{\text{fermionic}}$ (see (3.78)),

$$\mathcal{W}^{\text{fermionic}} \equiv -I \left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times \omega^s.$$

We choose damping term D_ω to be a sum of two Gaussians, centered at $\omega = .2$ and $\omega = 1$ respectively. We then make a series of five numerical experiments, where we choose pumping term F_ω to be a Gaussian centered at .44, .52, .6, .68, .76 respectively. In these numerical experiments we numerically evaluate (3.97) until distribution reaches its steady state. In Figure (3.6) we present the forms of pumping/damping, as well as the steady values for fluxes for one such numerical experiment. We see that the fluxes are constants in the windows of transparency, i.e. in the regions where there is now pumping or damping.

To check if (3.57) holds, we plot $-Q_R \omega_R / P_R$, $-Q_L \omega_L / P_L$ and

$$-Q_R / Q_L \frac{\omega_R - \omega_0}{\omega_0 - \omega_L}$$

as a function of ω_0 for all five numerical runs (see Figure (3.7)). According to (3.56) and (3.57) these quantities should relax to unity for all five runs. Deviation from unity can be explained by noting that (3.56) derived by assuming that pumping and damping are delta-functions, while in practice there is always some width associated with pumping/damping domains. We also verify that $Q_0 = Q_L - Q_R$ with accuracy of 10^{-3} .

To conclude, we verified numerically the validity of (3.56) and (3.57).

Stationary Fluxes and Pumping/Dumping

FIGURE 3.6. The stationary values of fluxes as a functions of ω , as well as pumping and damping profiles.

Flux of particles Q is shown by the thick solid line, flux of energy P is shown by the thin solid line. Pumping and damping profiles are also shown by dashed lines. $\omega_L = .2$, $\omega_0 = .52$. $\omega_R = 1$. Fluxes are constants in inertial regions.

Verification of formulas for Left/Right Fluxes

FIGURE 3.7. Verification of formulas for the magnitude of particle and energy fluxes to the right and to the left.

$-Q_R\omega_R/P_R$, $-Q_L\omega_L/P_L$ and $-Q_R/Q_L \frac{\omega_R - \omega_0}{\omega_0 - \omega_L}$ are shown for different values of ω_0 . $-Q_R\omega_R/P_R$ shown by small circles, $-Q_L\omega_L/P_L$ shown by big circles and $-Q_R/Q_L \frac{\omega_R - \omega_0}{\omega_0 - \omega_L}$ is shown by disks. Theoretically these quantities should be equal to unity.

Chapter 4

DIFFERENTIAL QKE -TWO PARTICLE CASE

4.1 Derivation of the 2-particle DQKE.

So far we were dealing with the scattering of one type of particles, say, electrons. But in a "real" semiconductor there are at least two types of particles - electrons and holes. Therefore we have to generalize all our theory to include these two kinds of particles.

We start from writing down the Hamiltonian for interacting electrons and holes (2.55). This Hamiltonian is nothing but (1.3) with wiped out phonons ($c_k, c_k^\dagger \rightarrow 0$) and neglected field $\mathcal{E} \rightarrow 0$:

$$\begin{aligned}
 H = & \hbar \sum_{\mathbf{k}} ((\epsilon_{ek} + \epsilon_{gap}) a_{\mathbf{k}}^+ a_{\mathbf{k}} + \epsilon_{hk} b_{-\mathbf{k}}^+ b_{-\mathbf{k}}) \\
 & + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}', \mathbf{q} \neq 0} V_{\mathbf{q}} (a_{\mathbf{k}+\mathbf{q}}^+ a_{\mathbf{k}'-\mathbf{q}}^+ a_{\mathbf{k}'} a_{\mathbf{k}} + b_{\mathbf{k}+\mathbf{q}}^+ b_{\mathbf{k}'-\mathbf{q}}^+ b_{\mathbf{k}'} b_{\mathbf{k}} - 2a_{\mathbf{k}+\mathbf{q}}^+ b_{\mathbf{k}'-\mathbf{q}}^+ b_{\mathbf{k}'} a_{\mathbf{k}}),
 \end{aligned} \tag{4.1}$$

here $a_{\mathbf{k}}^\dagger, a_{\mathbf{k}}$ are creation/annihilation operators for electrons, $b_{\mathbf{k}}^\dagger, b_{\mathbf{k}}$ are creation /annihilation operators for holes. First line in this Hamiltonian represents electron and hole kinetic energies, second line describes the carrier-carrier interaction through the screened Coulomb potential $V_{\mathbf{q}}$ (2.54).

We then should write down evolution equations for operators $a_{\mathbf{k}}^\dagger, a_{\mathbf{k}}$ and $b_{\mathbf{k}}^\dagger, b_{\mathbf{k}}$ (see (3.4)) in order to derive evolution equations for electron distribution function $n_{\mathbf{k}} = \langle a_{\mathbf{k}}^+ a_{\mathbf{k}} \rangle$ and hole distribution function $m_{\mathbf{k}} = \langle b_{-\mathbf{k}}^+ b_{-\mathbf{k}} \rangle$. These equations would be coupled to four-operator averages composed of electron-hole creation/annihilation operators. Not to redo all the analyses of

Chapter 3. let us simplify the life by saying that in everything said in Chapter 3. we imply that index k contains not only corresponding moment, but band index also $\mathbf{k} \rightarrow \mathbf{k}, \lambda = e, h$. Integrations over $\mathbf{k}$ would then include the summations over band index $\int d\mathbf{k} \rightarrow \sum_{\lambda=e,h} \int d\mathbf{k}$. Then it is straightforward to generalize QKE (3.39) to the two particle case. The result is given by

$$\begin{aligned}
\frac{\partial}{\partial t} n_k &= 4\pi \int |T_{kk_1k_2k_3}|^2 (n_{\mathbf{k}_2} n_{\mathbf{k}_3} (1 - n_{\mathbf{k}_1}) (1 - n_{\mathbf{k}}) \\
&\quad - n_{\mathbf{k}} n_{\mathbf{k}_1} (1 - n_{\mathbf{k}_2}) (1 - n_{\mathbf{k}_3})) \\
&\times \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \delta(\omega_{\mathbf{k}}^e + \omega_{\mathbf{k}_1}^e - \omega_{\mathbf{k}_2}^e - \omega_{\mathbf{k}_3}^e) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 + \\
&4\pi \int |T_{kk_1k_2k_3}|^2 (n_{\mathbf{k}_2} m_{\mathbf{k}_3} (1 - m_{\mathbf{k}_1}) (1 - n_{\mathbf{k}}) \\
&\quad - n_{\mathbf{k}} m_{\mathbf{k}_1} (1 - n_{\mathbf{k}_2}) (1 - m_{\mathbf{k}_3})) \\
&\times \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \delta(\omega_{\mathbf{k}}^e + \omega_{\mathbf{k}_1}^h - \omega_{\mathbf{k}_2}^e - \omega_{\mathbf{k}_3}^h) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3,
\end{aligned} \tag{4.2}$$

where $n_{\mathbf{k}}$ is the distribution function of electrons, $\omega_{\mathbf{k}}^e$ is electron energy, and $m_{\mathbf{k}}$ is the hole distribution function with $\omega_{\mathbf{k}}^h$ being hole energy. The evolution equation for $m_{\mathbf{k}}$ can also be obtained:

$$\begin{aligned}
\frac{\partial}{\partial t} m_k &= 4\pi \int |T_{kk_1k_2k_3}|^2 (m_{\mathbf{k}_2} m_{\mathbf{k}_3} (1 - m_{\mathbf{k}_1}) (1 - m_{\mathbf{k}}) \\
&\quad - m_{\mathbf{k}} m_{\mathbf{k}_1} (1 - m_{\mathbf{k}_2}) (1 - m_{\mathbf{k}_3})) \\
&\times \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \delta(\omega_{\mathbf{k}}^h + \omega_{\mathbf{k}_1}^h - \omega_{\mathbf{k}_2}^h - \omega_{\mathbf{k}_3}^h) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3 + \\
&4\pi \int |T_{kk_1k_2k_3}|^2 (m_{\mathbf{k}_2} n_{\mathbf{k}_3} (1 - n_{\mathbf{k}_1}) (1 - m_{\mathbf{k}}) \\
&\quad - m_{\mathbf{k}} n_{\mathbf{k}_1} (1 - m_{\mathbf{k}_2}) (1 - n_{\mathbf{k}_3})) \\
&\times \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \delta(\omega_{\mathbf{k}}^h + \omega_{\mathbf{k}_1}^e - \omega_{\mathbf{k}_2}^h - \omega_{\mathbf{k}_3}^e) d\mathbf{k}_1 d\mathbf{k}_2 d\mathbf{k}_3,
\end{aligned} \tag{4.3}$$

Note that (4.3), (4.2) include only differences of electrons and holes energies: $\omega_{\mathbf{k}}^e + \omega_{\mathbf{k}_1}^h - \omega_{\mathbf{k}_2}^e - \omega_{\mathbf{k}_3}^h$, $\omega_{\mathbf{k}}^e + \omega_{\mathbf{k}_1}^e - \omega_{\mathbf{k}_2}^e - \omega_{\mathbf{k}_3}^e$ so that ϵ_{gap} cancels from these equations. Consequently we take $\omega^e = \frac{\hbar^2 k^2}{2\mu_e}$ but this is legitimate as long

as *differences* of electron energies is considered. As in Chapter 3, we take $\hbar = 1$ ¹.

4.1.1 Effective mass and effective frequency.

To consider both electrons and holes we have to introduce the concept of effective mass kinetic energy. First we introduce reduced mass as

$$\mu_r = \frac{\mu_e + \mu_h}{\mu_e \mu_h}, \quad (4.4)$$

where μ_e is an electron mass and μ_h is a hole mass. We then introduce “reduced kinetic energy” ω

$$\begin{aligned} \omega^{(e)} &= \frac{k^2}{2\mu_e} = \frac{\mu_r}{\mu_e} \omega, \\ \omega^{(h)} &= \frac{k^2}{2\mu_h} = \frac{\mu_r}{\mu_h} \omega, \\ \omega &= \frac{k^2}{2\mu_r}, \\ \frac{\partial}{\partial \omega^{(e)}} &= \frac{\mu_e}{\mu_r} \frac{\partial}{\partial \omega}, \\ \frac{\partial}{\partial \omega^{(h)}} &= \frac{\mu_h}{\mu_r} \frac{\partial}{\partial \omega}. \end{aligned} \quad (4.5)$$

This effective mass kinetic energy is a convenient independent variable.

¹ $\hbar = 1$ through Chapters 3 and 4.

4.1.2 Derivation.

Then we can rewrite QKE in terms of ω . After doing the standard angular-averaging one has

$$\begin{aligned}
\frac{\partial}{\partial t} n_\omega &= \frac{1}{\Omega_0 k^{d-1} \left(\frac{dk}{d\omega} \right)} \int d\omega_1 d\omega_2 d\omega_3 \mathcal{S}_{\omega, \omega_1, \omega_2, \omega_3} \\
&\times \left(\delta \left(\frac{\mu_r}{\mu_e} (\omega + \omega_1 - \omega_2 - \omega_3) \right) \times \mathcal{K}_{\omega, \omega_1, \omega_2, \omega_3} + \right. \\
&\quad \left. \delta \left(\frac{\mu_r}{\mu_e} (\omega - \omega_2) + \frac{\mu_r}{\mu_h} (\omega_1 - \omega_3) \right) \mathcal{W}_{\omega, \omega_1, \omega_2, \omega_3} \right), \\
\mathcal{K}_{\omega, \omega_1, \omega_2, \omega_3} &= n_{\omega_2} n_{\omega_3} (1 - n_{\omega_1}) (1 - n_\omega) - n_\omega n_{\omega_1} (1 - n_{\omega_2}) (1 - n_{\omega_3}), \\
\mathcal{W}_{\omega, \omega_1, \omega_2, \omega_3} &= n_{\omega_2} m_{\omega_3} (1 - m_{\omega_1}) (1 - n_\omega) - n_\omega m_{\omega_1} (1 - n_{\omega_2}) (1 - m_{\omega_3}), \\
\mathcal{S}_{\omega, \omega_1, \omega_2, \omega_3} &= \Omega^4 (k k_1 k_2 k_3)^{d-1} < |T_{\omega \omega_1 \omega_2 \omega_3}|^2 \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) > \frac{dk dk_1 dk_2 dk_3}{d\omega d\omega_1 d\omega_2 d\omega_3}.
\end{aligned} \tag{4.6}$$

Let us multiply both sides of (4.6) by an arbitrary function $\Phi(\omega)$ and integrate with respect to ω . The result is analogous to (3.66)

$$\begin{aligned}
\int \dot{N}_\omega \Phi(\omega) d\omega &= \int \int \int \left(\mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) \times \mathcal{S}_{\omega, \omega_1, \omega_2, \omega_3} \delta(\omega + \omega_1 - \omega_2 - \omega_3) \frac{\mu_e}{\mu_r} \right. \\
&\quad \left. + \mathcal{W}_{\omega, \omega_1, \omega_2, \omega_3} \mathcal{S}_{\omega, \omega_1, \omega_2, \omega_3} \delta \left(\frac{\mu_r}{\mu_e} (\omega - \omega_2) + \frac{\mu_r}{\mu_h} (\omega_1 - \omega_3) \right) \right) \\
&\times \Phi(\omega) d\omega d\omega_1 d\omega_2 d\omega_3.
\end{aligned} \tag{4.7}$$

Symmetrise the RHS of Eqn. (4.7) to get

$$\begin{aligned}
\int \dot{N}_\omega \Phi(\omega) d\omega &= \int \int \int d\omega d\omega_1 d\omega_2 d\omega_3 \\
&\times \left[\mathcal{K}(\omega, \omega_1, \omega_2, \omega_3) \times S_{\omega, \omega_1, \omega_2, \omega_3} \left(\frac{\mu_e}{\mu_r} \right) \delta(\omega + \omega_1 - \omega_2 - \omega_3) \right. \\
&\times \frac{1}{4} (\Phi(\omega) + \Phi(\omega_1) - \Phi(\omega_2) - \Phi(\omega_3)) \\
&+ \mathcal{W}(\omega, \omega_1, \omega_2, \omega_3) \times S_{\omega, \omega_1, \omega_2, \omega_3} \delta \left(\frac{\mu_r}{\mu_e} (\omega - \omega_2) + \frac{\mu_r}{\mu_h} (\omega_1 - \omega_3) \right) \\
&\times \frac{1}{4} (\Phi(\omega) - \Phi(\omega_2)) \\
&+ \mathcal{W}(\omega_1, \omega, \omega_3, \omega_2) \times S_{\omega, \omega_1, \omega_2, \omega_3} \delta \left(\frac{\mu_r}{\mu_h} (\omega - \omega_2) + \frac{\mu_r}{\mu_e} (\omega_1 - \omega_3) \right) \\
&\times \frac{1}{4} (\Phi(\omega_1) - \Phi(\omega_3)) \left. \right].
\end{aligned} \tag{4.8}$$

We then introduce $\omega_i = \omega + \Delta_i$ and expand the collision kernel around ω (see also 3.69):

$$\begin{aligned}
\mathcal{W}_{\omega+\Delta_0, \omega+\Delta_1, \omega+\Delta_2, \omega+\Delta_3} &\simeq (-\Delta_1 + \Delta_3) n_\omega m'_\omega (1 - n_\omega) \\
&\quad - (\Delta_0 - \Delta_2) (1 - m_\omega) m_\omega n'_\omega.
\end{aligned} \tag{4.9}$$

We also expand

$$\begin{aligned}
\Phi(\omega) - \Phi(\omega + \Delta_2) &\simeq -\Delta_2 \Phi'(\omega), \\
\Phi(\omega_1) - \Phi(\omega + \Delta_3) &\simeq (\Delta_1 - \Delta_3) \Phi'(\omega),
\end{aligned} \tag{4.10}$$

along with (3.68). Finally integrating by parts the term proportional to electron-hole interaction, using delta function to integrate over Δ_2 and inte-

grating “self” term by part twice we get

$$\begin{aligned} \frac{\partial n_\omega}{\partial t} = & -\left(\frac{\mu_e}{\mu_r}\right) \frac{1}{\Omega k^{d-1} \left(\frac{dk}{d\omega}\right)} \frac{\partial^2}{\partial \omega^2} I_1 \omega^{\gamma+6} \left(n_\omega^4 (n_\omega^{-1})'' + n_\omega^2 (\ln n_\omega)'' \right) \\ & + \frac{\mu_e}{\Omega k^{d-1} \left(\frac{dk}{d\omega}\right)} \frac{\partial}{\partial \omega} I_2 \omega^{\gamma+4} (-\mu_h n m' (1-n) + \mu_e (1-m) m n') \end{aligned} \quad (4.11)$$

$$\begin{aligned} \frac{\partial m_\omega}{\partial t} = & -\left(\frac{\mu_h}{\mu_r}\right) \frac{1}{\Omega k^{d-1} \left(\frac{dk}{d\omega}\right)} \frac{\partial^2}{\partial \omega^2} I_1 \omega^{\gamma+6} \left(m_\omega^4 (m_\omega^{-1})'' + m_\omega^2 (\ln m_\omega)'' \right) \\ & - \frac{\mu_h}{\Omega k^{d-1} \left(\frac{dk}{d\omega}\right)} \frac{\partial}{\partial \omega} I_2 \omega^{\gamma+4} (-\mu_h n m' (1-n) + \mu_e (1-m) m n') \end{aligned} \quad (4.12)$$

$$(\cdot)' = \frac{\partial}{\partial \omega}, \quad n_\omega = n(\mathbf{k}(\omega)), \quad m_\omega = m(\mathbf{k}(\omega)).$$

Here we also wrote down equation for $\dot{m}_\omega$. As in one-particle case, γ is the degree of homogeneity of function S - see (3.71). I_1^2 and I_2 are positive-definite interaction strengths which are obviously different:

$$\begin{aligned} I_1 &= \frac{1}{4} \int d\delta_1 d\delta_2 \mathcal{S}(1, 1 + \delta_1, 1 + \delta_2, 1 + \delta_1 - \delta_2) \delta_2^2 (\delta_1 - \delta_2)^2, \\ I_2 &= \frac{\mu_e \mu_h}{4} \int d\delta_1 d\delta_2 (\delta_1 - \delta_3)^2 \\ &\quad \times \left(\frac{\mu_e^2}{\mu_h \mu_r} \mathcal{S}(1, 1 + \delta_1, 1 + \frac{\mu_e}{\mu_h} (\delta_1 - \delta_3), 1 + \delta_3) \right. \\ &\quad \left. \frac{\mu_h^2}{\mu_e \mu_r} \mathcal{S}(1, 1 + \delta_1, 1 + \frac{\mu_h}{\mu_e} (\delta_1 - \delta_3), 1 + \delta_3) \right). \end{aligned} \quad (4.13)$$

where $\Delta_i = \omega \delta_i$. We refer reader to Chapter 4 for complete details on these equations.

From the form of (4.11,4.12) one sees that only the constant-particle-flux solution $Q = \text{const}$ is available. *The (4.11,4.12) equations do not have individual constant-energy-flux solutions.* This is due to the fact, that energy is

² I_1 here is equivalent to I of Chapter three. For convenience of notation we prefer to keep both I and I_1 , to differentiate between one - species and two-species systems.

not a conserved quantity in a electron sub-system or hole sub-system individually. In order to get constant-energy-flux solutions for the electron-hole system, one has to consider electrons *and* holes together and correspondently consider (4.11,4.12) as a system of equations.

4.2 Properties and solutions of 2-DQKE.

4.2.1 Thermodynamic Equilibrium solutions.

One can check that Fermi-Dirac Functions

$$n_\omega = \frac{1}{e^{\frac{1}{T_e}(\frac{\mu_e}{\mu_e}\omega - \xi_e)} + 1}, \quad m_\omega = \frac{1}{e^{\frac{1}{T_h}(\frac{\mu_h}{\mu_h}\omega - \xi_h)} + 1}. \quad (4.14)$$

are steady solutions of the 2-particle DQKE, as long as the electron and hole temperatures are equal: $T_e = T_h$.

4.2.2 Role of the “cross” term.

The role of the “cross” term is to equilibrate the temperatures of the components of the electron-hole plasma. To proof this fact, let us define

$$n_\omega = \frac{1}{e^f + 1}, \quad m_\omega = \frac{1}{e^g + 1}$$

and rewrite (4.11,4.12) as

$$\begin{aligned} \frac{\partial n_\omega}{\partial t} &= \dots I_2 \frac{\mu_e}{\Omega k^{d-1} \left(\frac{dk}{d\omega}\right)} \frac{\partial}{\partial \omega} \left(\frac{e^f e^g}{(e^f + 1)^2 (e^g + 1)^2} \frac{\partial}{\partial \omega} (\mu_h g_\omega - \mu_e f_\omega) \right) \\ \frac{\partial m_\omega}{\partial t} &= \dots -I_2 \frac{\mu_h}{\Omega k^{d-1} \left(\frac{dk}{d\omega}\right)} \frac{\partial}{\partial \omega} \left(\frac{e^f e^g}{(e^f + 1)^2 (e^g + 1)^2} \frac{\partial}{\partial \omega} (\mu_h g_\omega - \mu_e f_\omega) \right), \end{aligned} \quad (4.15)$$

where we used dots “...” to designate one particle contributions.

Now let us assume that $I_2 \ll I_1, (I_1 \frac{\mu_h}{\mu_e})$ so that the distribution functions are (4.14) at all the times, with T_e and T_h being functions of time $T_e =$

$T_e(t)$, $T_h = T_h(t)$. Let us calculate the evolution equation for the rate of change of total electron energy ³

$$E^{(e)} = \int d\omega \left(\frac{\mu_r}{\mu_e} \omega + \epsilon_{gap} \right) N_\omega.$$

and total hole energy:

$$E^{(h)} = \frac{\mu_r}{\mu_h} \int d\omega \omega M_\omega.$$

Now

$$\begin{aligned} \dot{E}^{(e)} &= \frac{\mu_r}{\mu_e} \int d\omega \omega \dot{N}_\omega + \epsilon_{gap} \dot{N} \\ &= -\frac{\mu_r}{\mu_e} I_2 \int d\omega \left(\frac{e^f e^g}{(e^f + 1)^2 (e^g + 1)^2} \frac{\partial}{\partial \omega} (\mu_h g_\omega - \mu_e f_\omega) \right) \\ &= -I_2 \frac{\mu_r}{\mu_e} \int d\omega \frac{e^f e^g}{(e^f + 1)^2 (e^g + 1)^2} \left(\frac{1}{T_h} \frac{\mu_r}{\mu_h} - \frac{\mu_e}{\mu_h} \frac{1}{T_e} \frac{\mu_r}{\mu_e} \right), \\ \dot{E}^{(h)} &= \frac{\mu_r}{\mu_h} \int d\omega \omega \dot{M}_\omega = -\dot{E}^{(e)}, \\ N_\omega &= \Omega_0 k^{d-1} \left(\frac{dk}{d\omega} \right) n_\omega, \\ M_\omega &= \Omega_0 k^{d-1} \left(\frac{dk}{d\omega} \right) m_\omega. \end{aligned} \tag{4.16}$$

Here $N = \int d\omega N_\omega$ is the total number of electrons which is conserved, thus $\dot{N} = 0$. We also used the fact that one-particle contribution conserves the energy of the subsystems. Note that $\dot{E}^{(e)}$ is proportional to $(1/T_e - 1/T_h)$ times positive function and $\dot{E}^{(h)}$ is proportional to $(1/T_e - 1/T_h)$ times negative function. It means that energy goes from hot particles to cold particles.

Equations for $\dot{n}_\omega$ and $\dot{m}_\omega$ consist of two parts - first part is “self” interaction, proportional to I_1 , and second- “cross” interaction, proportional

³ We must include band gap to calculate electron energy. We will return to this point in subsection (4.5).

to I_2 . “Self” interaction term describes the interaction of particles among themselves (intraband scattering). “Cross” term describes the interaction of electron and hole subsystems (interband scattering). Holes being much heavier than electrons, reach their equilibrium faster than electrons. The cross term is then tries to equilibrate the temperature of two subsystems. However one can not neglect electron “self” interaction. Indeed, let us assume that electrons are very hot so that in wide ranges of ω we have $n \simeq \text{constant}$. Let us further assume that holes are very cold and their distribution function is almost heavy side functions. Then (we use “...” to designate one particle contributions)

$$\dot{M}_\omega \simeq \dots n(1-n)\mu_h \frac{\partial}{\partial \omega} m I_2 \omega^s \simeq \dots + m''$$

and we see that the cross term has m'' contribution in leading order. It means that effectively $\dot{M}_\omega \simeq$ positive function m'' which is heat-type equation. It means that a “step” of a step function will become less sharp so that the electron temperature will be increasing. Since the $\dot{V}_\omega$ will also have contribution proportional to m'' , one can not neglect self term in comparison to cross term.

4.2.3 Boltzmann H theorem.

By analogy with one particle case the entropy of electron-hole plasma may be defined as

$$\begin{aligned} \mathcal{S} = - \int d\mathbf{k} \quad & (\mu_e(n_k \log n_k + (1 - n_k) \log(1 - n_k)) \\ & + \mu_h(m_k \log m_k + (1 - m_k) \log(1 - m_k))) . \end{aligned} \quad (4.17)$$

Its time evolution is given by

$$\begin{aligned}
\dot{S} &= \int d\omega \frac{dk}{d\omega} k^{d-1} \Omega_0 \left(\mu_e \dot{n}_\omega \log\left(\frac{1-n_\omega}{n_\omega}\right) + \mu_h \dot{m}_\omega \log\left(\frac{1-m_\omega}{m_\omega}\right) \right) \\
&= \dots + \int d\omega \frac{dk}{d\omega} k^{d-1} \Omega_0 I_2 \left(\frac{\partial \text{Cross}}{\partial \omega} \right) \left(\mu_e \log \frac{1-n}{n} - \mu_h \log \frac{1-m}{m} \right) \\
&= \dots + \int d\omega \frac{dk}{d\omega} k^{d-1} \Omega_0 I_2 \left(\frac{\partial \text{Cross}}{\partial \omega} \right) \left(\log \left(\left(\frac{1-n}{n} \right)^{\mu_e} \cdot \left(\frac{m}{1-m} \right)^{\mu_h} \right) \right) \\
&= \dots - \int d\omega \frac{dk}{d\omega} k^{d-1} \Omega_0 I_2 \left(\frac{\partial}{\partial \omega} \log \left(\left(\frac{1-n}{n} \right)^{\mu_e} \cdot \left(\frac{m}{1-m} \right)^{\mu_h} \right) \right) \cdot \text{Cross},
\end{aligned} \tag{4.18}$$

where we integrated by parts once and defined $\text{Cross} = -\omega^{s-2} \times (\mu_e m n'(-1+m) - \mu_h n m'(-1+n))$. We also use dots “...” to designate terms proportional to the one particle DKE. These terms lead only to increase of entropy, as proven in preceding sections. Using the fact that

$$\frac{\partial}{\partial \omega} \log \left(\left(\frac{1-n}{n} \right)^{\mu_e} \cdot \left(\frac{m}{1-m} \right)^{\mu_h} \right) = \frac{\mu_h n m' (1-n) + \mu_e m n' (-1+m)}{(1-m)m(1-n)n} \tag{4.19}$$

one trivially gets⁴

$$\dot{S} \geq 0. \tag{4.20}$$

Thus we conclude that in the absence of external forcing the entropy of the system may only grow or, at best, stay the same. It is easy to see using variation principle, that maximum of entropy corresponds to a state where both n and m are given by Fermi-Dirac distribution functions with the same temperatures.

⁴Remember,

$$0 \leq n_\omega \leq 1$$

and

$$0 \leq m_\omega \leq 1,$$

because of Pauli exclusion principle.

4.2.4 Conservation Laws.

It is easy to see that 2DQKE conserves number of electrons and number of holes.

Since number of electrons is constant, and number of holes is constant, then total number of carriers is constant as well, so then for the sum of electrons and holes spectral densities $N_\omega + M_\omega$ defined as

$$\begin{aligned} N_\omega &= \Omega k^{d-1} \left(\frac{dk}{d\omega} \right) n_\omega \\ M_\omega &= \Omega_0 k^{d-1} \left(\frac{dk}{d\omega} \right) m_\omega, \end{aligned} \tag{4.21}$$

one has

$$\begin{aligned} \dot{N}_\omega + \dot{M}_\omega &= -\frac{I_1}{\mu_r} \frac{\partial^2}{\partial \omega^2} \omega^{\gamma+6} \left(\mu_e \left(n_\omega^4 (n_\omega^{-1})'' + n_\omega^2 (\ln n_\omega)'' \right) \right. \\ &\quad + \left. (I_1 \mu_h) \left(m_\omega^4 (m_\omega^{-1})'' + m_\omega^2 (\ln m_\omega)'' \right) \right) \\ &\quad + (\mu_e - \mu_h) \frac{\partial}{\partial \omega} I_2 \omega^{\gamma+4} (-\mu_h n m' (1 - n) + \mu_e (1 - m) m n'). \end{aligned} \tag{4.22}$$

with can be written in a continuity equation form. It is straightforward task to write down constant-particle- flux solutions for (4.22).

The total energy of the combined electron-hole system is constant as well. Total electron and hole energies along with respective spectral energies are

given by

$$\begin{aligned}
E &= \int d\omega ((M_\omega + N_\omega)\omega + \epsilon_{gap} N_\omega), \\
E &= E^e + E^h + \epsilon_{gap} \int d\omega N_\omega, \\
E^e &= \int d\omega E_\omega^e, \quad E_\omega^e = \omega N_\omega, \\
E^h &= \int d\omega E_\omega^h, \quad E_\omega^h = \omega M_\omega.
\end{aligned} \tag{4.23}$$

The time evolution of spectral energy density $E_\omega = E_\omega^e + E_\omega^h$ is given by

$$\begin{aligned}
\dot{E}_\omega &= -\frac{I_1}{\mu_r} \omega \frac{\partial^2}{\partial \omega^2} \omega^{\gamma+6} \left(\mu_e \left(n_\omega^4 (n_\omega^{-1})'' + n_\omega^2 (\ln n_\omega)'' \right) \right. \\
&\quad \left. + \mu_h \left(m_\omega^4 (m_\omega^{-1})'' + m_\omega^2 (\ln m_\omega)'' \right) \right),
\end{aligned} \tag{4.24}$$

which can be presented as continuity equation for E_ω .

4.3 Boundary conditions.

Recall,

$$d\vec{k} = \Omega_0 k^{d-1} \frac{dk}{d\omega} = \frac{1}{2} \Omega_0 (2m_r)^{\frac{d}{2}} \omega^{\frac{d-2}{2}}. \tag{4.25}$$

Let us rewrite DKE's (4.11.4.12) in a form

$$\begin{aligned}
\dot{N}_\omega &= \frac{\partial^2}{\partial \omega^2} \mathcal{X} + \mu_e \frac{\partial}{\partial \omega} \mathcal{Y}, \\
\dot{M}_\omega &= \frac{\partial^2}{\partial \omega^2} \mathcal{Z} - \mu_h \frac{\partial}{\partial \omega} \mathcal{Y}, \\
\mathcal{X} &= \mu_e I_1 \omega^{\gamma+6} (-n'^2(2n-1) - nn''(1-n)) = \omega^s \mathcal{K}, \\
\mathcal{Y} &= I_2 \omega^{\gamma+4} \left(m_\omega n'_\omega (-1 + m_\omega) - \frac{\mu_e}{\mu_h} n_\omega m'_\omega (-1 + n_\omega) \right) = \omega^{s-2} \mathcal{M}, \\
\mathcal{Z} &= \mu_h I_1 \omega^{\gamma+6} (-m'^2(2m-1) - mm''(1-m)) = \omega^s \mathcal{L}.
\end{aligned} \tag{4.26}$$

Let us assume for a second that effective masses of electrons and holes are the same, moreover assume that $n_\omega = m_\omega$ initially. Then $\mathcal{Y} = 0$ initially in (4.26). It is easy to see then, that equations for $\dot{N}_\omega^{\text{elec}}$ and $\dot{N}_\omega^{\text{holes}}$ are the same. Therefore $n_\omega = m_\omega$ for all subsequent times because $\mathcal{Y} = 0$ for all times.

But now we know how to specify boundary conditions - in complete analogy with one particle case. Let us specify Q^e, Q^h, P^e, P^h at each side of computational domain and then use the wisdom of section (3.3.4).

Let us call $\mathcal{X}$ and $\mathcal{Z}$ terms “transport terms” as they transport particles and energy conservatively within subsystems. We can call the $\mathcal{Y}$ term “cross” term - it transports energy between subsystems. Note, that amount of energy taken from electrons is equal to amount of energy given to holes.

Let us now assume that $\mathcal{Y}$ term suddenly become nonzero. Then we still may specify Q^e, Q^h, P^e, P^h at the boundaries. Then the physical meaning of P^e and P^h will be somewhat arbitrary, only $P = P^e + P^h$ will have clear meaning. But we could still think of P^e and P^h as energy fluxes in subsystems. The energy will drive from one subsystem to another because of $\mathcal{Y}$ term, therefore we may think of P^e and P^h as being determined up to addition/subtraction of arbitrary same function. Then

$$\begin{aligned}
 Q^{(e)} &= \frac{\partial}{\partial \omega} \mathcal{X} + \mu_e \mathcal{Y} = s\omega^{s-1} \mathcal{K} + \omega^s \frac{\partial \mathcal{K}}{\partial \omega} + \mu_e \omega^{s-2} \mathcal{M} \\
 Q^{(h)} &= \frac{\partial}{\partial \omega} \mathcal{Z} - \mu_h \mathcal{Y} = s\omega^{s-1} \mathcal{L} + \omega^s \frac{\partial \mathcal{L}}{\partial \omega} - \mu_h \omega^{s-2} \mathcal{M} \\
 &= \\
 P^{(e)} &= \left(\mathcal{X} - \omega \frac{\partial \mathcal{X}}{\partial \omega} \right) = \omega^s \mathcal{K} (1 - s) - \omega^{s+1} \frac{\partial \mathcal{K}}{\partial \omega} \\
 P^{(h)} &= \left(\mathcal{Z} - \omega \frac{\partial \mathcal{Z}}{\partial \omega} \right) = \omega^s \mathcal{L} (1 - s) - \omega^{s+1} \frac{\partial \mathcal{L}}{\partial \omega}.
 \end{aligned} \tag{4.27}$$

From the definition of P fluxes it follows

$$\begin{aligned}\frac{\partial \mathcal{K}}{\partial \omega} &= \omega^{-s} (\mathcal{K} \omega^{s-1} (1-s) - P^{(e)}/\omega) \\ \frac{\partial \mathcal{L}}{\partial \omega} &= \omega^{-s} (\mathcal{L} \omega^{s-1} (1-s) - P^{(h)}/\omega).\end{aligned}\tag{4.28}$$

We substitute it to the equations for Q 's to get

$$\begin{aligned}Q^{(e)} &= \mu_e \omega^{s-2} \mathcal{M} + \omega^{s-1} \mathcal{K} - P^{(e)}/\omega \\ Q^{(h)} &= -\mu_h \omega^{s-2} \mathcal{M} + \omega^{s-1} \mathcal{L} - P^{(h)}/\omega.\end{aligned}\tag{4.29}$$

or

$$\begin{aligned}\omega^{1-s}(Q^{(e)}\omega + P^{(e)}) &= \\ &I_2 \mu_e (\mu_e m_\omega n'_\omega (1 - m_\omega) - \mu_h n_\omega m'_\omega (1 - n_\omega)) \\ &+ \mu_e I_1 \omega (-n'^2 (2n - 1) - n n'' (1 - n)) \\ \omega^{1-s}(Q^{(h)}\omega + P^{(h)}) &= \\ &-I_2 \mu_h (\mu_e m_\omega n'_\omega (1 - m_\omega) - \mu_h n_\omega m'_\omega (1 - n_\omega)) \\ &+ (I_1 \mu_h) \omega (-m'^2 (2m - 1) - m m'' (1 - m)).\end{aligned}\tag{4.30}$$

We now use the relations between first and second derivatives at the boundaries of computational domain, analogous to (3.92). We write them in a form

$$\begin{aligned}n' &= \alpha + \beta n'', \quad m' = \gamma + \delta m'' \\ \text{Left side} \quad \alpha &= (n_2 - n_1)/\Delta, \quad \beta = \delta = -\Delta/2, \quad \gamma = (m_2 - m_1)/\Delta, \\ \text{Right side} \quad \alpha &= (n_N - n_{N-1})/\Delta, \quad \beta = \delta = \Delta/2, \quad \gamma = (m_N - m_{N-1})/\Delta,\end{aligned}\tag{4.31}$$

Then one gets the system of equations for n'' and m''

$$\begin{aligned}
a_1 n''^2 + b_1 n'' + c_1 + d_1 m'' &= 0 \\
a_2 m''^2 + b_2 m'' + c_2 + d_2 n'' &= 0 \\
a_1 &= -(\beta^2 I_1 \mu_e (-1 + 2n) \omega) \\
b_1 &= \beta I_2 (-1 + m) m \mu_e^2 - I_1 \mu_e (1 - n) n \omega - 2\alpha \beta I_1 \mu_e (-1 + 2n) \omega \\
c_1 &= -\omega^{1-s} (Q^{(e)} \omega + P^{(e)}) + \alpha I_2 (-1 + m) m \mu_e^2 \\
&\quad - \gamma I_2 \mu_e \mu_h (-1 + n) n - \alpha^2 I_1 \mu_e (-1 + 2n) \omega \\
d_1 &= -(\delta I_2 \mu_e \mu_h (-1 + n) n) \\
a_2 &= -(\delta^2 I_1 (-1 + 2m) \mu_h \omega) \\
b_2 &= \delta I_2 \mu_h^2 (-1 + n) n - I_1 (1 - m) m \mu_h \omega - 2\delta \gamma I_1 (-1 + 2m) \mu_h \omega \\
c_2 &= -\omega^{1-s} (Q^{(h)} \omega + P^{(h)}) - \alpha I_2 (-1 + m) m \mu_e \mu_h + \\
&\quad \gamma I_2 \mu_h^2 (-1 + n) n - \gamma^2 I_1 (-1 + 2m) \mu_h \omega \\
d_2 &= -(\beta I_2 (-1 + m) m \mu_e \mu_h).
\end{aligned} \tag{4.32}$$

Equations (4.32) may be transformed into single *quartic* equation for, say, n'' . Although analytical solution for quartic equation is available, a quartic equation has four roots (fundamental theorem of algebra). Not to deal with root selections, we solve (4.32) iteratively at each time step.

4.4 Numerical Results.

Here we present results of a couple of numerical experiments.

Let us take as an initial condition two Fermi-Dirac distributions with different temperatures and model their evolution as given by 2DQKE. Results are shown below in figures (4.1).

FIGURE 4.1. Evolution of electron (a) and hole (b) distribution functions as given by the 2DQKE.

Initial distributions, chosen to be Fermi Dirac distributions, are shown by thin lines. Final distributions are shown by thick lines. Final Distributions are Fermi-Dirac Distributions with the equal temperatures. Vertical axis is the value of distribution function, horizontal axis is the frequency in meV.

To check if final distributions has the same temperature, we introduce “temperature” of the distribution as

$$T^e = \frac{\mu_r}{\mu_e} \left[\frac{\partial}{\partial \omega} \frac{1}{\omega_1 - \omega_2} \int_{\omega_1}^{\omega_2} d\omega \log((1/n_\omega - 1)) \right]^{-1}. \quad (4.33)$$

for electrons and

$$T^h = \frac{\mu_r}{\mu_h} \left[\frac{\partial}{\partial \omega} \frac{1}{\omega_1 - \omega_2} \int_{\omega_1}^{\omega_2} d\omega \log((1/m_\omega - 1)) \right]^{-1}. \quad (4.34)$$

for holes. Then, if a distributions are Fermi-Dirac distributions (4.14) we have

$$\begin{aligned} \frac{\mu_r}{\mu_e} \left[\frac{\partial}{\partial \omega} \log((1/n_\omega - 1)) \right]^{-1} &= T_e, \\ \frac{\mu_r}{\mu_h} \left[\frac{\partial}{\partial \omega} \log((1/m_\omega - 1)) \right]^{-1} &= T_h. \end{aligned} \quad (4.35)$$

Then the evolution of electrons and holes “temperatures”, in a (4.33,4.34) sense, are shown on figure (4.2). We see that the equilibrium corresponds to electrons and holes having the same temperature. We check that the final distributions are indeed of the form (4.14) so that our definition of “temperature” is well defined.

Let us take as an initial condition two arbitrary distributions (distorted Fermi-Dirac Distributions) and model their evolution as given by 2DQKE. Results are shown below in figures (4.3). We see that distributions first tend to become FD-like and then they equilibrate their temperatures.

To check if final distributions has the same temperature again calculate the “temperature” of electrons and hole. Results are shown shown on figure (4.4): We see that the equilibrium corresponds to electrons and holes having the same temperature. We check that the final distributions are indeed of the form (4.14) so that our definition of “temperature” is well defined.

FIGURE 4.2. Evolution of electrons and holes “temperature”. Temperature of electrons is shown by short-dashed line and temperature of holes is shown by long-dashed line. “Temperature” is defined as (4.33) for electrons and (4.34) for holes. We see, that equilibrium corresponds to electrons and holes having the same “temperature”. Time shown in arbitrary units.

FIGURE 4.3. Evolution of electron (a) and hole (b) distribution functions as given by 2DQKE.

Initial distributions, chosen to be distorted Fermi Dirac distributions, are shown by thin lines. Few intermediate states are shown by dashed lines. Final distributions are shown by thick lines. Final Distributions are Fermi-Dirac Distribution with equal temperatures. Vertical axis is the value of distribution function, horizontal axis is the frequency in meV.

FIGURE 4.4. Evolution of electrons and holes “temperature”. Temperature of electrons is shown by short-dashed line and temperature of holes is shown by long-dashed line. We see, that equilibrium corresponds to electrons and holes having the same “temperature”. Time shown in arbitrary units. Note that until distribution reaches Fermi-Dirac state, our definition of the temperature has little or no sense.

4.5 Setup for input-output fluxes for the case of semiconductor.

Taking into account that the conduction band is separated by the energy $\mathcal{E}_{gap}$ from the valence band, we generalize (3.56) for the case of semiconductor. There we have (see Figure (4.5)) four particle fluxes $Q_L^e, Q_L^h, Q_R^e, Q_R^h$ and energy fluxes P_L, P_R across inertial ranges.

Then (3.56) generalizes to

$$\begin{aligned}
 Q_0^e &= Q_L^e - Q_R^e \\
 Q_0^h &= Q_L^h - Q_R^h \\
 -P_0 = P_R - P_L &= (\epsilon_{gap} + \omega_0 \frac{\mu_r}{\mu_e}) Q_0^e + \omega_0 \frac{\mu_r}{\mu_h} Q_0^h \\
 -P_L &= (\epsilon_{gap} + \omega_L \frac{\mu_r}{\mu_e}) Q_L^e + \omega_L \frac{\mu_r}{\mu_h} Q_L^h \\
 -P_R &= (\epsilon_{gap} + \omega_R \frac{\mu_r}{\mu_e}) Q_R^e + \omega_R \frac{\mu_r}{\mu_h} Q_R^h.
 \end{aligned} \tag{4.36}$$

The first two relations in (4.36) express conservation of particles - electrons and holes. Third relation expresses the conservation of total energy. The last two express the fact that total energy carried to ω_L (ω_R) get absorbed there.

Charge neutrality is equivalent to one particle case. Let us assume that the rates of adding electrons and holes to the system are the same. Therefore we choose $Q_0^e = Q_0^h$ (charge neutrality means that electron and hole inputs are the same). Furthermore, assume that $Q_L^e = Q_L^h = Q_L$. In the semiconductor laser context this correspond to stating that operating laser uses the same amount of electrons and holes to operate (every electron needs a hole to

FIGURE 4.5. Setup for input-output fluxes.

Carriers and energy are added at ω_0 . The rate of adding electrons is $Q_0^{(e)}$, the rate of adding holes is $Q_0^{(h)}$. The rate of adding energy is P_0 . Energy and some carriers are dissipated at $\omega_R > \omega_0$ (an idealization) and carriers and some energy are absorbed by the laser at ω_L . Finite flux stationary solutions are realized in the windows (ω_L, ω_0) and (ω_0, ω_R) although in practice there will be some losses through both of these regions. The electron and hole fluxes to the left are $Q_L^{(e)}$ and $Q_L^{(h)}$ respectively. The electron and hole fluxes to the right are $Q_R^{(e)}$ and $Q_R^{(h)}$ respectively. The rate of energy flowing to the left (right) is P_L (P_R). Note that fluxes of particles is defined to be positive if flow leftwards, therefore $Q_L^s > 0$, $Q_R^s < 0$. Energy fluxes are defined to be positive if flow rightwards thus $P_L < 0$, $P_R > 0$.

recombine with). Now (4.36) gives

$$\begin{aligned}
 Q_0^e &= Q_0^h = Q_0 \\
 Q_L^e &= Q_L^h = Q_L \\
 Q_R^e &= Q_R^h = Q_R \\
 Q_0 &= Q_L - Q_R \\
 -P_0 &= P_R - P_L = (\epsilon_{gap} + \omega_0)Q_0 \\
 -P_L &= (\epsilon_{gap} + \omega_L)Q_L \\
 -P_R &= (\epsilon_{gap} + \omega_R)Q_R.
 \end{aligned}
 \tag{4.37}$$

We introduced Q_0 - number of added electrons (and holes), Q_L electron (and hole) flux to the left, Q_R electron (and hole) flux to the right and used the fact $1/\mu_r = 1/\mu_e + 1/\mu_h$. Note that this is generalization of (3.56) for the case of semiconductors, when the conduction band is separated from the valence band by the energy gap. Solving (4.37) we get⁵

$$\begin{aligned}
 P_R &= -\frac{(\omega_0 - \omega_L)(\epsilon_{gap} + \omega_R)Q_0}{(\omega_L - \omega_R)}, \\
 P_L &= -\frac{(\epsilon_{gap} + \omega_L)(\omega_0 - \omega_R)Q_0}{(\omega_L - \omega_R)}, \\
 Q_L &= \frac{(\omega_0 - \omega_R)Q_0}{(\omega_L - \omega_R)}, \\
 Q_R &= \frac{(\omega_0 - \omega_L)Q_0}{(\omega_L - \omega_R)}
 \end{aligned}
 \tag{4.38}$$

This is nothing but generalization of (3.56). Note that total input energy is given by

$$-P_0 = P_R - P_L = (\epsilon_{gap} + \omega_0)Q_0.$$

⁵Remember, $\hbar = 1$ in Chapters 3 and 4 so that all frequencies are measured in energy units. That is why we have terms like $(\epsilon_{gap} + \omega_R)$. Strictly speaking we should write such terms as $(\epsilon_{gap} + \hbar\omega_R)$.

Also

$$\frac{Q_L}{Q_0} = \frac{\omega_R - \omega_0}{\omega_R - \omega_L}. \quad (4.39)$$

It means that only $\frac{\omega_R - \omega_0}{\omega_R - \omega_L}$ portion of the input particle flux goes to the left to the lasing region. If possible we would like to design lasers to maximize this ratio. This ratio is equal to unity for $\omega_r \rightarrow \infty$ so that to design a better laser we would like to push high frequency sink as far to the right as possible.

Chapter 5

PHONONS

Phonon - quantum of lattice vibrational energy. In analogy to a photon, the phonon can be viewed as a wave packet with particle-like properties.

5.1 System Hamiltonian.

One of the principle sinks of energy (besides lasing and inhomogeneous broadening) of pumped semiconductor is the material lattice vibrations (called phonons) which interacts with electrons and holes through what is called carrier-phonons collisions.

We are going to simplify descriptions of phonons by taking equal mass, single species approximation so as to develop general ideas.

The extra term in the Hamiltonian describing this interaction is

$$\mathcal{H}_{e-p} = \sum_k \epsilon_k a_k^\dagger a_k + \sum_q \hbar \omega_q c_q^\dagger c_q + \sum_{\mathbf{k}, \mathbf{q}} \hbar G_q a_{\mathbf{k}+\mathbf{q}}^\dagger a_{\mathbf{k}} (c_{\mathbf{q}} + c_{-\mathbf{q}}^\dagger). \quad (5.1)$$

where $a_{\mathbf{q}}, a_{-\mathbf{q}}^\dagger$ are the annihilation and creation operators of electrons and $c_{\mathbf{q}}, c_{-\mathbf{q}}^\dagger$ are the annihilation and creation operators of phonons. *In this Chapter* we assume that ϵ_k is the energy of electrons *including* band gap energy: $\epsilon_k = \epsilon_{gap} + \epsilon_{e,k}$. Since the number of electrons is conserved and only energy differences enters into resulting kinetic equations, it will not affect the final result.

The matrix element of the interaction is *screened* Coulomb potential:

$$G_q^2 = \frac{4\pi e^2}{q^2 + \kappa^2}. \quad (5.2)$$

The first term in the Hamiltonian is the electron kinetic energy, the second is phonon kinetic energy and third is the phonon-electron interaction term.

Later we will restrict our consideration to LO (longitudinal optical) phonons only.

In principle, one should add to the Hamiltonian electron-electron interaction part which will lead to the QKE considered in the first part, and Phonon-phonon interaction terms. However, we will use the concept of “heat bath” and assume phonons to be in thermodynamical equilibrium with themselves.

5.2 Equation of motion.

Phononic equations of motion ($i\hbar\dot{F} = [F, H]$):

$$\begin{aligned}
 i\hbar\dot{a}_k &= \epsilon_k a_k + \sum_q G_q (c_{-q}^\dagger + c_q) a_{k-q} \\
 i\hbar\dot{a}_k^\dagger &= -\epsilon_k a_k - \sum_q G_q^* (c_{-q} + c_q^\dagger) a_{k-q} \\
 i\hbar\dot{c}_k &= \hbar\omega_q c_q + \sum_q G_{-q} a_{k-q}^\dagger a_k \\
 i\hbar\dot{c}_k^\dagger &= -\hbar\omega_q c_q - \sum_q G_{-q}^* a_k^\dagger a_{k-q}.
 \end{aligned}
 \tag{5.3}$$

5.3 Kinetic Equation for carrier-phonon scattering.

We are interested in time evolution of $n_k = \langle a_k^\dagger a_k \rangle$ which is going to depend on

$g_q = \langle c_k^\dagger c_k \rangle$. Then

$$\begin{aligned}
 i\hbar\dot{n}_k &= \sum_q G_q (T_{kq}^I + G_q T_{kq}^{II} - G_q^* T_{kq}^{III} - G_q^* T_{kq}^{IV}), \\
 T_{kq}^I &= b_{-q}^\dagger a_k^\dagger a_{k-q}, \\
 T_{kq}^{II} &= c_q a_k^\dagger a_{k-q}, \\
 T_{kq}^{III} &= c_q a_{k-q}^\dagger a_k, \\
 T_{kq}^{IV} &= c_q^\dagger a_{k-q}^\dagger a_k.
 \end{aligned} \tag{5.4}$$

Then one has to write down the equations of time evolution for the T_{kq} 's. The RHS of the resulting equations may be factorized by using Hartree-Fock factorization. Then, for example,

$$i\hbar\dot{T}_{kq}^I = (\epsilon_{k-q} - \hbar\omega_{-q} - \epsilon_k) (G_q^* n_{k-q}(n_k - 1) + G_{-q} g_{-q} n_k - G_q^* g_{-q} n_{k-q}). \tag{5.5}$$

and one can formally integrate this equation in time to get

$$i\hbar T_{kq}^I = \int_{t_0}^t dt' e^{-\frac{i}{\hbar}(\epsilon_{k-q} - \hbar\omega_{-q} - \epsilon_k)(t-t')} (G_q^* n_{k-q}(n_k - 1) + G_{-q} g_{-q} n_k - G_q^* g_{-q} n_{k-q}). \tag{5.6}$$

Assuming, that the interaction term is varying slowly compared to the exponentials, we evaluate the integral by moving n, N terms out of the integral:

$$i\hbar T_{kq}^I = \frac{(G_q^* n_{k-q}(n_k - 1) + G_{-q} g_{-q} n_k - G_q^* g_{-q} n_{k-q})}{-\frac{i}{\hbar}(\epsilon_{k-q} - \hbar\omega_{-q} - \epsilon_k) - \gamma}, \tag{5.7}$$

where we phenomenologically added a decay constant γ to the denominator.

The resulting KE is

$$\begin{aligned} \frac{dn_k}{dt} \Big|_{e-p} = & -2\pi \sum_q G_q^2 \\ & \times (\delta(\epsilon_k - \epsilon_{k-q} - \hbar\omega_0) (n_k(1 - n_{k-q})(g_q + 1) - (1 - n_k)n_{k-q}g_q) \\ & + \delta(\epsilon_k - \epsilon_{k-q} + \hbar\omega_0) (n_k(1 - n_{k-q})g_{-q} - (1 - n_k)n_{k-q}(g_{-q} + 1))) . \end{aligned} \quad (5.8)$$

The meaning of this equation is transparent:

- The first term in first line $n_k(1 - n_{k-q})(g_q + 1)$ describes the emission of the phonon with momentum q by $k \rightarrow (k - q)$ electron scattering
- The second term in first line $(1 - n_k)n_{k-q}g_q$ describes the absorption of phonon by $(k - q) \rightarrow k$ electron scattering
- The first term in second line $n_k(1 - n_{k-q})g_{-q}$ describes the absorption of the phonon with momentum $-q$ due to $k \rightarrow (k - q)$ electron scattering
- The second term in second line $(1 - n_k)n_{k-q}(g_{-q} + 1)$ describes phonon emission due to $(k - q) \rightarrow k$ electron scattering

It is a mixed fermionic (electron)- boson (phonon) equation, similar to a three-wave equation. The probability of electron $k_1 \rightarrow k_2$ electron scattering is proportional to $n_{k_1}(1 - n_{k_2})$, and the probability of absorbing (emitting) phonon is proportional to $g_k (1 + g_k)$. We now make this equation look nicer by introducing integration instead of summation. Assume, that we redefine

G_q in such a way, that it contains all volume factors. Then

$$\begin{aligned}
\frac{dn_k}{dt} \Big|_{e-p} &= -2\pi \int d\mathbf{q} d\mathbf{p} \delta(\mathbf{p} - \mathbf{k} + \mathbf{q}) G_q^2 \\
&\times (\delta(\epsilon_k - \epsilon_p - \hbar\omega_0) (n_k(1 - n_p)(g_q + 1) - (1 - n_k)n_p g_q) \\
&+ \delta(\epsilon_k - \epsilon_p + \hbar\omega_0) (n_k(1 - n_p)g_{-q} - (1 - n_k)n_p(g_{-q} + 1))) .
\end{aligned} \tag{5.9}$$

Let us assume spherical isotropy. Then the interaction coefficient is invariant with regards to rotations in $\mathbf{k}$ -space and, consequently may be considered as a function of only absolute values of wave vectors. Since $\omega(k)$ and n_k are also isotropic, then the only angular dependence is in the delta-function of the wavevectors. Then for $d = 2$ here, $d = 3$ earlier

$$\begin{aligned}
&\int \delta(k - k_1 \cos \theta_1 - k_2 \cos \theta_2) \delta(k_1 \sin \theta_1 + k_2 \sin \theta_2) d\theta_1 d\theta_2 \\
&= (k k_1 \sin \theta_1)^{-1} = \Delta_2^{-1}
\end{aligned}$$

where Δ_2 is the area of triangle formed by the vectors k, k_1, k_2 :

$$\Delta_2 = (1/2) (2(k^2 k_1^2 + k^2 k_2^2 + k_1^2 k_2^2) - k^4 - k_1^4 - k_2^4)^{1/2} .$$

In the same way, for $d = 3$ introducing the spherical coordinates (k, θ, ϕ) :

$$\begin{aligned}
&\int (k - k_1 \cos \theta_1 - k_2 \cos \theta_2) \delta(k_1 \sin \theta_1 \sin \phi_1 + k_2 \sin \theta_2 \sin \phi_2) \\
&\times \delta(k_1 \sin \theta_1 \cos \phi_1 + k_2 \sin \theta_2 \cos \phi_2) d\cos \theta_1 d\phi_1 d\cos \theta_2 d\phi_2 = \\
&\int \delta(k - k_1 \cos \theta_1 - k_2 \cos \theta_2) \delta(k_1 \sin \theta_1 + k_2 \sin \theta_2) \frac{\sin \theta_1 d\theta_1 d\theta_2}{2k_2} \\
&= \frac{1}{2k k_1 k_2} = \Delta_3 .
\end{aligned} \tag{5.10}$$

We then change the integration from modulus of wavevectors to the frequency space via $\omega(p) = \omega_p$:

$$\begin{aligned} \frac{dn_\omega}{dt}_{e-p} &= -2\pi \frac{1}{k^{d-1}\Omega_0(dk/d\omega)} \times \int d\omega_p d\omega_q S_{\omega,\omega_p,\omega_q}^{\text{phon}} \\ &\times \left(\delta(\omega_k - \omega_p - \omega_0) (n_\omega(1 - n_{\omega_p})(g_{\omega_q} + 1) - (1 - n_\omega)n_{\omega_p}g_q) \right. \\ &\left. + \delta(\omega - \omega_p + \omega_0) (n_\omega(1 - n_{\omega_p})g_{\omega_q} - (1 - n_\omega)n_{\omega_p}(g_{\omega_q} + 1)) \right). \end{aligned} \quad (5.11)$$

where $S_{\omega,\omega_p,\omega_q}^{\text{phon}}$ is angle-averaged potential with all the necessary factors, namely

$$S_{\omega,\omega_p,\omega_q}^{\text{phon}} = \frac{dkdpdq}{d\omega d\omega_p d\omega_q} (kpq)^{d-1} \Delta_d G_{k,p,q}. \quad (5.12)$$

We then rewrite KE as

$$\begin{aligned} \frac{dn_\omega}{dt}_{e-p} &= -2\pi \frac{1}{k^{d-1}\Omega_0(dk/d\omega)} \times \int d\omega_1 d\omega_2 S_{\omega,\omega_1,\omega_2}^{\text{phon}} \\ &\times \left(\delta(\omega_k - \omega_1 - \omega_0) (n_\omega(1 - n_1)(g_2 + 1) - (1 - n_\omega)n_1g_2) \right. \\ &\left. + \delta(\omega - \omega_1 + \omega_0) (n_\omega(1 - n_1)g_2 - (1 - n_\omega)n_1(g_2 + 1)) \right). \end{aligned} \quad (5.13)$$

Now we use the known fact, that optical phonon dominates the process of electron cooling. We then limit our consideration of phonons to LO phonons. Then for optical phonons (in Einstein approximation) its population is frequency-independent function, which should be computed self-consistently. Therefore, after dropping the argument of g , the integration

over ω_2 can be easily performed:

$$\begin{aligned} \frac{dn_\omega}{dt}_{e-p} = & -2\pi \frac{1}{k^{d-1}\Omega_0(dk/d\omega)} \times \int d\omega_1 S_{\omega,\omega_1}^{\text{phon}} \\ & \times (\delta(\omega_k - \omega_1 - \omega_0) (n_\omega(1 - n_1)(g + 1) - (1 - n_\omega)n_1g) \\ & + \delta(\omega - \omega_1 + \omega_0) (n_\omega(1 - n_1)g_\omega - (1 - n_\omega)n_1(g + 1))) . \end{aligned} \quad (5.14)$$

with $S_{\omega,\omega_1}^{\text{phon}} = \int d\omega_2 S_{\omega,\omega_1,\omega_2}^{\text{phon}}$. The integration over ω_1 is again can be easily performed by using the delta-function:

$$\begin{aligned} \frac{dn_\omega}{dt}_{e-p} = & -2\pi \frac{1}{k^{d-1}\Omega_0(dk/d\omega)} \times \\ & \times \left(S_{\omega,\omega-\omega_0}^{\text{phon}} (n_\omega(1 - n_{\omega-\omega_0})(g + 1) - (1 - n_\omega)n_{\omega-\omega_0}g) \right. \\ & \left. + S_{\omega,\omega+\omega_0}^{\text{phon}} (n_\omega(1 - n_{\omega+\omega_0})g - (1 - n_\omega)n_{\omega+\omega_0}(g + 1)) \right) . \end{aligned} \quad (5.15)$$

The phonons, however, are often considered to be in thermal equilibrium with the room temperature (heat bath), so we may take

$$g_\omega = \frac{1}{\exp\left(\frac{\hbar\omega_0}{kT}\right) - 1} . \quad (5.16)$$

which is Bose-Einstein distribution with zero chemical potential (for obvious reasons phonons has zero chemical potential¹). For typical Ga As the ω_0 is 36 meV, while room temperature correspond to 25 meV, thus the concentration of optical phonons is about 0.5. It is easy to see, that if n_ω is FD with the same temperature as (5.16), then the RHS of (5.15) is zero.

¹The chemical potential by the definition is $\mu = \frac{\partial F}{\partial N}$ where F is the systems free energy and N is number of particles. Since phonons are quasi particles which can be created or annihilated, the number of phonons is defined self consistently by $\frac{\partial F}{\partial N} = 0$, so that chemical potential of phonons is indeed zero.

5.4 Stability of FD distribution.

Suppose we perturbed initial carrier Fermi-Dirac distribution by some small perturbation. Then it is again easy to see, that in leading order the perturbation will try to decrease in magnitude, so that (5.15) drives the system towards thermodynamical equilibrium with temperature of the phonon gas. Indeed, let

$$n_{\omega} = \frac{1}{\exp(\alpha\omega + \beta) + 1} + m_{\omega} \quad g_{\omega} = \frac{1}{\exp(\alpha\omega_0) - 1},$$

where $m_{\omega} \ll 1$ is the small local perturbation having its support around ω_{pert} . Then (5.15) takes the form

$$\begin{aligned} \frac{dm_{\omega_{\text{pert}}}}{dt} \Big|_{e-p} &= -2\pi \frac{1}{k^{d-1} \Omega_0 (dk/d\omega_{\text{pert}})} \times \\ &\times \left(S_{\omega_{\text{pert}}, \omega_{\text{pert}} - \omega_0}^{\text{phon}} (m_{\omega_{\text{pert}}} (1 - n_{\omega_{\text{pert}} - \omega_0}) (g + 1) + \right. \\ &\quad \left. m_{\omega_{\text{pert}}} n_{\omega_{\text{pert}} - \omega_0} g) \right. \\ &\quad \left. + S_{\omega_{\text{pert}}, \omega + \omega_0}^{\text{phon}} (m_{\omega_{\text{pert}}} (1 - n_{\omega_{\text{pert}} + \omega_0}) g + \right. \\ &\quad \left. m_{\omega_{\text{pert}}} n_{\omega_{\text{pert}} + \omega_0} (g + 1)) \right). \end{aligned} \tag{5.17}$$

It is now easy to see, that m_{ω} decays with time exponentially (remember $0 \leq n_k \leq 1$), so that carrier-phonon interaction tries to bring carrier distribution towards thermodynamical equilibrium.

5.5 Phononic conclusion.

To consider the time evolution of LO phonon concentration self consistently, one has to take into account acoustical phonons and consider electron-phonon (acoustic), electron-phonon(optical), and acoustic-optical phonon interactions (along with interactions of phonons within themselves). However, the

electron-acoustic phonon interactions are three to four orders of magnitude slower, than electron-optical phonon interactions, which in term, say, five times slower than carrier-carrier interaction. Therefore in what follows we will include carrier-carrier interaction phenomenologically through pumping-damping terms.

Chapter 6

LIGHT-MATTER INTERACTION

6.1 Polarization.

6.1.1 Classical definition of polarization.

How does matter react to an external electric field?

Let us first consider a “classical” crystal, where the electrons are bound to positively charged ions which are, fixed in space. Then an external electric field (assumed to be polarized in x direction) causes a displacement $\mathbf{r}$ of an electron with charge e from its equilibrium position. This results in chain acquiring some dipole moment. Let us define *polarization* as dipole moment per unit volume :

$$\mathbf{P} = \frac{\mathbf{P}}{L^3} = -n_0 e \mathbf{r} = -n_0 \mathbf{d}, \quad (6.1)$$

where $\mathcal{V} = L^3$ is the volume of a crystal, $\mathbf{d} = e \mathbf{r}$ is the electric dipole moment, n_0 is the average electron density.

The electron acquires some additional energy due to interaction with electric field so that interaction Hamiltonian is equal to

$$H_I = -e \mathbf{r} \mathcal{E} = -\mathbf{d} \mathcal{E}, \quad (6.2)$$

where $\mathcal{E}$ is external applied electrical field.

6.1.2 The Interband polarization.

In this manuscript we consider electromagnetic effects *semiclassically*. That is to say we introduce classical electrical fields instead of writting down photonic Hamiltonian with photonic creation/annihilation operators. Let us

consider a situation, when an electron is excited from the valence band to the conduction band by, say, absorbing a light quantum. Then there is a positively charged quasi particle left behind - a hole. Then an interband polarization is created: two charged particles separated by some distance. Let us define the macroscopic inter band polarization as the average value of the electric dipole $e\mathbf{r}$:

$$\mathbf{P}(t) = \int d\mathbf{r} \left\langle \hat{\psi}^\dagger(\mathbf{r}, t) e\mathbf{r} \hat{\psi}(\mathbf{r}, t) \right\rangle, \quad (6.3)$$

where $\hat{\psi}^\dagger(\mathbf{r}, t)$, $\hat{\psi}(\mathbf{r}, t)$ are *field operators* see (2.37). In the case of a spatially homogeneous system, the Bloch wave functions $\psi(\mathbf{k}, \mathbf{r})$ may be used as an appropriate basis for expanding the field operators:

$$\hat{\psi}(\mathbf{r}, t) = \sum_{\mathbf{k}, \lambda=c,v} a_{\lambda\mathbf{k}} \psi_\lambda(\mathbf{k}, \mathbf{r}), \quad (6.4)$$

Inserting (6.4) into (6.3) one gets:

$$\mathbf{P}(t) = \sum_{\lambda, \lambda', \mathbf{k}, \mathbf{k}'} \langle a_{\lambda\mathbf{k}}^\dagger a_{\lambda'\mathbf{k}'} \rangle \int d\mathbf{r} \psi_\lambda^*(\mathbf{k}, \mathbf{r}) e\mathbf{r} \psi_{\lambda'}(\mathbf{k}', \mathbf{r}). \quad (6.5)$$

This integral is computed in the literature. (see, e.g. [25]). The result for polarization of a spatially homogeneous system is given by

$$\mathbf{P}(t) = \sum_{\lambda, \lambda', \mathbf{k}} \langle a_{\lambda\mathbf{k}}^\dagger a_{\lambda'\mathbf{k}} \rangle \mathbf{d}_{\lambda\lambda'\mathbf{k}} = \sum_{\lambda, \lambda', \mathbf{k}} p_{\lambda\lambda'\mathbf{k}} \mathbf{d}_{\lambda\lambda'\mathbf{k}}, \quad (6.6)$$

where we defined polarization pair function

$$p_{\lambda\lambda'\mathbf{k}} = \langle a_{\lambda\mathbf{k}}^\dagger a_{\lambda'\mathbf{k}} \rangle. \quad (6.7)$$

The optical dipole matrix element $\mathbf{d}_{\lambda\lambda'\mathbf{k}}$ is commonly taken to be

$$d_{\lambda\lambda'\mathbf{k}} = \frac{d_{k=0}}{(1 + \epsilon_k/\epsilon_{\text{gap}})}, \quad (6.8)$$

$d_{k=0}$ is dipole matrix element value for $k = 0$ point. In second quantization the Hamiltonian of matter interacting with the light acquires the form:

$$\mathcal{H}_I = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r})(-e\mathbf{r})\mathcal{E}(\mathbf{r}, t)\hat{\psi}(\mathbf{r}). \quad (6.9)$$

Let us consider the case when electric field has a monochromatic spacial dependence

$$\mathcal{E}(\mathbf{r}, t) = \mathcal{E}(t) (\exp(i\mathbf{q} \cdot \mathbf{r}) + c.c.), \quad (6.10)$$

and using expansion (6.4) for spatially homogeneous systems, one gets:

$$\mathcal{H}_I \simeq - \sum_{\mathbf{k}} \mathcal{E}(t) (a_{c,\mathbf{k}}^\dagger a_{v,\mathbf{k}} d_{\mathbf{k}} + a_{c,\mathbf{k}} a_{v,\mathbf{k}}^\dagger d_{\mathbf{k}}^*), \quad (6.11)$$

6.2 Many Body Hamiltonian

Consider the semiconductor system with electrons and holes interacting with electric field. The model Hamiltonian is then the sum of interaction Hamiltonian (6.11) and electron-hole interaction Hamiltonian (2.55):

$$\begin{aligned} H = & \hbar \sum_{\mathbf{k}} ((\epsilon_{ek} + \epsilon_{gap}) a_{\mathbf{k}}^+ a_{\mathbf{k}} + \epsilon_{hk} b_{-\mathbf{k}}^+ b_{-\mathbf{k}}) \\ & + \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}', \mathbf{q} \neq 0} V_{\mathbf{q}} (a_{\mathbf{k}+\mathbf{q}}^+ a_{\mathbf{k}'-\mathbf{q}}^+ a_{\mathbf{k}'} a_{\mathbf{k}} + b_{\mathbf{k}+\mathbf{q}}^+ b_{\mathbf{k}'-\mathbf{q}}^+ b_{\mathbf{k}'} b_{\mathbf{k}} - 2a_{\mathbf{k}+\mathbf{q}}^+ b_{\mathbf{k}'-\mathbf{q}}^+ b_{\mathbf{k}'} a_{\mathbf{k}}) \\ & - \sum_{\mathbf{k}} \mathcal{E} (d_{\mathbf{k}} a_{\mathbf{k}}^+ b_{-\mathbf{k}}^+ + d_{\mathbf{k}}^* a_{\mathbf{k}} b_{-\mathbf{k}}) \end{aligned} \quad (6.12)$$

where $a_{\mathbf{k}}^\dagger, a_{\mathbf{k}}, b_{\mathbf{k}}^\dagger, b_{\mathbf{k}}$ are creation/annihilation operators for electrons and holes, $\mathcal{E}$ is the value of electrical field (scalar), $V_{\mathbf{q}}$ is the screened Coulomb potential (2.54). We are interested in obtaining the set of equations for

density of electrons, holes and polarization. These quantities are given in this representation as

$$\begin{aligned} p_{\mathbf{k}} &= \langle b_{-\mathbf{k}} a_{\mathbf{k}} \rangle, \\ n_{\mathbf{k}} &= \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle, \\ m_{\mathbf{k}} &= \langle b_{-\mathbf{k}}^{\dagger} b_{-\mathbf{k}} \rangle. \end{aligned} \tag{6.13}$$

6.3 Semiconductor Bloch Equations

To obtain the time evolution of these operators we use the Heisenberg equation: $\dot{X}_{\mathbf{k}} = \frac{i}{\hbar}[H, X]$ with Hamiltonian (6.12) and fermionic commutation relations (2.39) The result is

$$\begin{aligned} \dot{p}_{\mathbf{k}} &= -\epsilon_{\mathbf{k}} p_{\mathbf{k}} - \frac{i}{\hbar} d_{\mathbf{k}} E(z, t) (n_{\mathbf{k}} + m_{\mathbf{k}} - 1) \\ &\quad + \frac{i}{\hbar} \sum_{\mathbf{k}', \mathbf{q} \neq 0} V_{\mathbf{q}} \left[\langle a_{\mathbf{k}'+\mathbf{q}}^{\dagger} b_{-\mathbf{k}} a_{\mathbf{k}'} a_{\mathbf{k}+\mathbf{q}} \rangle + \langle b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{\mathbf{k}'} a_{\mathbf{k}} b_{-\mathbf{k}-\mathbf{q}} \rangle \right. \\ &\quad \left. - \langle a_{\mathbf{k}'+\mathbf{q}}^{\dagger} b_{-\mathbf{k}'+\mathbf{q}} a_{\mathbf{k}'} a_{\mathbf{k}} \rangle - \langle b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{-\mathbf{k}} b_{\mathbf{k}'} a_{\mathbf{k}-\mathbf{q}} \rangle + \langle b_{-\mathbf{k}+\mathbf{q}} a_{\mathbf{k}-\mathbf{q}} \rangle \delta_{\mathbf{k}'}^{\mathbf{k}} \right], \\ \dot{n}_{\mathbf{k}} &= \frac{i}{\hbar} (d_{\mathbf{k}} p_{\mathbf{k}}^* - d_{\mathbf{k}}^* p_{\mathbf{k}}) E(z, t) \\ &\quad + \frac{i}{\hbar} \sum_{\mathbf{k}', \mathbf{q} \neq 0} V_{\mathbf{q}} \left[\langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}'} \rangle - \langle a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'-\mathbf{q}}^{\dagger} a_{\mathbf{k}} a_{\mathbf{k}'} \rangle \right. \\ &\quad \left. + \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}-\mathbf{q}} b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{\mathbf{k}'} \rangle - \langle a_{\mathbf{k}+\mathbf{q}}^{\dagger} a_{\mathbf{k}'} b_{-\mathbf{k}-\mathbf{q}}^{\dagger} b_{\mathbf{k}'} \rangle \right], \\ \dot{m}_{\mathbf{k}} &= \frac{i}{\hbar} (d_{\mathbf{k}} p_{\mathbf{k}}^* - d_{\mathbf{k}}^* p_{\mathbf{k}}) E(z, t) \\ &\quad + \frac{i}{\hbar} \sum_{\mathbf{k}', \mathbf{q} \neq 0} V_{\mathbf{q}} \left[\langle b_{-\mathbf{k}}^{\dagger} b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{-\mathbf{k}-\mathbf{q}} b_{\mathbf{k}'} \rangle - \langle b_{-\mathbf{k}+\mathbf{q}}^{\dagger} b_{\mathbf{k}'-\mathbf{q}}^{\dagger} b_{-\mathbf{k}} b_{\mathbf{k}'} \rangle \right. \\ &\quad \left. + \langle a_{\mathbf{k}'+\mathbf{q}}^{\dagger} a_{\mathbf{k}'} b_{-\mathbf{k}}^{\dagger} b_{-\mathbf{k}+\mathbf{q}} \rangle - \langle a_{\mathbf{k}'+\mathbf{q}}^{\dagger} a_{\mathbf{k}'} b_{-\mathbf{k}-\mathbf{q}}^{\dagger} b_{\mathbf{k}} \rangle \right], \end{aligned} \tag{6.14}$$

So the Coulomb interaction is coupling the evolution of two operator averages to evolution of higher moments exactly as it was in previous chapters.

To proceed, we need to employ some kind of approximation or method to decouple the hierarchy. Applying the same kind of analyses as in Chapter 3, we get

$$\begin{aligned} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}^\dagger a_{\mathbf{p}} a_{\mathbf{p}'} \rangle &\simeq n_{\mathbf{k}} n_{\mathbf{k}'} (\delta_{\mathbf{p}}^{\mathbf{k}} \delta_{\mathbf{p}'}^{\mathbf{k}'}) + h.o.t \\ \langle a_{\mathbf{k}'+\mathbf{q}} b_{\mathbf{q}-\mathbf{k}} a_{\mathbf{k}'} a_{\mathbf{k}} \rangle &\simeq n_{\mathbf{k}} p_{\mathbf{k}} \delta_{\mathbf{k}-\mathbf{q}}^{\mathbf{k}'} + h.o.t. \end{aligned} \quad (6.15)$$

where h.o.t. stands for high order terms. This is essentially equivalent to Hartree-Fock factorization.

So we use Hartree-Folk or Random Phase Approximation, namely to factorize six-order terms into products of two. This corresponds to neglecting all higher order cumulants and neglecting of the interactions in the system and instead considering particles to be moving in the self-consistent potential produced by all the particles. Obviously, this is valid only for weakly interacting particles.

The rules of Hartree-Folk factorization are equivalent to rules of Chapter 3 -take *all* possible combinations of splitting four-operator averages into products of two operators averages. The result is

$$\begin{aligned} & \left[i \frac{d}{dt} - (\epsilon_{ek} + \sum_{\mathbf{q} \neq 0} V_{\mathbf{q}} n_{\mathbf{k}+\mathbf{q}} + \epsilon_{hk} + \sum_{\mathbf{q}} V_{\mathbf{q}} m_{\mathbf{k}+\mathbf{q}}) \right] p_{\mathbf{k}} \\ &= (n_{ek} + n_{hk} - 1) \frac{1}{\hbar} (d_{\mathbf{k}} \mathcal{E} + \sum_{\mathbf{q} \neq \mathbf{k}} V_{\mathbf{q}-\mathbf{k}} p_{\mathbf{q}}) \\ \dot{n}_{ek} &= 2I_m \left[\frac{1}{\hbar} (d_{\mathbf{k}} \mathcal{E} + \sum_{\mathbf{q} \neq \mathbf{k}} V_{\mathbf{q}-\mathbf{k}} p_{\mathbf{q}}) \cdot p_{\mathbf{k}}^* \right] \\ \dot{n}_{hk} &= 2I_m \left[\frac{1}{\hbar} (d_{\mathbf{k}} \mathcal{E} + \sum_{\mathbf{q} \neq \mathbf{k}} V_{\mathbf{q}-\mathbf{k}} p_{\mathbf{q}}) \cdot p_{\mathbf{k}}^* \right]. \end{aligned} \quad (6.16)$$

Now define

$$\begin{aligned}
 e_{ek} &= \epsilon_{ek} + \sum_q V_q n_{k+q} \\
 e_{hk} &= \epsilon_{hk} + \sum_q V_q m_{k+q} \\
 \omega_{r,k} &= \frac{1}{\hbar} (d_k \mathcal{E} + \sum_{q \neq k} V_q p_{k-q})
 \end{aligned} \tag{6.17}$$

These formulas correspond to the Field-Energy renormalization. Finally we write the Bloch equations as

$$\begin{aligned}
 \left[\frac{d}{dt} + i(e_{ek} + e_{hk}) \right] p_k &= -i(n_k + m_k - 1)\omega_{rk} \\
 \dot{n}_k &= 2\text{Im}[\omega_{r,k} \cdot p_k^*] \\
 \dot{m}_k &= 2\text{Im}[\omega_{r,k} \cdot p_k^*]
 \end{aligned} \tag{6.18}$$

6.4 Slowly varying Maxwell equations.

Let us write down Maxwell's equations in the absence of free charges, current flows, and magnetization. These equations are

$$\begin{aligned}
 \nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t}, \\
 \nabla \cdot \mathbf{D} &= 0 \\
 \nabla \times \mathbf{H} &= \frac{\partial \mathbf{D}}{\partial t}, \\
 \nabla \cdot \mathbf{B} &= 0.
 \end{aligned} \tag{6.19}$$

To complete the description of the system we write down following constitutive relations.

$$\mathbf{B} = \mu_0 \mathbf{H}, \mathbf{D} = \epsilon \mathbf{E} = \epsilon_0 \mathbf{E} + \mathbf{P}, \tag{6.20}$$

where ϵ is the permittivity of the semiconductor medium. $\mathbf{P}$ is the induced electric polarization and $\mu_0\epsilon_0 = 1/ch^2$. The semiconductor lattice has a background index of refraction, $n \simeq 3$, which is included in ϵ via $\epsilon = n^2\epsilon_0$, where ϵ_0 is the permittivity of the vacuum. Combining the field equations (6.19) with the constitutive relations (6.20) we get a following wave equation

$$\nabla^2 \mathbf{E} - \frac{n^2}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} - \nabla(\nabla \cdot \mathbf{E}) = \mu_0 \frac{\partial^2 \mathbf{P}}{\partial t^2}. \quad (6.21)$$

If one also makes the assumption that electric field is singularly polarized and $\mathbf{E}$ propagates mostly along the z -axis, we ignore $\nabla(\nabla \cdot \mathbf{E})$ and get

$$\nabla^2 \mathbf{E} - \frac{n^2}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = \frac{1}{\epsilon_0 c^2} \frac{\partial^2 \mathbf{P}}{\partial t^2}, \quad (6.22)$$

where n is the background index of refraction. Now we will assume that $\mathbf{E}$ and $\mathbf{P}$ are traveling waves with cavity frequency Ω :

$$\mathbf{E} = \hat{e} A(x, y, z, t) e^{ikz - i\Omega t} + c.c.$$

$$\mathbf{P} = \hat{e} \lambda(x, y, z, t) e^{ikz - i\Omega t} + c.c.$$

Here we have assumed that we have a singularly polarized, $\hat{e}$, and unidirectional traveling, e^{ikz} wave in open medium. Substituting this into (6.22) and separating $\nabla^2 = \nabla_T^2 + \partial_z^2$, where $\nabla_T^2 = \partial_x^2 + \partial_y^2$,

$$\nabla_T^2 A + 2ik \frac{\partial A}{\partial z} + \frac{\partial^2 A}{\partial z^2} - \frac{n^2}{c^2} \frac{\partial^2 A}{\partial t^2} + 2i \frac{\Omega n^2}{c^2} \frac{\partial A}{\partial t} = \frac{1}{\epsilon_0 c^2} \frac{\partial^2 \lambda}{\partial t^2} - 2i \frac{\Omega}{\epsilon_0 c^2} \frac{\partial \lambda}{\partial t} - \frac{\Omega^2}{\epsilon_0 c^2} \lambda \quad (6.23)$$

Here we have used the linear dispersion relationship $k^2 = n^2 \Omega^2 / c^2$.

Using the slowly varying envelop approximation, we arrive at the following

$$\frac{n}{c} \frac{\partial A}{\partial t} - \frac{ic}{2n\Omega} \nabla_T^2 A = \frac{i\Omega}{2\epsilon_0 nc} \lambda. \quad (6.24)$$

adding in an phenomenologically loss term $\frac{\kappa}{c} A$ where $\kappa = \left(\frac{\sigma}{\epsilon_0}\right) + \left(\frac{c}{L}\right) \ln\left(\frac{1}{\sqrt{R}}\right)$. The term $\frac{\sigma}{\epsilon_0}$ represents the losses due to finite conductivity, and $\frac{c}{L} \ln\left(\frac{1}{\sqrt{R}}\right)$

represents the mirror losses. Finally,

$$\frac{n}{c} \frac{\partial \mathcal{A}}{\partial t} - \frac{ic}{2n\Omega} \nabla_T^2 \mathcal{A} + \frac{\kappa}{c} \mathcal{A} = \frac{i\Omega}{2\epsilon_0 n c} \Lambda. \quad (6.25)$$

In this manuscript we will be dealing with the semiconductor lasers in its simplified description. We neglect transversal effects in the system $\nabla_T^2 \mathcal{A} \simeq 0$ because we are looking mainly at cavity mode, i.e. assuming single mode operation. We further rewrite polarization Λ in terms of (6.6). This brings us to the equation which we will use in our modeling of the laser:

$$\frac{\partial e}{\partial t} = i \frac{\Omega}{2\epsilon_0} \frac{V}{(2\pi)^d} \int d\mathbf{k} p_{\mathbf{k}} d\mathbf{k} - \gamma_E e, \quad (6.26)$$

where γ_E is electrical field decay constant.

Chapter 7

LASERS

We make a *prima facie* case that finite flux solutions of the kinetic equation can be important in the context of semiconductor lasers and show how they might be used to enhance laser performance.

7.1 Basic Physics of Lasers.

LASER - a device that uses the principle of amplification of electromagnetic waves by stimulated emission of radiation and operates in infrared, visible or ultraviolet region. The word laser is an acronym derived from "light amplification by stimulated emission of radiation" (see, e.g. [31]).

To motivate why to work so hard on a semiconductor laser theory we try to put lasers in perspective and to give some historical review in sections (7.1-7.3). This material was heavily borrowed from the Internet (many useful links were found starting at [32]) and that is why the English is so much better in these sections.

Quantum mechanics teaches us that atoms and molecules can be in many different states characterized by their energy level. By supplying energy to the system, one can excite atoms or molecules from lower energy states to higher energy states. After staying at high energy state the particles can spontaneously return to lower energy states. By doing so they give off the extra energy, usually in a form of a light quantum (photon). In "conventional" light sources the many excited atoms or molecules emit light independently of each other, in many different colors (wavelengths) and not in phase. If,

however, during the brief instant that atom is excited, light of a certain wavelength impinges on it, the atom can be stimulated to emit radiation that is in phase with the wave that stimulated it. The new emission thus amplifies the passing wave. This physical process is called “stimulated emission”. If one constructs the situation when the phenomenon of stimulated emission can be multiplied sufficiently, then the resulting beam, made up of wholly coherent light (i.e., light of a single frequency and in phase with each other), may be quite powerful.

Albert Einstein discovered the existence of stimulated emission in 1917, but only in the 1950s were ways found to use it in devices. The American physicists Charles H. Townes and A.L. Schawlow showed that it was possible to construct such a device. Two Soviet physicists proposed related ideas independently. The first laser was constructed in 1960 by Theodore H. Maiman of the United States. Since then many types of lasers have been built...

So in order to achieve lasing, the following conditions should be met (see, e.g. [26]):

- The medium should be able to amplify the passing light. (Sometimes the weird term “negative absorption” is used.) That is, the medium should be able to store the energy by exciting its electrons or atoms into higher *meta stable* energy states.
- There should be some mechanism of pumping the energy into the system. This pumping process is usually incoherent, that is to say, the input energy is provided at many frequencies.
- There should be some kind of optical feedback to put the light back into the system in order to achieve a higher level of amplification. There are several ways to achieve this goal. For example, one can trap the

beam between two curved mirrors (Fabry-Perot cavity), or in a circular arrangement between three or more mirrors in a ring cavity. The length of the cavity is chosen to select (or to resonate with) the modes with the wavelength of the photons emitted by lasing the lasing medium.

7.2 Different types of lasers.

- *Optically pumped solid-state lasers.*

It is possible to excite the atoms to the higher energy level for laser action to take place by illuminating the laser material with light of a frequency higher than that which the laser is to emit. Such process is called optical pumping. Optical pumping must be of high intensity, because the process is rather inefficient.

An optically pumped solid-state laser consists of a rod of the material, with its ends polished flat, parallel and coated with mirrors to reflect the laser light. The sides are left clear to admit the light from the pumping lamp, for example a pulsed gas discharge, flashing on and off like a photographers electronic flash. The first operating laser employed a rod of pink ruby, an artificial crystal of sapphire (aluminum oxide). Other rare-earth elements have since been employed, the most widely used being neodymium. The output power of the order of thousands of watts can be obtained.

- *Liquid lasers.* Solid-state lasers have the disadvantage of occasional breakdown and damage at higher power levels because of the intense heat generated within the device and by the pumping lamp. The liquid laser is less susceptible to such damage. In liquid lasers the crystalline or glassy rod is replaced by a transparent cell containing a suitable

liquid, usually a solution of neodymium oxide or chloride in selenium oxychloride. Such cells can be made as large as desired to increase power output. Unfortunately, only a small number of inorganic liquids will function as lasers.

- *Dye lasers.* Certain organic dyes are capable of fluorescing—i.e., re-radiating light of a different wavelength. Though the excited state of their atoms lasts only a small fraction of a second and the light emitted is not concentrated in a narrow band, many such dyes have been made to exhibit laser action. They can be tuned to a wide range of frequencies.

Dyes such as rhodamine 6G, which emits orange-yellow light, can be made to lase (provide laser action) by excitation by another laser. Rhodamine 6G was the first dye for which continuous, rather than pulsed, operation was achieved, making possible the production of a continuous beam of tunable laser light. Another type of dye, methylumbelliferone, with the addition of hydrochloric acid, can be made to lase at wavelengths varying across the wide portion of light spectrum ranging from ultraviolet to yellow, thus producing laser output of almost any desired frequency within this range.

- *Gas-discharge lasers.* Atoms in a gas discharge can be excited to radiate, as in a neon sign. Occasionally, a particular energy level will cause an exceptionally high number of atoms to accumulate within it. If mirrors are attached properly to the ends of the discharge tube, laser action may take place. Though this conditions are unusual and occur for only a few of the many wavelengths at which the discharge emits, most gases can be made to exhibit laser action at some wavelength

under certain conditions.

- *Gas dynamic lasers.* If a hot gas is cooled rapidly, the number of molecules in a low-energy state may decrease more rapidly and fall below the number in a higher energy state, thus permitting laser action. This condition can be achieved by expanding burning carbon monoxide mixed with nitrogen through jet nozzles. High power outputs of order of 30.000 watts can be obtained.
- *Chemical lasers.* Certain chemical reactions produce enough high-energy atoms to permit laser action to occur. For example laser action can occur in carbon dioxide if it is present when the elements hydrogen and fluorine are reacting to produce hydrogen fluoride. Relatively large amounts of energy can be released when only moderate amounts of the appropriate materials react.
- *Semiconductor lasers.* Semiconductor laser, the main hero of this manuscript, consist of a flat junction of two pieces of semiconductor material, each of which has been treated with a different type of impurity. Such junction is called p-n junction. Aluminum gallium arsenide and gallium arsenide are most commonly used in semiconductor lasers, though pairs of other so-called III-V compound semiconductors may be employed. When an electrical current is passed through such a device, electrons and holes are brought together in a relatively thin region, called active zone. Then laser light emerges from the active zone. Although power output is limited, the low cost, small size, and comparatively high efficiency make these devices suitable for use in many applications, such as optical fiber communications systems (see below), compact digital audio disc players and so on.

- *Free-electron lasers.* Lasers of this type are more efficient than any other variety in producing beams of very high power radiation. Furthermore, these devices are tunable, so that they can be made to operate at microwave to ultraviolet wavelengths. In a free-electron laser, free electrons (i.e., those not bound to nuclei) from, say, a particle accelerator are passed through a modulator ("wiggler"), a device consisting of a linear array of electromagnets. An alternating magnetic field in the modulator bends the electrons into a spiral trajectories, whereby electrons are accelerated to very high velocities approaching the speed of light. Electrons then emit energy in the form of synchrotron radiation. The intensity and wavelength of this radiation can be adjusted by modifying certain parameters of the magnetic field. Because of this ability to produce laser light tunable over a broad range of wavelengths and high efficiency, many researchers believe that the free-electron laser, with further development, will prove especially suitable in many applications such as isotope separation, semiconductor research, and even ballistic missile defense (namely, as a laser beam weapon).
- *Lasers producing short and intense pulses.* A shutter placed between the amplifying column and the end mirrors of a laser can prevent laser action as long as it is closed. If conditions are otherwise correct for laser action and the shutter is suddenly opened, then the stored energy is released in a form of a giant pulse of light lasting only a tiny fraction of a second and having a peak power up to several hundred megawatt. Such device is called a Q-switch. The Q-switch may be a mechanical shutter or even a liquid crystal or solid optical shutter that is normally opaque but can be made transparent by the application of an electrical pulse. Normally a laser oscillates in several modes—i.e.,

at several different frequencies. By synchronizing these modes, a process called mode-locking, even shorter, more powerful pulses can be in principle obtained. Such pulses are useful in scientific investigations and in puncturing holes so rapidly that the surrounding material is not affected.

7.3 Few words about applications.

The light produced by lasers is in general far more monochromatic, directional, powerful, and coherent than that from any other light sources. Nevertheless, the individual kinds of lasers differ greatly in these properties as well as in wavelength, size, cost and efficiency. There is no single laser suitable for all purposes, but some of the combinations of properties can do things that were difficult if not impossible before lasers were developed.

A continuous visible beam from a gas laser provides a nearly ideal straight line for all kinds of alignment applications. The beam from such a laser typically diverges by less than one part in a thousand, approaching the theoretical limit. The beam's divergence can be reduced by passing it backward through a telescope, although fluctuations in the atmosphere then limit the sharpness of a beam over a long path. Lasers have come to be widely used for alignment in large construction—for example to guide machines for drilling tunnels and for laying pipelines.

A pulsed laser can be used in a light radar, sometimes called LIDAR, and the narrowness of its beam permits sharp definition of targets. As with radar, the distance to an object is measured by the time taken for the light to reach and return from it, since the speed of light is known. LIDAR echoes have been returned from the Moon, facilitated by a multiprism reflector that was placed there by the first astronauts to land there. Distances can be

measured from an observatory on Earth to the lunar mirror with an accuracy of several centimeters. Simultaneous measurements of the mirrors distance and direction from two observatories on different parts of the Earth could give very accurate value for the distance between the two observatories. A series of such measurements can tell the rate at which continents are drifting relative to each other.

A vertically directed laser radar in an airplane can serve as a fast, high-resolution device for mapping fine details, such as the contours of a stadium or even the shape of the roof of a house. With a pulsed laser radar, returns can be obtained from dust particles and even from air molecules at higher altitudes. Therefore air densities can be measured and air currents can sometimes be traced.

The high coherence of a laser's output is very helpful in precise measurement and other applications involving interference of light beams. If a light beam is separated into two parts that travel different paths, then when the beams come together producing interference patterns. Such devices are called laser interferometers. Very small displacements can be detected, and larger distances can be measured with great precision. With lasers, these measurements can be carried out over extremely long distances. For example laser interferometers are used to monitor small displacements in the Earth's crust across geological faults.

Lasers can be so monochromatic that a small shift in the light frequency can be detected. Light reflected from an object that is moving toward the laser is raised in frequency by an amount depending on the velocity of the object (Doppler effect). For a receding object, the frequency is lowered. In either case, if some of the original and the shifted light are recombined at a photo-detector, a signal at the difference frequency is observed, and even

small velocities can be measured. Big velocities can be measured too, and police laser guns operates on this principle.

The brightness and coherence of laser light make it especially suitable for visual effects and holography.

The light from many lasers is relatively powerful and can be focused by a conventional lens system to a small spot of great intensity. Thus even a moderately small pulsed laser can evaporate a small amount of any substance and drill narrow holes in the hardest materials. Ruby lasers, for example, are used to drill holes in diamonds for wire drawing dies and in sapphire for watch bearings. For biological research, a finely focused laser can vaporize parts of a single cell, thus permitting micro surgery of chromosomes.

Strong heating can be produced by a laser at a place where no mechanical contact is possible. Thus one of the earliest applications of lasers was for surgery on the retina of the eye.

The high brightness, pure color, and directionality of laser light make it ideally suited for experiments on light scattering. Even a small amount of light that is scattered with a change of wavelength or direction can be readily identified. In particular, a type of scattering known as the Raman effect produces characteristic wavelength shifts by which molecular species can be identified. With laser sources and sensitive spectrography, small samples of transparent liquids, gases or solids can be analyzed. It is even possible to measure contaminants in the atmosphere at a considerable distance by the Raman scattering of light from a laser beam.

It would probably be true to say that the most common type of laser is semiconductor laser. Indeed, semiconductor lasers may be found in people homes (countless CD players, laser printers, laser jet printers, CD readers in computers, laser pointers, etc) while other types of lasers are only in labs

and factories.

Laser beams can be used for communications. Because the light frequency is so high (around 5 times 10^{14} hertz for visible light), the intensity can be rapidly altered to encode very complex signals. In principle, one laser beam could carry as much information as all existing radio channels. Laser light can, however, be blocked by rain, fog, or snow so that, for reliable communications on Earth, the laser beam would need to be enclosed in a protective medium. Optical fibers made of glass and covered with a cladding material are employed for this purpose. Waveguides of this kind have been used increasingly in long-distance telephone systems since the early 1980s. This is the area of very intensive research now, since optical telecommunication lines operating on solitons can operate on rates of gigabits per second.

Semiconductor laser technology is integral to optical disc recording and storage systems. In such a system, digital data are recorded by burning a series of microscopic holes, commonly referred to as pits, with a laser beam into thin metallic film on the surface of an optical disc. In this manner, information from magnetic tape is encoded on a master disc, which is replicated by a process known as stamping. In the read mode, laser light of low intensity is reflected off the disc surface and is "read" by light-sensitive diodes. The amount of light received by the diodes varies according to the presence or the absence of the pits, and this input is digitized by the diode circuits. Then digital signals are converted to analog video or audio information.

Semiconductor lasers also are used in a major type of computer printer. Laser printers employ a laser beam and a system of optical devices to etch images on a photo-conductor drum. The images are carried from the drum to manuscript by means of electrostatic photocopying.

FIGURE 7.1. Basic principles of semiconductor laser operation.

In a ground state electrons occupy the valence band, but can be excited to conduction band, leaving behind a positively charged vacancy - hole. In a reverse process electron *recombines* with its hole, emitting quantum of light - photon. The frequency ν of emitted photon is equal to the energy difference between electron and hole states $\hbar\nu = E_1 - E_2 \equiv \hbar\omega_\kappa$, see (2.34).

7.4 Basic principles of semiconductor laser operation.

In many ways, semiconductor lasers are similar to two level lasers in that the coherent light output is associated with the in-phase transitions of an electron from a higher to lower energy state. In semiconductors, the lower energy state is the valence band, from which sea electrons are removed leaving behind positively charged holes. The higher energy state is the conduction band. The quantum of energy released corresponds to an excited electron in the conduction band combining with a hole directly below (because the emitted photon has negligible momentum) in the lower band (see Figure (7.1)).

However, there are several important ways in which the semiconductor

laser differs from and is more complicated than the traditional two-level laser model. First, in order for there to be lasing, there must be both an electron and hole available at the same momentum (and spin) absolute¹ value whereas, in the traditional two level laser, the ground state is always available for an excited electron. As a result, the excitation levels of both electrons and holes must be above a certain level. Second, there is a continuum of transition energies parameterized by the electron momentum $\mathbf{k}$ and the laser output is a weighted sum of contributions from polarizations corresponding to electron-hole pairs at each momentum value. In this feature, the semiconductor laser resembles an inhomogeneously broadened two level laser. Third, electrons and holes interact with each other via Coulomb forces. Although this interaction is screened by the presence of many electrons and holes, it is nonetheless sufficiently strong to lead to a nonlinear coupling between electrons and holes at different momenta. It is this effect that gives rise to the coupling coefficient $T_{\mathbf{k}\mathbf{k}_1,\mathbf{k}_2\mathbf{k}_3}$ of the earlier sections of this manuscript. The net effect of these collisions is a redistribution of carriers (the common name for both electrons and holes) across the momentum spectrum. In fact it is the fastest (≈ 100 fs.) process (for electric field pulses of duration greater than picoseconds) and because of this, the gas of carriers essentially relaxes to a distribution corresponding to an equilibrium of this collision process. This equilibrium state is commonly taken to be that of thermodynamic equilibrium for fermion gases, the Fermi-Dirac distribution characterized by two parameters, the chemical potential μ and temperature T , slightly modified by the presence of broadband pumping and damping. However, as we have shown, in situations where there is applied forcing and damping and in particular where these

¹Individual recombination event consist of electron of momentum $\mathbf{k}$ and spin s to recombine with hole of momentum $-\mathbf{k}$ and spin $-s$ to emit quantum of light (photon) with negligible momentum and zero spin.

processes take place in separate regions of momentum space, it is the finite flux equilibrium which is more relevant (see e.g. [1],[33],[34]).

In the semiconductor laser the applied forcing is usually the electrical pumping process. The low-energy sink is the actual lasing process, i.e. stimulated emission at the laser frequency. The second sink has contributions from a variety of processes. One contribution is due to that fact that some of the charge carriers with high kinetic energies can leave the optically active region and, therefore, contribute to the electrical pumping current without contributing to the light amplification. Other processes acting as sinks are less well localized at high energies. They are distributed over an extended range of momentum values. Examples are non-radiative recombination of electron-hole pairs mediated by impurities, dislocations, interface roughness, etc. In addition, Auger processes contribute significantly to the damping (i.e., loss of charge carriers).

Although it is beyond the scope of this manuscript, we should like to mention that, for a complete description of relaxation and thermalization processes in semiconductor lasers, one would also have to take electron-phonon scattering into consideration. This interaction insures that the temperature of the electron-hole plasma is driven towards the lattice temperature. The main electron-phonon interactions involve longitudinal optical and acoustic phonons. The former couple via the Fröhlich interaction to the charge carriers and typical thermalization times are almost as short as those due to carrier-carrier interaction in semiconductor lasers (within a factor of about 5). Much slower (three to four orders of magnitude) is the deformation potential coupling with acoustic phonons. Making the assumption that the electron-electron interaction dominates over electron-phonon interactions, we proceed now and investigate the role of equilibrium distributions other than

Fermi-Dirac distributions in laser performance. As we have shown in previous sections, there are finite flux equilibria, for which there is a finite and constant flux of carriers and energy across a given spectral window. It is the aim of this work to suggest that these finite flux equilibria are more relevant to situations in which energy and carriers are added in one region of the spectrum, redistributed via collision processes to another region where they are absorbed. In conventional diode lasers, pumping is a process in which charge carriers are injected into the depletion layer region in a p-n or p-i-n structure (see, for example, [35]). If the active layer is bulk-like, this process is based on a regular drift-diffusion current, whereas in quantum-well lasers there is the additional processes of carrier capture into the quantum well by means of inelastic scattering processes. In the following we restrict ourselves to the simplest model for injection pumping that neglects the intrinsically anisotropic aspect of injection pumping but includes the basic features of Pauli blocking effects in the pump process [24]. Within this model, the rate of change of the carrier distribution is proportional to $\Lambda_k(1 - n_k)$, where the pump coefficient Λ_k is taken as a Fermi function with a given density modeling the incoming equilibrated carriers, n_k is the actual carrier distribution in the active region, and $(1 - n_k)$ takes into account the Pauli blocking effects. This means that only non-occupied states can be filled by the pump current. Since Λ_k is a function that extends over a large range of k-values, we call this pump model “broad band pumping.” In contrast to broad band pumping one can also pump a laser locally in momentum space. However, usually such a local pump process is narrow-band optical pumping, but this is not commonly used to pump semiconductor lasers. There are, however, also electrical pumping schemes available, which are based on resonant tunneling of electrons through arrays of multiple quantum wells. Such resonant

tunneling allows for selective and localized pumping and damping (see, e.g., [36]).

7.5 Application of Quantum Weak Turbulence to Semiconductor Lasers.

We will now investigate the relevance of finite flux solutions in the context of semiconductor lasers. In the following we will examine the laser process and discuss, in particular, the influence of the pumping process and its relation to the equilibrium distribution function in stationary laser operation.

In this section we are going to present the main and surprising result of this manuscript. This result persists across quite a big range of parameters - pumping and damping strengths, different mass ratios of electron and holes, etc. *It turns out that for the same amount of carriers pumped and approximately same amount of energy pumped the output power ($|e|^2$) in the narrow band pumping case, when a finite flux distribution is excited, is consistently higher than in the broad band case, when carrier distributions have zero or small flux.*

We base our numerical solutions on a greatly simplified laser model. We make the following assumptions:

- We first assume that the distribution functions for electrons and holes are identical (in other words, we assume electrons and holes to have identical effective masses). We are going to relax this assumption in the following sections.
- we model the cavity losses by a simple phenomenological loss term in the propagation equation for the light field amplitude;
- we assume ideal single-mode operation;

- we make the rotating wave approximation in the equation for the distribution functions and the optical polarization function p_k ;
- we neglect all electron-hole Coulomb correlations (the so-called Coulomb enhancement, see, e.g., [24]);
- we neglect bandgap energy renormalization;
- we treat electron-phonon interaction phenomenologically through damping term.

In spite of the approximations made, our model still captures the basic processes in a semiconductor laser.

7.5.1 One-particle model.

The equations of motion are a form of the semiconductor Maxwell-Bloch equations, (see, e.g., [24], [25]). We take (6.18) and neglect field and bandgap renormalizations. We add phenomenologically polarization decay term $-\gamma_p p_k$ to the polarization equation. We include in the equation for n_k the collision term, and we add phenomenologically terms describing pumping $\Lambda_k(1 - n_k)$ and nonradiative damping $-\gamma_k n_k$ of carriers. We also assume, as mentioned above, $n_k = m_k$. We use (6.26) as equation of motion for electric field. The resulting equations read:

$$\frac{\partial e}{\partial t} = i \frac{\Omega}{2\epsilon_0} \frac{V}{(2\pi)^d} \int d_k p_k d\mathbf{k} - \gamma_E e, \quad (7.1)$$

$$\frac{\partial p_k}{\partial t} = (i\Omega - i\tilde{\omega}_k - \gamma_p) p_k - \frac{id_k}{2\hbar} (2n_k - 1) e, \quad (7.2)$$

$$\frac{\partial n_k}{\partial t} = \Lambda_k(1 - n_k) - \gamma_k n_k + \left(\frac{\partial n_k}{\partial t} \right)_{\text{collision}} - \frac{i}{2\hbar} (d_k p_k e^* - d_k p_k^* e). \quad (7.3)$$

Here $e(t)$ and $p_k(t)$ are the electric field and polarization (at momentum $\mathbf{k}$) envelopes of the carrier wave $\exp(-i\Omega t + iKz)$ where $\Omega = 1440\text{meV}^{-1}$ is the cavity frequency (we assume single mode operation only) and n_k is the distribution function for electrons and holes. The constants $\gamma_E = 6 \times 10^{10}/\text{sec}$, $\gamma_p = 10^{13}/\text{sec}$ model electric field losses and polarization decay (dephasing), ϵ_0 is the dielectric constant, d_k is the weighting accorded to different $\mathbf{k}$ momentum values and is modeled by $d_k = d_{k=0}/(1 + \epsilon_k/\epsilon_{\text{gap}})$, $d_{k=0} = 3/10^{10}\text{Me}$. e is the electron charge, $\gamma_k = 10^{10}/\text{sec}$ represent nonradiative carrier damping. In (7.8), Λ_k is the pumping due to the injection current (taken to be between 0.001ps^{-1} and 0.01ps^{-1}) and in (7.7) $\hbar\tilde{\omega}_k = \epsilon_{\text{gap}} + \epsilon_{e,k} + \epsilon_{h,k}$ (see (2.34)). We further assume that all fields are isotropic and make a convenient transformation from k ($= |\mathbf{k}|$) to ω ³ via the dispersion relation $\omega = \omega(\mathbf{k})$ defining the carrier density $n_\omega = n(\mathbf{k}(\omega))$ and approximate the collision term $\left(\frac{\partial n_k}{\partial t}\right)_{\text{collision}} = \left(\frac{\partial n_{k(\omega)}}{\partial t}\right)_{\text{collision}}$ by the differential kinetic expression (3.72):

$$\begin{aligned} \left(\frac{\partial n_{k(\omega)}}{\partial t}\right)_{\text{collision}} &= -\frac{1}{\Omega_0 k^{d-1}(dk/d\omega)} \\ &\quad \times \frac{\partial^2}{\partial \omega^2} \left[\left(n_\omega^4 \frac{\partial^2}{\partial \omega^2} \left(\frac{1}{n_\omega} \right) + n_\omega^2 \frac{\partial^2}{\partial \omega^2} (\ln(n_\omega)) \right) \times I \times \omega^s \right], \end{aligned} \quad (7.4)$$

We choose the value of the constant I to ensure that solutions of (7.4) relax with characteristic relaxation time of of 100 fs to its equilibrium value and s turns out to be 7.

²We measure all frequencies Ω , ω_0 , ω_L , ω_R , ω , $\tilde{\omega}$ in energy units (meV).

³ $\hbar\omega$ is the reduced mass kinetic energy, defined in (4.5).

Let us make convenient transformation to the non-dimensional variables:

$$\begin{aligned}
 e &= \bar{e} \times \frac{\hbar \gamma_p}{d_{k=0}}, \\
 d_k &= \tilde{d}_k d_{k=0}, \\
 t &= \frac{\tilde{t}}{\gamma_p}, \\
 \omega &= \hbar^2 |\mathbf{k}|^2 / (2m), \quad \omega = \tilde{\omega} \hbar \gamma_p, |\tilde{\mathbf{k}}| = \sqrt{\tilde{\omega}}
 \end{aligned} \tag{7.5}$$

where we denote non dimensional variables with tilde. Remember, that n_k and p_k are dimensionless quantities between zero and one. Now drop the tilde's and rewrite (7.1-7.3) as

$$\frac{\partial e}{\partial t} = i \frac{\Omega d_{k=0}^2 V}{2 \gamma_p^2 \epsilon_0 \hbar} \int d\mathbf{k} d_k p_k - \frac{\gamma_E}{\gamma_p} e, \tag{7.6}$$

$$\frac{\partial p_k}{\partial t} = \left(i \frac{\Omega}{\gamma_p} - i \frac{\tilde{\omega}_k}{\gamma_p} - 1 \right) p_k - i d_k (2n_k - 1) e. \tag{7.7}$$

$$\frac{\partial n_k}{\partial t} = \frac{\Lambda_k}{\gamma_p} (1 - n_k) - \frac{\gamma_k}{\gamma_p} n_k + \frac{1}{\gamma_p} \left(\frac{\partial n_k}{\partial t} \right)_{\text{collision}} - i (d_k p_k e^* - d_k p_k^* e). \tag{7.8}$$

We now compare the laser efficiencies in two numerical experiments in which we arrange to: (i) Pump broadly across a wide range of momenta, so that the effective carrier distribution equilibrium has zero (or small⁴) flux. We take the pump profile to be given by the Fermi-Dirac distribution. (ii) Pump carriers and energy into a narrow band of frequencies about ω_0 and simulate this by specifying carrier and energy flux rates Q_L and P_L at the boundary $\omega = \omega_0$. P_L chosen so that the energy absorbed by the laser is

⁴Even for broad band pumping the small amount (much smaller than in local band pumping) of P and Q fluxes are also excited, because the form of the pumping f_k gets effectively multiplied by the Pauli blocking $(1 - n_k)$ term. But these fluxes are much smaller and relatively local in k space.

consistent with the number of carriers absorbed (see (4.37)). $\omega = \omega_L < \omega_0$ is the frequency at which the system lases.

Definitions - broad band pumping.

- The total number of *carriers* supplied to the laser per unit time in the broad band pumping case is

$$\int \Lambda_k d\mathbf{k} (1 - n_k)$$

- The total amount of *energy* supplied to the laser per unit time in the broad band pumping case is

$$\begin{aligned} \int d\mathbf{k} \left(\Lambda_k^{(e)} (1 - n_k) \left(\frac{\hbar^2 k^2}{2\mu_e} + \epsilon_{gap} \right) + \Lambda_k^{(h)} (1 - m_k) \frac{\hbar^2 k^2}{2\mu_h} \right) \\ \simeq \epsilon_{gap} \int d\mathbf{k} \Lambda_k^{(e)} (1 - n_k), \end{aligned}$$

because the band gap energy is 1400 meV, and majority of carriers have kinetic energy less than 200 meV. Here μ_e and μ_h are the masses of electron and hole respectively, μ_r is the reduced mass. $1/\mu_r = 1/\mu_e + 1/\mu_h$.

Remember that in this section $\Lambda_k = \Lambda_k^{(e)} = \Lambda_k^{(h)}$.

Definitions - narrow band pumping.

- The total number of *carriers* supplied per unit time in narrow band pumping is

$$Q_0$$

- The total amount of *energy* pumped to the system per unit time is

$$-P_0 = P_R - P_L = (\epsilon_{gap} + \omega_0 \frac{\mu_r}{\mu_e}) Q_0^e + \omega_0 \frac{\mu_r}{\mu_h} Q_0^h \simeq \epsilon_{gap} Q_0^e,$$

see (4.36).

Remember that in this section $Q_L^e = Q_L^h = Q_L$. Also the band gap energy is 1400 meV, and majority of carriers have kinetic energy less than 200 meV.

We compare only cases in which the total amount of carriers supplied per unit time is the same and energy supplied per unit time is approximately the same.

Experimental setup. We would like to set up numerical experiments in such a way that total amounts of carriers supplied to the laser in narrow band and broad band pumping cases are the same. Therefore we choose

$$\int \Lambda_k d\mathbf{k} (1 - n_k) = Q_0, \quad (7.9)$$

so that the number of carriers available to the system is the same in broad band and narrow band cases. We choose $Q_0 = Q_L$ so that all carriers pumped to the system go to the left. This is an *assumption*. We also may choose Q_L consistent with (4.36), but this would employ some kind of arbitrariness (in choosing ω_R). Note that choosing $Q_L < Q_0$ will make the narrow band pumping less effective, but it is still will be more effective, at least with lower levels of pumping.

P_L chosen so that the energy absorbed by the laser is consistent with the number of carriers absorbed (see (4.37)).

The total number of energy pumped per unit time to the system is

$$\simeq \epsilon_{gap} \int d\mathbf{k} \Lambda_k^{(e)} (1 - n_k)$$

is almost equal to amount of energy pumped in the narrow band pumping case:

$$\simeq \epsilon_{gap} Q_0^e,$$

because of (7.9).

Results of numerical experiments. In the first numerical experiment, we show that for a very small amount of pumping the laser operates for the narrow band pumping, while it fails to operate in the broad band pumping case (i.e. the threshold pumping value for narrow band pumping is much lower than in the broad band case). The carriers supplied through the pumping process get totally absorbed by the global damping $-\gamma_k n_k$ in the broad band pumping case. There no lasing occurs. In the local band pumping case, for the same amount of carriers and approximately same amount of energy supplies, the laser operates. This is the qualitative difference between two cases.

The results of this numerical experiment are presented in Figure (7.2) (see also Figure (7.5)). The narrow-band pumped laser switches on and generates a nonzero output power (by power we mean output light intensity $|e|^2$). We pump in the narrow region around $\omega_0 \simeq 200\text{meV}$ and we model this by specifying the boundary conditions at ω_0 to correspond to carrier and energy flux rates Q_L and P_L respectively. The initial value of the distribution function (shown by a thin line), taken to be just below the lasing threshold, builds up because of the influx of particles and energy from the right boundary (dashed lines) until the laser switches on. The final (steady) distribution function is shown by a thick solid line and corresponds to a flux of particles and energy from the right boundary (where we add particles and energy) to the left boundary, where the system lases. The output power as a function of time is also shown (Figure (7.2)).

Time is measured in units of relaxation times $\tau_{\text{relax}} = 100fs$. In the contrast, the broad-band pumped laser fails to switch on for such weak pumping.

We then increase the level of pumping, to a point where the laser turns on for both the broad band and narrow band pumping cases, and examine

FIGURE 7.2. Time dependence of distributions (a) and output laser intensity (b) according to (7.6-7.8).

Local-band pumping is modeled by specifying the carrier and energy flux rates Q_L and P_L at the right ($\omega_0 \simeq 200\text{meV}$) boundary. The initial distribution function (shown by a thin line in this and consequent figures) evolves through a number of intermediate states shown by dashed lines, until the laser switches on. The final (steady) distribution function is shown by a thick solid line (in this and subsequent figures). Lasing frequency is marked by arrow on this and subsequent pictures and is equal to $1440\text{meV} = \epsilon_{gap} + 40\text{meV}$. Time is given in units of the relaxation time $\tau_{\text{relax}} = 100\text{fs}$ on this and subsequent figures. The laser fails to switch on in the broad-band pumping case for these levels of pumping.

the output power in both cases. It turns out that for the same amount of carriers pumped and approximately same amount of energy pumped the output power in the narrow band case is higher by a factor of 10 than in the broad band case. The results are presented in Figures (7.3-7.4). We first pump broadly, so that the effective carrier distribution has (almost) zero flux. The initial distribution function (thin line, Figure (7.3)) builds up because of a global pumping (dashed lines) until the laser switches on. The final (steady) distribution function is shown by the thick solid line. The output power as a function of time is also shown.

If we pump in the narrow region around $\omega_0 \simeq 200\text{meV}$ and we model this by specifying the carrier and energy flux rates Q_L and P_L , then the initial distribution function (thin line) builds up because of an influx of particles and energy from the right boundary (dashed lines) until the laser switches on. The final (steady) distribution function is shown by a thick solid line and corresponds to a flux of particles and energy from the right boundary (where we add particles and energy) to the left boundary, where the system lases (Figure (7.4)). The output power as a function of time is also shown.

Analysis. Let us integrate (7.3) with respect to $\mathbf{k}$ over computational domain. Since dn_ω/dt is a perfect derivative of of a flux Q whose values at ω_0 is Q_L and at ω_L is zero the resulting equation read

$$\frac{\partial}{\partial t} \int n_k d\mathbf{k} = \int d\mathbf{k} (\lambda_k(1 - n_k) - \gamma_k n_k) + Q_L - \frac{i}{2\hbar} \int d\mathbf{k} (d_k p_k e^* - d_k p_k^* e) \quad (7.10)$$

The value of $\int d\mathbf{k} d_k p_k$ may be obtained from (7.1):

$$\int d_k p_k d\mathbf{k} = -i \frac{2\epsilon_0 (2\pi)^d}{\Omega V} \left(\frac{\partial e}{\partial t} + \gamma_E e \right), \quad (7.11)$$

FIGURE 7.3. Same as in Figures (7.2) but for increased pump rate. Broad-band pumping case.

Lasing frequency is marked by arrow and is equal to $1440\text{meV} = \epsilon_{\text{gap}} + 40\text{meV}$.

FIGURE 7.4. Same as in Figure (7.2) and with same pump rate as in Figure (7.3). Narrow band pumping.

Combining these two formulas together,

$$\frac{\partial}{\partial t} \int n_k d\mathbf{k} = \int d\mathbf{k} (\Lambda_k(1 - n_k) - \gamma_k n_k) + Q_L - \frac{2\epsilon_0 (2\pi)^d}{\hbar\Omega V} (\gamma_E + \frac{\partial}{\partial t}) |e|^2 \quad (7.12)$$

If one assumes steady state in the above expression, then

$$|e|^2 = \frac{\hbar\Omega}{2\epsilon_0} \frac{V}{(2\pi)^d} \frac{1}{\gamma_E} \left(\int d\mathbf{k} (\Lambda_k(1 - n_k) - \gamma_k n_k) + Q_L \right) \quad (7.13)$$

We see that the pumping can be done through the pumping current Λ_k or through input of the particle fluxes Q_L to the computational domain. The former then excites the finite flux solutions which carry energy and carriers from the right boundary of computational domain to the ω_L where they are absorbed by a laser. Note that pumping Λ_k or Q_L is balanced with losses $-\gamma_k n_k$ and “radiative sink” - laser output. In order to have lasing, the pumping strength Λ_k or Q_L should overcome nonradiative losses $-\gamma_k n_k$. The output intensity $|e|^2$ is then proportional to the value of pumping current Λ_k or to the input flux Q_L .

We also perform a series of numerical experiments with different levels of pumping. In Figure (7.5) we plot the output power as a function of pumping strength for both narrow-band and broad band pumping. We use thick points to show the output power for narrow band pumping and thin points to show the output power for broad band pumping. We see that for bigger amounts of pumping, narrow band pumping is still more effective.

We also verify the predictions of (7.13). For each run performed we use the numerical values of the stationary distribution functions n_k to evaluate the theoretical output power as predicted by (7.13). Predictions of (7.13) almost coincide with numerical results. We fit a polynomial through the theoretical

points predicted by (7.13). Polynomial fit for narrow band pumping is shown by thick continuous line, while polynomial fit for broad band pumping is shown by thin continuous line. The theoretical points are not shown as they virtually coincide with the numerical results.

We also want to note that

1. We assumed that all added carriers go to the left: $Q_L = Q_0$. If we assume that some carriers go to the right, the narrow band pumping case will be still more effective for lower values of pumping.
2. Since induced fluxes effectively lower the carrier temperature (see Chapter 3), the lasing is more effective as more carriers concentrated around lasing region creating bigger level of inversion and effectively decreasing nonradiative losses $-\int d\mathbf{k} \gamma_k n_k$.
3. For the same level of pumping it takes less time for narrow band pumping to start to operate, due to less noticeable Pauli blocking effects.

Pauli Blocking. In all of the above we have assumed that there is no “energetical punishment” for the Pauli blocking. In other words we have assumed that if we try to fill an already filled electron state then we do not spend energy for this unsuccessful attempt.

It may seem from the first principle consideration that this is the case. Indeed, let us consider for the simplicity of the arguments that we pump the semiconductor laser optically (not by the electrical current). One may think about an active zone of a laser as three dimensional atomic lattice. Let us consider a specific site of the lattice. If photon “approaches” this site, then there could be two cases :

- *atom is not excited.* Then the photon will be absorbed by the atom, and electron will be transferred from valence band to the conduction

FIGURE 7.5. The output power as a function of pumping strength for narrow-band and broad-band pumping, one particle model.

Narrow band output power is shown by thick points, broad band output power is shown by thin points. Theoretical curves, obtained by interpolating (polynomial fitting) predictions of (7.13), are shown for narrow band pumping by thick and for broad band by thin lines. Predictions of (7.13) are pretty accurate.

band, thus creating electron-hole pair. This electron-hole pair may later radiate.

- *atom is excited.* Then the “passing” photon will not be absorbed by the atom and will go to the next atom of the lattice.

This consideration supports the idea that there is no energy losses due to Pauli blocking. However one should remember that semiconductor lasers are pumped by the electrical current. Before reaching an active zone the current has to pass through the bulk of semiconductor, because the active zone is a small part of the actual crystal. Therefore some energy will be spend by electrons outside the active zone. The power loss outside active zone W may be estimated as current through the crystal I times the voltage drop U outside active zone: $W = I \times U$. The current may be determined by the Ohm’s law ($I = U/R$). This effect (resistivity of the bulk of the crystal) makes the overall efficiency of semiconductor lasers of the order of 10% (see, e.g. [37]). Therefore, even if an electron passes through the crystal and does not contribute to the inversion (due to Pauli blocking), one still needs to spend the extra energy needed to drag the electron through the crystal!

In this manuscript we do not consider the transport phenomena and focus entirely on the understanding (and modeling) of the physics of the active zone. Thus it is consistent to count the number of electrons provided to the laser as $\int \Lambda_k(1 - n_k)dk$. We want to stress, however, that because of the extra energy needed to be spent to drag an electron across the crystal (even if an electron does not contribute to the inversion!) there may be additional advantages in the proposed local band pumping scheme.

7.5.2 Two particle model.

We now generalize (7.1-7.3) to a two-component electron-hole plasma. To do that we replace $2n_k$ in (7.1) by $n_k + m_k$ and write a separate equation for evolution of m_k . The result is

$$\frac{\partial e}{\partial t} = i \frac{\Omega}{2\epsilon_0} \frac{V}{(2\pi)^d} \int d_k p_k d\mathbf{k} - \gamma_E e. \quad (7.14)$$

$$\frac{\partial p_k}{\partial t} = (i\Omega - i\bar{\omega}_k - \gamma_p) p_k - \frac{id_k}{2\hbar} (n_k + m_k - 1) e. \quad (7.15)$$

$$\begin{aligned} \frac{\partial n_k}{\partial t} &= \lambda_k^e (1 - n_k) - \gamma_k n_k + \left(\frac{\partial n_k}{\partial t} \right)_{\text{collision}} - \frac{i}{2\hbar} (d_k p_k e^* - d_k p_k^* e), \\ \frac{\partial m_k}{\partial t} &= \lambda_k^h (1 - m_k) - \gamma_k m_k + \left(\frac{\partial m_k}{\partial t} \right)_{\text{collision}} - \frac{i}{2\hbar} (d_k p_k e^* - d_k p_k^* e). \end{aligned} \quad (7.16)$$

We use (4.11-4.12) to model $\left(\frac{\partial n_k}{\partial t} \right)_{\text{collision}}$ and $\left(\frac{\partial m_k}{\partial t} \right)_{\text{collision}}$:

$$\begin{aligned} \frac{\partial n_\omega}{\partial t} &= -\left(\frac{\mu_e}{\mu_r} \right) \frac{1}{\Omega k^{d-1} \left(\frac{dk}{d\omega} \right)} \frac{\partial^2}{\partial \omega^2} I_1 \omega^{\gamma+6} \left(n_\omega^4 (n_\omega^{-1})'' + n_\omega^2 (\ln n_\omega)'' \right) \\ &\quad + \frac{\mu_e}{\Omega k^{d-1} \left(\frac{dk}{d\omega} \right)} \frac{\partial}{\partial \omega} I_2 \omega^{\gamma+4} (-\mu_h n m' (1 - n) + \mu_e (1 - m) m n') \\ \frac{\partial m_\omega}{\partial t} &= -\left(\frac{\mu_h}{\mu_r} \right) \frac{1}{\Omega k^{d-1} \left(\frac{dk}{d\omega} \right)} \frac{\partial^2}{\partial \omega^2} I_1 \omega^{\gamma+6} \left(m_\omega^4 (m_\omega^{-1})'' + m_\omega^2 (\ln m_\omega)'' \right) \\ &\quad - \frac{\mu_h}{\Omega k^{d-1} \left(\frac{dk}{d\omega} \right)} \frac{\partial}{\partial \omega} I_2 \omega^{\gamma+4} (-\mu_h n m' (1 - n) + \mu_e (1 - m) m n') \\ &\quad ()' = \frac{\partial}{\partial \omega}, \quad n_\omega = n(\mathbf{k}(\omega)), \quad m_\omega = m(\mathbf{k}(\omega)), \end{aligned}$$

where μ_e and μ_h are the masses of electron and hole respectively, μ_r is the reduced mass, $1/\mu_r = 1/\mu_e + 1/\mu_h$, I_1 and I_2 are positive-definite interaction

strengths (4.13):

$$\begin{aligned}
 I_1 &= \frac{1}{4} \int d\delta_1 d\delta_2 \mathcal{S}(1, 1 + \delta_1, 1 + \delta_2, 1 + \delta_1 - \delta_2) \delta_2^2 (\delta_1 - \delta_2)^2, \\
 I_2 &= \frac{\mu_e \mu_h}{4} \int d\delta_1 d\delta_2 (\delta_1 - \delta_3)^2 \\
 &\quad \times \left(\frac{\mu_e^2}{\mu_h \mu_r} \mathcal{S}(1, 1 + \delta_1, 1 + \frac{\mu_e}{\mu_h} (\delta_1 - \delta_3), 1 + \delta_3) \right. \\
 &\quad \left. \frac{\mu_h^2}{\mu_e \mu_r} \mathcal{S}(1, 1 + \delta_1, 1 + \frac{\mu_h}{\mu_e} (\delta_1 - \delta_3), 1 + \delta_3) \right).
 \end{aligned} \tag{7.17}$$

where $\Delta_i = \omega \delta_i$. We refer reader to Chapter 4 for more details on differential kinetic equations.

Transformation to non dimensionless variables is the same as in one particle case. The result is

$$\frac{\partial e}{\partial t} = i \frac{\Omega d_{k=0}^2 V}{2 \gamma_p^2 \epsilon_0 \hbar} \int d\mathbf{k} d_k p_k - \frac{\gamma_E}{\gamma_p} e, \tag{7.18}$$

$$\frac{\partial p_k}{\partial t} = \left(i \frac{\Omega}{\gamma_p} - i \frac{\tilde{\omega}_k}{\gamma_p} - 1 \right) p_k - i d_k (n_k + m_k - 1) e, \tag{7.19}$$

$$\frac{\partial n_k}{\partial t} = \frac{\Lambda_k^e}{\gamma_p} (1 - n_k) - \frac{\gamma_k}{\gamma_p} n_k + \frac{1}{\gamma_p} \left(\frac{\partial n_k}{\partial t} \right)_{\text{collision}} - i (d_k p_k e^* - d_k p_k^* e),$$

$$\frac{\partial m_k}{\partial t} = \frac{\Lambda_k^h}{\gamma_p} (1 - m_k) - \frac{\gamma_k}{\gamma_p} m_k + \frac{1}{\gamma_p} \left(\frac{\partial m_k}{\partial t} \right)_{\text{collision}} - i (d_k p_k e^* - d_k p_k^* e). \tag{7.20}$$

Definitions - broad band pumping.

- The total number of electrons (holes) supplied to the laser per unit time in the broad band pumping case is

$$\begin{aligned}
 &\left[\int (\Lambda_k^e (1 - n_k)) d\mathbf{k} \right] \quad \text{Number of electrons per unit time} \\
 &\left[\int (\Lambda_k^h (1 - m_k)) d\mathbf{k} \right] \quad \text{Number of holes per unit time}
 \end{aligned}$$

- The total number of *energy* supplied to the laser per unit time in the broad band pumping case is

$$\begin{aligned} \int d\mathbf{k} \left(\Lambda_k^{(e)}(1 - n_k) \left(\frac{\hbar^2 k^2}{2\mu_e} + \epsilon_{gap} \right) + \Lambda_k^{(h)}(1 - m_k) \frac{\hbar^2 k^2}{2\mu_h} \right) \\ \simeq \epsilon_{gap} \int d\mathbf{k} \Lambda_k^{(e)}(1 - n_k). \end{aligned} \quad (7.21)$$

because the band gap energy is 1400 meV, and the maximum width of steady-state carrier distribution is about 200 meV.

Definitions - narrow band pumping.

- The total number of *carriers* supplied per unit time in broad band pumping is

$$Q_0^e + Q_0^h.$$

To preserve charge neutrality we choose $Q_0^e = Q_0^h$.

- The total number of *energy* pumped to the system per unit time is

$$-P_0 = P_R - P_L = (\epsilon_{gap} + \omega_0 \frac{\mu_r}{\mu_e}) Q_0^e + \omega_0 \frac{\mu_r}{\mu_h} Q_0^h \simeq \epsilon_{gap} Q_0^e.$$

see (4.36).

We compare only cases in which the total amount of carriers supplied (per unit time) is the same and energy supplied is approximately the same.

Experimental setup. We would like to set up numerical experiments in such a way that total amount of carriers supplied to the laser are the same. Therefore we choose

$$\int \Lambda_k^e d\mathbf{k} (1 - n_k) = Q_0^e, \quad (7.22)$$

so that the number of electrons available to the system is the same in broad band and narrow band cases. We choose $Q_0^e = Q_L^e$ so that all electrons pumped to the system go to the left. This is an *assumption*. We also may choose Q_L consistent with (4.36), but this would employ some kind of arbitrariness (in choosing ω_R).

P_L chosen so that the energy absorbed by the laser is consistent with the number of carriers absorbed (see (4.37)).

Due to Pauli exclusion principle the amount of electrons absorbed by the system is $\int \Lambda_k^e d\mathbf{k}(1 - n_k)$ for broad band pumping case. Therefore to preserve charge neutrality of a laser we adjust Λ_k^h at every time step in such a way that

$$\int \Lambda_k^e d\mathbf{k}(1 - n_k) = \int \Lambda_k^h d\mathbf{k}(1 - m_k),$$

so that the total number of electrons and holes added are the same. We adjust Λ_k^h to match Λ_k^e (and not vice versa) because Pauli blocking is more significant for electrons.

The total number of energy pumped per unit time to the system is

$$\simeq \epsilon_{gap} \int d\mathbf{k} \Lambda_k^{(e)} (1 - n_k)$$

is almost equal to amount of energy pumped per unit time in the narrow band pumping case:

$$\simeq \epsilon_{gap} Q_0^e,$$

because of (7.22).

We choose the hole-hole interaction rate $\mu_h I_1$ (see (4.13)) to insure that holes relax to its equilibrium with typical relaxation time of 100 fs. We choose the electron-hole interaction strength I_2 (see (4.13)) to insure that electrons relaxes to hole temperature with typical relaxation time of 300 fs.

The constant s is again equal to 7. All other material parameters are the same as in the one-particle case.

Holes is two times heavier than electrons. Numerical results. We first take holes to be 2 times heavier than electrons:

$$\mu_h = 2\mu_e, \quad \mu_r = \frac{2}{3}\mu_e.$$

It turns out that for the same amount of carriers pumped and for the approximately same amount of energy pumped the output power in the narrow band case is higher especially for lower levels of pumping. The results of numerical simulations are presented in Figures (7.6-7.8) and summarized in Figure (7.9).

In the first numerical experiment, we show that for a very small amount of pumping the laser operates for the narrow band pumping, while it fails to operate in the broad band pumping case (i.e. the threshold pumping value for narrow band pumping is much lower than in the broad band case). The carriers supplied through the pumping process get totally absorbed by the global damping $-\gamma_k n_k$ in the broad band pumping case. There no lasing occurs. In the local band pumping case, for the same amount of carriers and approximately same amount of energy supplies, the laser operates. This is the qualitative difference between two cases.

We first pump broadly, so that the effective carrier distribution has (almost) zero flux. Then the laser fails to generate any output power. For the case of narrow-band pumping, when we pump in the narrow region around $\omega_0 \simeq 200\text{meV}$ and we model this by specifying the carriers and energy flux rates Q_L^e , Q_L^h and P_L , the laser does generate nonzero output power. The initial distribution functions (thin lines (7.6)) build up because of an influx of particles and energy from the right boundary (dashed lines) until the laser

switches on. The final (steady) distribution functions are shown by the thick dashed lines (longer and thinner dashing - electrons, shorter and thicker - holes distribution functions). The laser output power as a function of time is also shown.

We then increase the level of pumping to a point where the laser turns on for both the broad band and narrow band pumping cases, and examine the output power in both cases. It turns out that for the same amount of carriers pumped and approximately same amount of energy pumped the output power in the narrow band case is significantly higher than in the broad band case. The results are presented in Figures (7.7-7.8).

We assumed that all injected carriers go the left $Q_L = Q_0$. If we relax this assumption, the narrow-band pumping case will still be more effective than broad-band pumping for lower levels of pumping.

We now make a series of numerical experiments for different strengthes of narrow-band and broad-band pumping. Results are summarized In Figure (7.9) where we show the output power (field intensity) as a function of pumping strengths. We again observe that narrow band laser is significantly better in regions of small pumping. In regions of strong pumping the narrow band laser is still more effective.

We now consider the realistic electron to hole mass ratios.

Holes is six times heavier then electrons. We then take holes to be 6 times heavier than electrons:

$$\mu_h = 6\mu_e, \quad \mu_r = \frac{6}{7}\mu_e.$$

This is the typical value for electron-hole mass ratio.

Again it turns out that for the same amount of carriers pumped and approximately same amount of energy pumped the output power in the narrow

FIGURE 7.6. Time dependence of distributions (a) and output laser intensity (b) according to (7.18-7.20). Narrow pumping case.

Local-band pumping is modeled by specifying the carrier and energy flux rates Q_L^s and P_L at the right ($\omega_0 \simeq 200\text{meV}$) boundary. The initial distribution functions (shown by solid thin lines in this and consequent figures, thinner line - electrons, thicker line - holes) evolves through a number of intermediate states shown by dashed lines, until the laser switches on. The final (steady) distributions functions are shown by thick dashed lines (longer and thinner dashing - electrons, shorter and thicker - holes distribution functions). Output laser intensity as a function of time is also shown. Time is given in units of the relaxation time $\tau_{\text{relax}} = 100\text{fs}$ on this and subsequent figures. Lasing frequency is $1440\text{meV} = \epsilon_{\text{gap}} + 40\text{meV}$ and is marked by arrow. $\mu_h/\mu_e = 2$.

FIGURE 7.7. Same as on Figure (7.6) for increased pumping rate. Broad band pumping case. $\mu_h/\mu_e = 2$.

FIGURE 7.8. Same as on Figure (7.6) for narrow band pumping. Pumping rate is the same as in Figure (7.7). $\mu_h/\mu_e = 2$.

FIGURE 7.9. The output power as a function of pumping strength for narrow-band and broad-band pumping. $\mu_h/\mu_e = 2$.

Narrow band output power is shown by thick points, broad band output power is shown by thin points. We also draw lines connecting the numerical points.

band case is higher than in the broad band case. The results are presented in Figures (7.10-7.11) and summarized in Figure (7.12).

We now make a series of experiments for different strengthes of pumping. In Figure (7.12) we show the output power (field intensity) as a function of pumping strengths. We again observe that narrow band laser is significantly better in regions of small pumping. In regions of strong pumping the narrow band laser is still more effective.

7.6 Analysis.

We presented the results of numerical simulations for one- and two-species models of semiconductor lasers. We consistently observe that the laser operating on narrow band pumping has lower lasing thresholds (i.e. switches on for lower levels of pumping than broad-band pumped laser). Consequently the output power of narrow-band pumped laser is much bigger for weaker pumping rates. For bigger pumping rates narrow band laser is still slightly better then the broad band one. These effects can be explained qualitatively by noting that finite fluxes effectively lower the temperature of carriers, by redistributing carriers in such a way that bigger fraction of carriers occupies lower-energy part of the spectrum. Such redistribution creates bigger inversion in the lasing region as well as lowers the nonradiative carrier losses $\int \gamma_k n_k d\mathbf{k}$.

Note that while comparing efficiencies of different pumping schemes we have assumed that there is no energy cost associated with Pauli blocking. This is consistent, because we do not consider transport phenomena in the present manuscript. In reality, however, the carriers have to travel through the bulk of semiconductor crystal before having chance of contributing to the inversion. Since semiconductors have finite resistivity, one has to spend

FIGURE 7.10. Same as on Figure (7.6) for broad pumping case. $\mu_h/\mu_e = 6$.

FIGURE 7.11. Same as on Figure (7.6) for narrow pumping case. Pumping rate is the same as on Figure (7.10). $\mu_h/\mu_e = 6$.

FIGURE 7.12. The output power as a function of pumping strength for narrow-band and broad-band pumping. $\mu_h/\mu_e = 6$. Narrow band power is shown by thin points, narrow band output is shown by thick points. We also draw lines connecting the numerical points.

energy for “dragging” carrier through the crystal, even if the carrier does not contribute to inversion. Therefore it might be the case that there is a energy cost of Pauli blocking. Than the local band pumping is even more advantageous! To minimize Pauli blocking one has to chose the place of pumping to insure that Pauli blocking factor $(1 - n_{\omega_0})$ is sufficiently small (because n_{ω_0} is small) and at the same time amount of extra energy to spend is also small.

These results certainly suggest that the possibility of using narrow band pumping and the resulting finite flux equilibrium of the QKE is an option which is worth exploring further.

Chapter 8

CONCLUSION AND REMAINING CHALLENGES

We have shown that, for weak coupling, the full BBGKY hierarchy of operator equations has a natural asymptotic closure consistent with Hartree-Fock factorization and complex frequency renormalization.

We have demonstrated that the QKE has a new class of steady (equilibrium) solutions which carry constant fluxes of particles and energy across momentum space. We have explored these solutions by using the differential approximation to the collision integral.

We have then applied these ideas to semiconductor lasers and shown that the output power is consistently higher when the finite flux equilibrium is excited. We have also shown that finite-flux-equilibria lasers has lower lasing threshold.

While we do not claim that, if we take all effects into account, the advantages of narrow-band pumping will necessary remain, we do suggest that the evidence suggests that it is a possibility worth pursuing further.

Although the theory developed so far provides a qualitative understanding of possible, more effective semiconductor laser design, to gain a better quantitative understanding one has to solve a number of exciting challenges:

- It is known that phonons play a crucial role in “cooling” the semiconductor laser. One has to develop a self-consistent theory of semiconductor lasers starting from first principles, taking into account carrier-carrier, carrier-phonon and phonon-phonon interactions.
- We have treated the kernel of the Kinetic Equation by a differential

approximation. One has to go beyond this approximation by both considering higher order terms in expansion for collision operator and by studying full (integral) collision operators.

- We were considering isotropic cases only. Nonisotropic solutions of QKE may of great interest also.
- Considering systematically the kinetic-like equation for the polarization and its solutions is another direction of research with possibly a high impact in the area of optical communications.

These questions certainly have potential of entertain researches beyond the year of 2000.

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