THEORY OF PHOTO-INDUCED FERRO-MAGNETISM IN DILUTE MAGNETIC SEMICONDUCTORS

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by

SUBODHA MISHRA

Dr. Sashi Satpathy, Dissertation Supervisor

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The undersigned, appointed by the Dean of the Graduate School, have examined the dissertation entitled:

THEORY OF PHOTO-INDUCED FERRO-MAGNETISM IN DILUTE MAGNETIC SEMICONDUCTORS

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and hereby certify that in their opinion it is worthy of acceptance.

Prof. S. Satpathy

Prof. S. K. Loyalka

Prof. H. R. Chandrasekhar

Prof. P. Pfeifer

Prof. S. Zhang

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ABSTRACT

This thesis is a theoretical study of photo-induced ferro-magnetism in Dilute Magnetic Semiconductors. When light is incident on these systems, electrons and holes are created across the band gap. These particles interact with the impurity magnetic moments and mediate ferro-magnetism when temperature is lowered. This is a situation similar to the famous Rabi problem of a two state system coupled to time-dependent oscillating electric field. Ours is a multi-state system with electrons and holes coupled to an oscillating electric field. This is a generalization of the Rabi problem which shows also a phase transition from para to ferromagnetic state. We first study some model one and two state systems. We show by performing appropriate unitary transformations, it is possible to eliminate the time from the time-dependent Hamiltonians and get the eigen energies. Since our system of electrons and holes in contact with the photon bath is in a steady state, we calculate the free energy of the system. We study the problem of phase transition in two different ways , one by constructing Bogoliubov-Valatin quasi particles and the other by BCS wave function approach as in the low-temperature superconducting phenomenon. We calculate magnetization of the system in a self-consistent mean-field way. The magnetization and thereby the critical temperature is dependent on the photon energy incident on the system. By increasing the light coupling to the particles the transition temperature increases. Also by increasing the frequency of the light, the transition temperature is increased. Since more and more of the electrons and holes are created, these carriers mediate more with the magnetic moments and flip their moments into the ferro-magnetic state. It is also found that even when light energy is below the band-gap there is still magnetization and a ferro-magnetic state is still possible. It is interesting to find a linear dependence of critical temperature T_c on the square of the coupling.

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Chapter 1

Introduction

This thesis is a study of photo-induced ferro-magnetism in dilute magnetic semiconductors. When light falls on the semiconductor, it creates electron-hole pairs across the band gap. These carriers interact with the impurity magnetic atoms and so induce ferromagnetic coupling among magnetic moments and thereby create a ferromagnetic state in these semiconductors when temperature is lowered. Figure1.1 schematically describes the process.

1.1 Spintronics

The ability to control the properties of a system by acting on the spin of its charge carriers is the subject of the new field of "Spintronics" [1–4], and is believed to hold the promise to developing devices which combine storage functionalities (such as memory devices) together with information processing functionalities. Diluted Magnetic Semiconductors (DMS) have recently attracted a great deal of attention for their potential in combining ferro-magnetism and semiconductor properties in a single material. The DMS material is $Ga_{1-x}Mn_xAs$ (typically $x \approx (1 - 10\%)$) with the Mn ions substitutionally replacing Ga. Mn ions in $Ga_{1-x}Mn_xAs$ serve a dual purpose, acting both as dopants(acceptors in this case) and as magnetic impurities, whose spins align at the ferromagnetic transition (or,

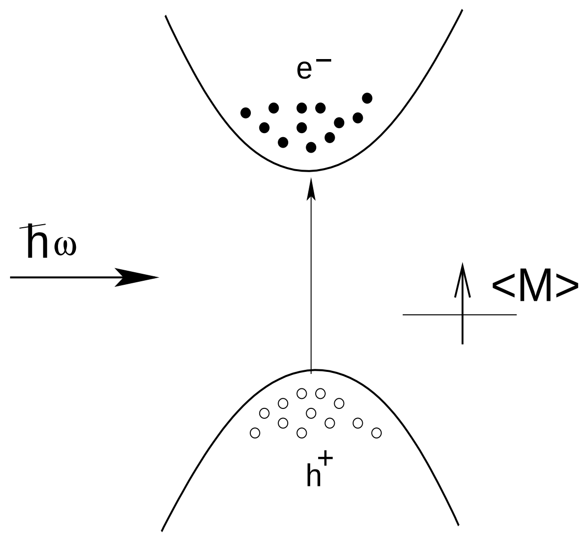

Figure 1.1: A schematic picture of light induced ferro-magnetism in dilute magnetic semiconductor. The electrons and holes that are created across the band gap interact with the magnetic moments and when temperature is lowered, system changes from para to ferro-magnetic phase.

equivalently, the Curie temperature) $T_c \approx$ 10-100K. Other DMS materials of current interest include $In_{1-x}Mn_xAs$, $Ga_{1-x}Mn_xP$ and $Ga_{1-x}Mn_xSb$. Prospects for new device functionalities in all semiconductor spin-electronic structures rely on the realization of a ferromagnetic semiconductor operating at room temperature. An important discovery in this material research was the discovery [3] of ferro-magnetism in Mn-doped GaAs with the Curie temperature $T_c = 100K$. Mn provides a local moment $S = 5/2$ and a delocalized hole [5]. Though ferromagnetism and semiconducting properties coexist in magnetic semiconductors, such as europium chalcogenides and semiconducting spinels their electronic structure is quite different from that of Si and GaAs, also the crystal growth is very very difficult. Again II-VI-based DMSs (CdTe, ZnSe) have been difficult to dope to create p- and n-type and the magnetic interaction in II-VI DMSs is dominated by the anti-ferromagnetic exchange among the Mn spins, which shows as paramagnetic, anti-ferromagnetic or spin-glass behavior. The III-V semiconductors such as GaAs are already in use in industry such as in electronic equipments and optoelectronic devices, including cellular phones(microwave transistors), compact disks (semiconductor lasers) etc. So it will be interesting to examine how light can induce some kind of magnetization when incident on these semiconductors.

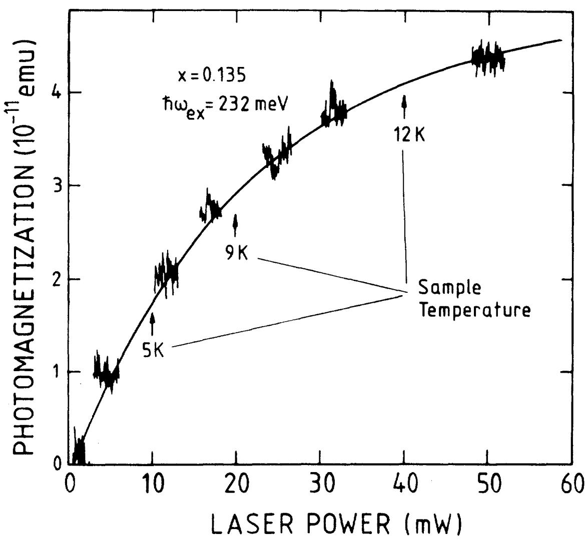

Figure 1.2: The dependence of photo-magnetization [7] in $Hg_{1-x}Mn_xTe$ ($x = 0.135$) on the impinging laser power. A linear relationship is observed only in the range up to 15 mW, below which most of the photo-magnetization experiments were performed. For higher laser powers the sample temperature increases and the signal deviates from proportionality.

1.2 The photo-induced ferro-magnetism: some experiments

In this section we discuss some experimental findings of how light can induce ferro-magnetism in DMS material. The idea is that the hole produced by the

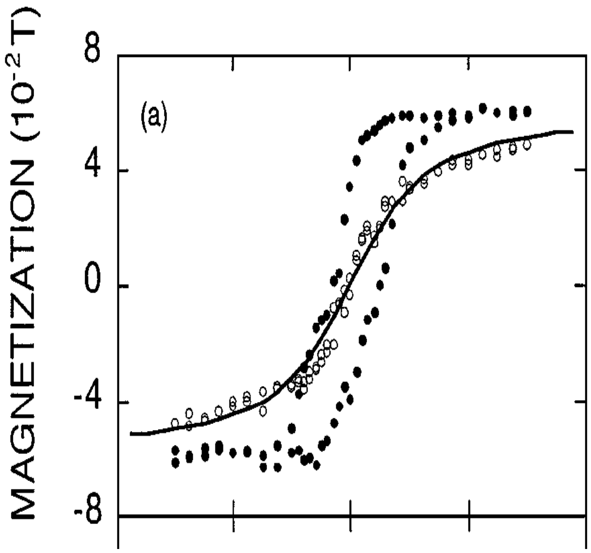

Figure 1.3: Magnetization curves [9] at 5 K observed before (open circles) and after (solid circles) light irradiation. Solid line shows a theoretical curve. x-axix is for magnetic field H(T) plotted from -0.30 to 0.30.

dopant Mn can interact with polarized light and be spin polarized and mediate ferromagnetic order between Mn moments. The photo-induced magnetization (PIM) has recently attracted a great deal of attention. The subject has acquired added importance in view of the search for materials with spin-polarized electrons to be relevant in the newly emerged area of spintronics [4], though dynamics of the carriers without spin has been studied in the past [6]. PIM was first demonstrated by Krenn et al [7, 8] who found a magnetization signal in $Hg_{1-x}Mn_xTe$ which depended characteristically on the degree of polarization of the exciting radiation which is shown in Fig.1.2. Interest has been focused recently on light induced magnetic phenomena in relatively important III-V based materials. In a recent paper Koshihara et al [9] observed the inducement of a ferromagnetic order by photo-generated carriers in the heterostructure (In,Mn)As/GaSb. Magnetization curves before and after the light irradiation are shown in Fig.1.3. At low

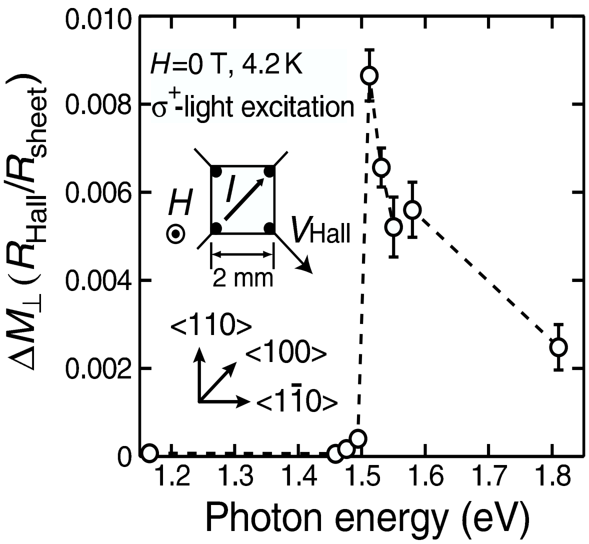

Figure 1.4: Dependence of photo-induced magnetization [10] ΔM extracted from anomalous Hall effect measurements on photon energy at 4.2 K for $Ga_{0.989}Mn_{0.011}As/GaAs$ sample with in-plane magnetic anisotropy. Illuminated light is σ^+ polarized. No magnetic field is applied. Excitation light power was about 600 mW/cm^2. The inset shows schematically the sample configuration.

temperatures, samples preserve ferromagnetic order even after light is switched off. They attribute the effect to hole transfer from GaSb to InMnAs in the heterostructure, which enhances a ferromagnetic spin exchange among Mn ions in the InMnAs layer. On the other hand, Oiwa et al [10] reported photo induced magnetization in ferromagnetic (Ga, Mn)As thin films caused by spin-polarized holes generated optically. Fig.1.4 shows dependence of photo-induced magnetization on photon energy. The observed results suggest that a small amount of non-equilibrium carrier spins can cause collective rotation of Mn spins presumably through p-d exchange interaction. While there have been a considerable number of experiments in this area, as is clear from the foregoing discussions, only recently have theorists focused on the problem. Piermarocchi et al [11] have reported a mechanism of coupling of spins localized in neighboring quantum dots by virtual excitation of delocalized exciton states in the host material by a light field. This indirect exchange interaction termed as ORKKY interaction, is analogous to a RKKY interaction ; the difference from the usual one is that the intermediate electron-hole pair is produced by external light. On the basis of the above ORKKY interaction, ferro-magnetism is predicted [12] in DMS illuminated by intense sub-band gap laser radiation.

1.3 Goals of this thesis

In this thesis we formulate the problem of photo-induced ferro-magnetism in Dilute Magnetic Semiconductors. We write down the Hamiltonian of the system and calculate energy and hence magnetization in the sample. The problem is studied using varieties of techniques such as, through the Bogoliubov-Valatin quasi-particle picture and also through the BCS-wave function approach.

In Chapter 2, we write down the Hamiltonian of the system and discuss the corresponding one-particle and two-particle pictures of the electrons and holes with up and down spins.

In Chapter 3, we study some model time-dependent Hamiltonians regarding their eigenenergy and then we construct an effective Hamiltonian for each one for their time evolution. We find that for these systems even if the Hamiltonians are time-dependent, their eigenenergies are not. We discuss the Rabi problem in detail in this chapter. We eliminate time from our Hamiltonian by an unitary transformation.

In Chapter 4, we construct Bogoliubov-Valatin transformations and transform our Hamiltonian of the system into this quasi particle picture. Then we diagonalize transformed Hamiltonian and calculate the energy of the system. Here we are able to get the energy of the excitations also.

In Chapter 5, we construct a BCS-type wavefunction for our problem and calculate energy of the system. Here we use a variational technique to calculate the ground state energy of the system.

In Chapter 6, we calculate the magnetization of the system and study the problem with different conditions of controlling parameters of the system.

In Chapter 7, we give the summary and conclusions of our work. We discuss some other ideas for further development in this field. In Appendix, we give the detail calculation of the BV transformations term by term and calculate some expectation values of some operators in the constructed BCS state of our problem.

Bibliography

[1] S. A. Wolff *et al* Science **294**, 1488 (2001).

[2] D. D. Awschalom, D. Loss and N. Samarth, Ed, *Semiconductor Spintronics and Quantum Computation*, (Springer, New York, 2002).

[3] H. Ohno, Science **281**, 951 (1998). H. Ohno *et al*, Nature (London) **408**, 944 (2000).

[4] S. Das Sarma, American Scientist, **89**, 516 (2001).

[5] T. Dietl *et al*, Scienc, **287**, 1019 (2000).

[6] C. Comte and G. Mahler, Phys. Rev. B, **38**, 10517 (1988).

[7] H. Krenn, K. Kaltenegger, T. Dietl, J. Spalek and G. Bauer, Phys. Rev. B, **39**, 10918 (1989).

[8] H. Krenn, W. Zawadzki and G. Bauer, Phys. Rev. Lett. **55**, 1510 (1985).

[9] S. Koshihara, A. Oiwa, M. Hirasawa, S. Katsumoto, Y. Iye, C. Urano, H. Takagi and H. Munekate, Phys. Rev. Lett. **78**, 4617,(1997).

[10] A. Oiwa, Y. Mitsumori, R. Moriya, T. Slupinski and H. Munekata, Phys. Rev. Lett. **88**, 137202-1 (2002).

[11] C. Piermarocchi, P. Chen, L. J. Sham and D. G. Steel, Phys. Rev. Lett. **89**, 167402-1(2002).

[12] J. Fernandez-Rossier, C. Piermarocchi, P. Chen, A. H. MacDonald and L. J. Sham, Phys. Rev. Lett. **93**, 127201 (2004).

Chapter 2

The Hamiltonian

2.1 The Hamiltonian of the problem

We consider a Hamiltonian describing a diluted magnetic semiconductor where electrons and holes generated by a light field are spin-split through an exchange interaction with the magnetic ions within mean field approximation. The Coulomb interaction includes electron-electron, hole-hole and electron-hole interactions. The semiconductor-light interaction is considered such that an electron-hole pair is created by absorption of light or an electron-hole pair recombines by emitting light. The light field is treated as a classical one. In the above situation, the Hamiltonian H is written as

$$H = H_{kin} + H_c + H_L(t) \tag{2.1}$$

where

$$H_{kin} = \sum_{\vec{k},\sigma} (\epsilon_{c\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \epsilon_{v\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma} d_{\vec{k}\sigma}) \tag{2.2}$$

$$H_c = H_{ee} + H_{hh} + H_{eh} \tag{2.3}$$

$$H_{ee} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} c^{\dagger}_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{2.4}$$

$$H_{hh} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} d^{\dagger}_{\vec{k}+\vec{q}\sigma} d^{\dagger}_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} d_{\vec{k}\sigma} \tag{2.5}$$

$$H_{eh} = - \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} d^{\dagger}_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{2.6}$$

$$H_L(t) = \lambda \sum_{\vec{k}} \rho_k [(c^{\dagger}_{\vec{k}\uparrow} d^{\dagger}_{-\vec{k}\downarrow} + c^{\dagger}_{\vec{k}\downarrow} d^{\dagger}_{-\vec{k}\uparrow}) e^{-i\omega t} + h.c] \tag{2.7}$$

In the above equations $c^{\dagger}$ and c are electron creation and destruction operators, $d^{\dagger}$ and d are the corresponding operators for holes. $V_{\vec{q}}$ denotes the particle-particle interaction. The negative sign in Eq.(2.6) denotes attractive interaction between electron and hole. We have parametrized the interaction of light with the particles. So we do not consider explicitly the matrix element of light-particle interaction [1] which comes from the $\lambda_k \sim < \psi_i | \hat{e}.\vec{p} | \psi_f >$ term when light interaction is treated in a semi-classical way. $\hat{e}$ is the polariastion vector of the light field. We take $\lambda_k = \lambda \rho_k$ and λ is the interaction strength of light-semiconductor coupling and momentum dependence of coupling is contained in ρ_k. σ, σ' denote the spin indices.

The single particle energy including the magnetic moment interaction, which is taken here in a mean field way can be written for the conduction band electron and valence band hole as:

$$\epsilon_{ck\uparrow(\downarrow)} = E_c(\vec{k}) \pm J_e(\langle M \rangle) \tag{2.8}$$

$$\epsilon_{vk\uparrow(\downarrow)} = E_v(\vec{k}) \pm J_h(\langle M \rangle) \tag{2.9}$$

here J_e and J_h are the electron and hole exchange interaction couplings with the localized magnetic moments (impurity atoms), $< M >$ is the average magnetization. The kinetic energy of the conduction band electron and that of valence band hole can be written as,

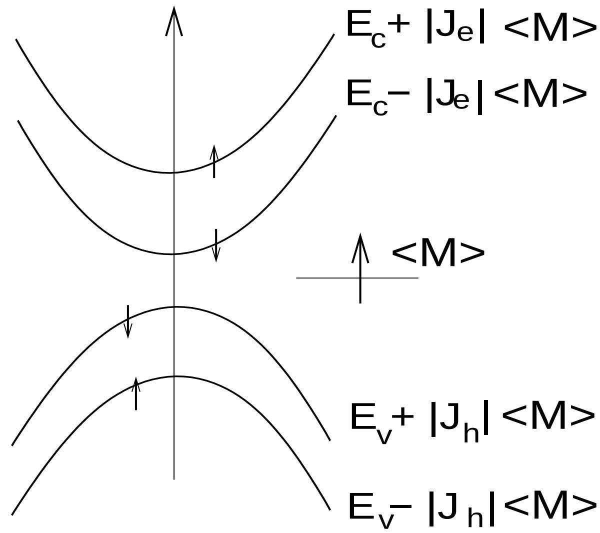

Figure 2.1: Spin-split one-particle energy band diagram for up electron and down electron as $E_c + |J_e| < M >$ and $E_c - |J_e| < M >$ in the conduction band and $E_v + |J_h| < M >$ and $E_v - |J_h| < M >$ for the down hole and up hole respectively in the valence band.

$$E_c(\vec{k}) = E_g + \frac{\hbar^2 k^2}{2m_e} \tag{2.10}$$

and

$$E_v(\vec{k}) = \frac{\hbar^2 k^2}{2m_h} \tag{2.11}$$

where E_g is the band gap and m_e and m_h are electron and hole effective masses respectively. This is shown pictorially in Fig.2.1. We also combine these single particle energies of spin up electron and spin down hole and spin down electron and spin up hole and show the band diagram in Fig.2.2.

2.2 Photon bath and Free energy

The system of electrons and holes is in contact with a light bath.This is shown pictorially in Fig.2.3. The chemical potential is the energy to add an particle to

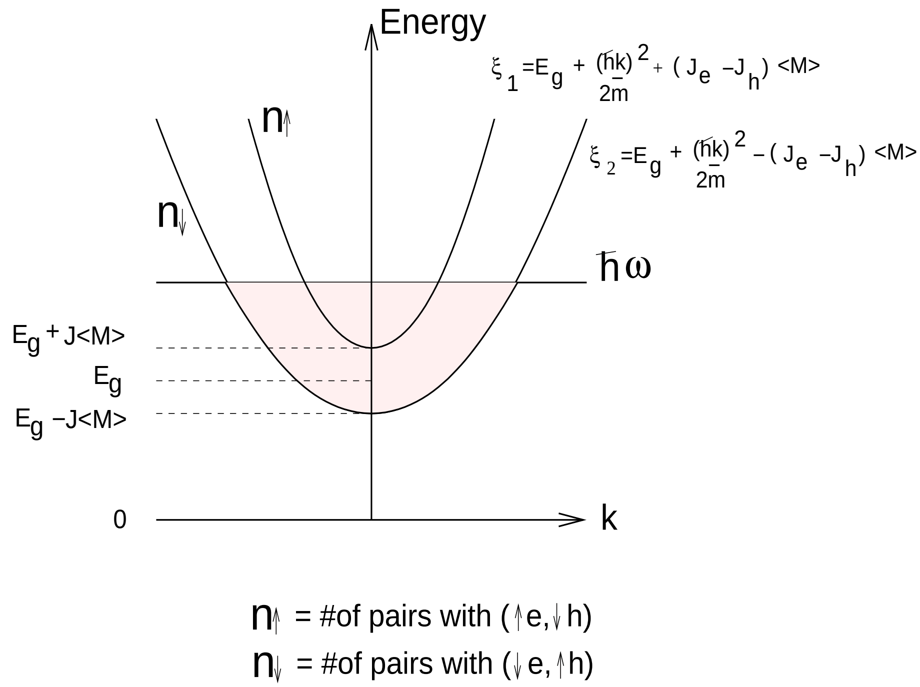

Figure 2.2: The two-particle energy band when light coupling $\lambda = 0$. Energy ξ_1 corresponds to $n\uparrow$ which refers to number of pairs with electron with up spin and hole with down spin and energy ξ_2 corresponds to $n\downarrow$ which refers to number of pairs with electron with down spin and hole with up spin. E_g refers to the highest position of the band gap. $E_g + J < M >$ and $E_g - J < M >$ refers to the highest positions of up and down two particle bands, split by the magnetic interaction energy $J < M >$.

the system. Here $\mu = \hbar\omega$ is required to create a hole and an electron. So the free energy to be minimized is given as

$$\begin{aligned} F &= H - \mu N_h \\ &= H - \mu \sum_{k\sigma} d^\dagger_{k\sigma} d_{k\sigma} \\ &= H - \frac{\mu}{2} \sum_{k\sigma} c^\dagger_{k\sigma} c_{k\sigma} - \frac{\mu}{2} \sum_{k\sigma} d^\dagger_{k\sigma} d_{k\sigma} \end{aligned} \tag{2.12}$$

where $\mu = \textit{chemical potential} = \hbar\omega$.

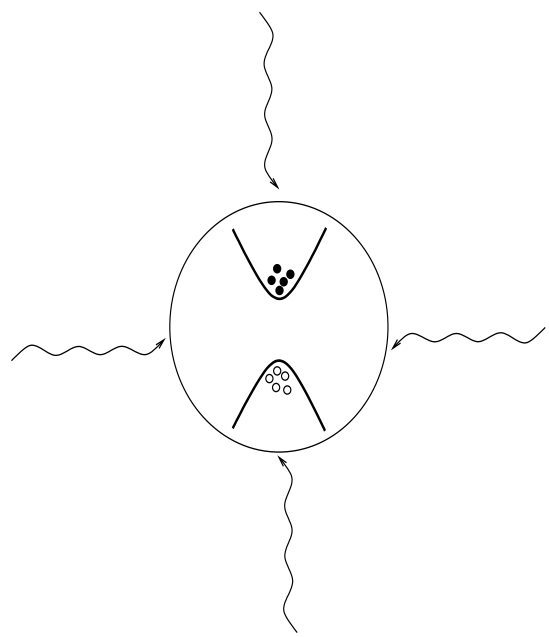

Figure 2.3: The system of electrons in the conduction band and holes in the valence band inside a light bath.

Bibliography

[1] F. Bassani and G. P. Parravicini, *Electronic states and optical transitions in solids*, (Pergamon, New York, 1975), p.151.

Chapter 3

Unitary transformations and elimination of time

3.1 Some model Hamiltonians

Since we will make an unitary transformation to eliminate time in our original Hamiltonian Eq.(2.1-2.7), we first study some simpler model Hamiltonians to illustrate the transformation. The physics of these Hamiltonians are related to our many-particle Hamiltonian. We study the effective Hamiltonian that is responsible for the time evolution of the system. Also by diagonalizing these original time dependent Hamiltonians, we calculate the energy eigenvalues of these particular Hamiltonians. We see that for some of these Hamiltonians, under certain condition the energy eigenvalues are time independent. The effective Hamiltonian of the problem gives the time evolution of the system. One can do a unitary transformation on time-independent or time-dependent Hamiltonians. However, if the unitary transformation itself is time-dependent, the transformed Schrodinger equation takes a modified form. Sometimes the time-dependent original Hamiltonian transforms into a time-independent Hamiltonian.

The Schrödinger equation is given as

$$\boxed{i\hbar\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t)} \tag{3.1}$$

where $H(t)$ is a time-dependent Hamiltonian. Let us now consider the time-dependent unitary operator,

$$U(t) = e^{iS(t)} \tag{3.2}$$

where $S(t)$ is Hermitian at all times. Then the transformed state vectors and operators are given by :

$$\tilde{\Psi}(t) = e^{-iS(t)}\Psi(t) \tag{3.3}$$

$$\tilde{O}(t) = e^{-iS(t)}O(t)e^{iS(t)} \tag{3.4}$$

Similarly,

$$\tilde{H}(t) = e^{-iS(t)}H(t)e^{iS(t)} \tag{3.5}$$

The rotation of operators and state vectors in Hilbert space does not change the eigenvalues so that the eigenvalues of H and $\tilde{H}$ are same. The Schrödinger equation that defines the evolution of $\tilde{\Psi}(t)$ does not follow $\tilde{H}$, but follow $\tilde{H}$ with an extra term added to it. Let us compute [1] how $\tilde{\Psi}(t)$ changes with time using Eq.(3.3),

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\tilde{\Psi}(t) &= i\hbar(\frac{\partial}{\partial t}e^{-iS(t)})\Psi(t) + i\hbar e^{-iS(t)}\frac{\partial}{\partial t}\Psi(t) \\ &= i\hbar(\frac{\partial}{\partial t}e^{-iS(t)})e^{iS(t)}\tilde{\Psi}(t) + \tilde{H}(t)\tilde{\Psi}(t) \\ &= [\tilde{H}(t) + i\hbar(\frac{\partial}{\partial t}e^{-iS(t)})e^{iS(t)}]\tilde{\Psi}(t) \\ &\equiv \tilde{H}_{eff}\tilde{\Psi}(t) \end{aligned} \tag{3.6}$$

Thus the effective transformed Hamiltonian (the transformed Hamiltonian which describes the evolution of $\tilde{\Psi}(t)$)is given as

$$\tilde{H}_{eff} = \tilde{H}(t) + i\hbar(\frac{\partial}{\partial t}e^{-iS(t)})e^{iS(t)} \tag{3.7}$$

This Hamiltonian may even be time-independent. Notice that $\tilde{\Psi}(t)$ does not evolve according to $\tilde{H}$, but rather according to $\tilde{H}_{eff}$.

3.1.1 One level system

Isolated one-level system without a light field

To begin with, we consider the trivial case of a one-level system

$$\boxed{H = \alpha c^\dagger c} \tag{3.8}$$

where $c^\dagger(c)$ is the particle creation(annihilation) operator. We make an unitary transformation of the form e^{iS}, where S is an Hermitian operator ($S^\dagger = S$) and it is given as

$$S = \omega t c^\dagger c \tag{3.9}$$

Then the transformed Hamiltonian reads

$$\boxed{\tilde{H} = e^{-iS} H e^{iS} = \alpha c^\dagger c} \tag{3.10}$$

Now we calculate the effective Hamiltonian for the one level system,

$$\tilde{H}_{eff} = \tilde{H} + i\hbar(\frac{\partial}{\partial t} e^{-iS})e^{iS} \tag{3.11}$$

$$= \tilde{H} + i\hbar(-i\omega c^\dagger c) \tag{3.12}$$

$$= (\alpha + \hbar\omega)c^\dagger c \tag{3.13}$$

$$\boxed{\tilde{H}_{eff} = (\alpha + \hbar\omega)c^\dagger c} \tag{3.14}$$

We now verify that we get the same answer for $\Psi(t)$ whether we calculate $\Psi(t)$ directly or calculate it by first evaluating $\tilde{\Psi}(t)$ which reads

$$|\tilde{\Psi}(t) > \equiv e^{-iS(t)}|\Psi(t) > \tag{3.15}$$

Now we see that the Schrödinger equations obeyed by H and $\tilde{H}_{eff}$ are

$$i\hbar\frac{\partial \Psi}{\partial t} = H\Psi \tag{3.16}$$

$$i\hbar\frac{\partial \tilde{\Psi}}{\partial t} = \tilde{H}_{eff}\tilde{\Psi} \tag{3.17}$$

But we know the wavefunction $\tilde{\Psi}(t)$ at time t is related to wavefunction at time t=0 as

$$\tilde{\Psi}(t) = e^{-i\int \tilde{H}_{eff}dt/\hbar}\tilde{\Psi}(0) \tag{3.18}$$

which can be simplified as

$$e^{-iS}\Psi(t) = e^{-i\tilde{H}_{eff}t/\hbar} \times e^{-S(t=0)}\Psi(0) \tag{3.19}$$

So the time evolution of $\Psi(t)$ which obeys the Hamiltonian H is given by

$$\begin{aligned} \Psi(t) &= e^{iS}e^{-i(\alpha+\hbar\omega)c^\dagger ct/\hbar}\Psi(0) && (3.20) \\ &= e^{-i\alpha c^\dagger ct/\hbar}\Psi(0) && (3.21) \\ &= e^{-i\frac{Ht}{\hbar}}\Psi(0) && (3.22) \end{aligned}$$

which checks that it has the right time evolution operator corresponding to the Hamiltonian H.

One-level system interacting with a light field

Now we consider another example. Here the one-level system is interacting with a light field. The Hamiltonian is given as

$$\boxed{H = \alpha c^\dagger c + \lambda(e^{-i\omega t} + e^{i\omega t})c^\dagger c} \tag{3.23}$$

where λ is the coupling strength of the classical light field with frequency ω and we have two terms due to the Hermitian conjugation. The eigenvalue of H is given as

$$eigenvalue = \alpha + \lambda(e^{-i\omega t} + e^{i\omega t}) \tag{3.24}$$

which oscillate between $\alpha + 2\lambda$ and $\alpha - 2\lambda$. We plot in Fig(3.1) eigenvalue as function of time t as given by Eq.(3.24). The graph shows the variation of eigenvalue from maximum $\alpha + 2\lambda$ to minimum $\alpha - 2\lambda$.

Now we make the unitary transformation e^{-iS}, where again,

$$S = \omega t c^\dagger c \tag{3.25}$$

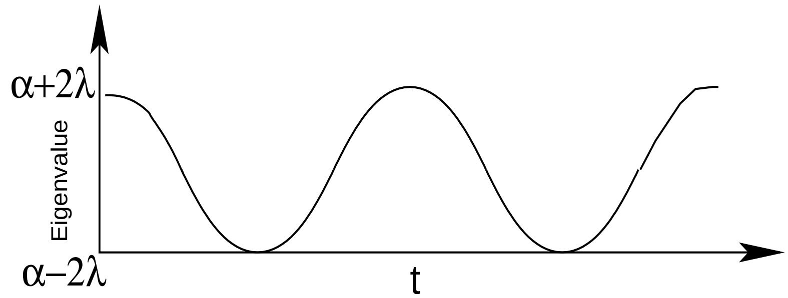

Figure 3.1: Eigenvalue as a function of time t as given by Eq.(3.24).The graph shows the variation of the eigenvalue between the two limits $\alpha + 2\lambda$ and $\alpha - 2\lambda$.

The transformed Hamiltonian is given as

$$\begin{aligned} \tilde{H} &= e^{-iS} H e^{iS} = \alpha c^\dagger c + e^{-i\omega t c^\dagger c} [\lambda c^\dagger c (e^{-i\omega t} + e^{i\omega t})] e^{i\omega t c^\dagger c} \\ &= \alpha c^\dagger c + \lambda c^\dagger c (e^{-i\omega t} + e^{i\omega t}) \end{aligned} \tag{3.26}$$

$$\boxed{\tilde{H} = \alpha c^\dagger c + \lambda c^\dagger c (e^{-i\omega t} + e^{i\omega t})} \tag{3.27}$$

Eigenvalues of H,$\tilde{H}$ are the same as expected because the unitary transformation is a rotation in Hilbert space at any specific time t. $\tilde{H}_{eff}$ is given as:

$$\begin{aligned} \tilde{H}_{eff} &= \tilde{H} + i\hbar (\frac{\partial}{\partial t} e^{-iS}) e^{iS} \\ &= \alpha c^\dagger c + \hbar\omega c^\dagger c + \lambda c^\dagger c (e^{-i\omega t} + e^{i\omega t}) \end{aligned} \tag{3.28}$$

$$\boxed{\tilde{H}_{eff} = \alpha c^\dagger c + \hbar\omega c^\dagger c + \lambda c^\dagger c (e^{-i\omega t} + e^{i\omega t})} \tag{3.29}$$

Note that $\tilde{H}_{eff}$ has a different eigenvalues than that of $\tilde{H}$. The eigenvalue is given as

$$eigenevalue = \alpha + \hbar\omega + \lambda(e^{-i\omega t} + e^{i\omega t}) \tag{3.30}$$

In Fig(3.2), we give a plot of eigenvalue as function of time t as given by Eq.(3.30).The graph shows the variation of eigenvalue from maximum $\alpha + 2\lambda + \hbar\omega$ to minimum $\alpha - 2\lambda + \hbar\omega$ Notice that the energy eigenvalue is determined from H or $\tilde{H}$, but not from $\tilde{H}_{eff}$. $\tilde{H}_{eff}$ merely describes the evolution of $|\tilde{\Psi}(t) >$.

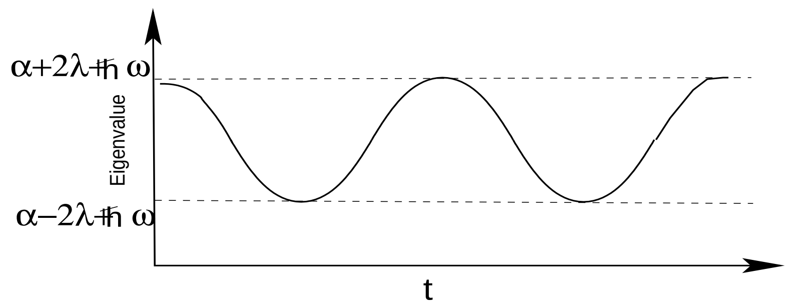

Figure 3.2: Eigenvalues of $\tilde{H}$ as a function of time t as given by Eq.(3.30).The graph shows the variation of the eigenvalue between the two limits $\alpha + 2\lambda + \hbar\omega$ and $\alpha - 2\lambda + \hbar\omega$.

3.1.2 The Rabi problem

A particle in a two state system when coupled to a light field oscillates between these two states. This is the famous Rabi problem.

Eigenenergies of Rabi problem

A particle in a two state system when coupled to a light field oscillates between these two states. This is the famous Rabi problem. Now we consider a Hamiltonian which describes a two state problem coupled two a light field. The electron creation operator is $c^\dagger$ in one level and is $d^\dagger$ in the other level. The electron is interacting with the light field of frequency ω. The coupling of light to electron is denoted by λ. We thus have a time-dependent potential that connects the two energy eigenstates of $H_0 = \alpha c^\dagger c + \beta d^\dagger d$. In other words, we can have a transition between the two states $|\alpha >\leftrightarrow |\beta >$.

$$\boxed{H = \alpha c^\dagger c + \beta d^\dagger d + \lambda(c^\dagger d e^{i\omega t} + d^\dagger c e^{-i\omega t})} \tag{3.31}$$

We have taken just two electron states here, which are coupled to light. The Hamiltonian can be written in matrix form as

$$H = \begin{pmatrix} \alpha & \lambda e^{i\omega t} \\ \lambda e^{-i\omega t} & \beta \end{pmatrix} \tag{3.32}$$

By diagonalizing the Hamiltonian we find the eigen values as:

$$eigenvalue = \frac{\alpha+\beta}{2} \pm \sqrt{(\frac{\alpha-\beta}{2})^2 + \lambda^2} \equiv \alpha_+, \beta_- \tag{3.33}$$

In Fig(3.3), we give a plot which shows schematically the eigenvalues as given by the Eq.(3.33).

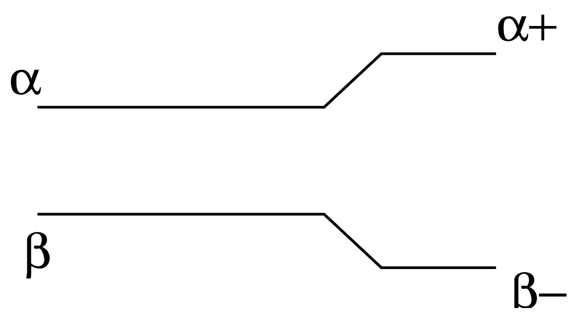

Figure 3.3: Eigenvalues α, β of the two-level system becomes modified to α_+, β_- due to coupling to the light. See Eq.(3.32) and Eq.(3.33).

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Note energy of the two-level system is shifted by the coupling λ. Now observe that even though the Hamiltonian is time dependent, the eigenvalues are not!

Unitary transformation and elimination of time.

We do not want time to stick around in the Hamiltonian, so we make an unitary transformation on the Hamiltonian H,

$$\tilde{H} = e^{-iS} H e^{iS} \tag{3.34}$$

where

$$S = \omega_1 t c^\dagger c + \omega_2 t d^\dagger d \tag{3.35}$$

We write

$$H = H_1 + H_2 + H_3 \tag{3.36}$$

Now we find that

$$\tilde{H}_1 = e^{-i\omega_1 c^\dagger c - i\omega_2 t d^\dagger d}(\alpha c^\dagger c)e^{i\omega_1 c^\dagger c + i\omega_2 t d^\dagger d} = \alpha c^\dagger c \tag{3.37}$$

Similarly

$$\tilde{H}_2 = \beta d^\dagger d \tag{3.38}$$

Now to compute $\tilde{H}_3$: we write

$$H_3 = T_1 + T_2 \tag{3.39}$$

where $T_1 = \lambda c^\dagger d e^{i\omega t}$ and T_2 is its Hermitian conjugate. We write

$$\begin{aligned}
\tilde{T}_1 &= e^{-i\omega_1 t c^\dagger c - i\omega_2 t d^\dagger d}(\lambda c^\dagger d e^{i\omega t})e^{i\omega_1 t c^\dagger c + i\omega_2 t d^\dagger d} && (3.40)\\
&= e^{itB} A e^{-itB} && (3.41)
\end{aligned}$$

Now we require to calculate [B,A]. We know that $[c^\dagger c, c^\dagger] = c^\dagger$, and $[d^\dagger d, d] = -d$. Hence

$$\begin{aligned}
[B, A] &= [-\omega_1 c^\dagger c - \omega_2 d^\dagger d, c^\dagger d]\lambda e^{i\omega t} && (3.42)\\
&= (-\omega_1 c^\dagger d + \omega_2 d c^\dagger)\lambda e^{i\omega t} && (3.43)\\
&= (-\omega_1 + \omega_2) c^\dagger d \lambda e^{i\omega t} && (3.44)
\end{aligned}$$

$$[B, [B, A]] = (-\omega_1 + \omega_2)^2 c^\dagger d \lambda e^{i\omega t} \tag{3.45}$$

So $\tilde{T}_1$ can be calculated as:

$$\begin{aligned}
\tilde{T}_1 &= A + it[B, A] + \frac{(it)^2}{2!}[B, [B, A]] + ... && (3.46)\\
&= \lambda c^\dagger d e^{i\omega t} + it(-\omega_1 + \omega_2)\lambda c^\dagger d e^{i\omega t} + \frac{(it)^2}{2!}(-\omega_1 + \omega_2)^2 \lambda c^\dagger d e^{i\omega t} + ...\\
&= \lambda c^\dagger d e^{i\omega t}[1 + it(-\omega_1 + \omega_2) + \frac{(it)^2}{2!}(-\omega_1 + \omega_2)^2 + ...]\\
&= \lambda c^\dagger d e^{i\omega t} e^{-it(\omega_1 - \omega_2)}
\end{aligned}$$

When $\omega = \omega_1 - \omega_2$, we have

$$\tilde{T}_1 = \lambda c^\dagger d \tag{3.47}$$

Similarly the other term $\tilde{T}_2$ can be found to be

$$\tilde{T}_2 = \lambda d^\dagger c \tag{3.48}$$

So the total transformed Hamiltonian under the condition that $\omega = \omega_1 - \omega_2$ can be written as

$$\boxed{\tilde{H} = \tilde{H}_1 + \tilde{H}_2 + \tilde{H}_3 = \alpha c^\dagger c + \beta d^\dagger d + \lambda(c^\dagger d + d^\dagger c)} \tag{3.49}$$

Note that $\tilde{H}$ became independent of time unlike H. $\tilde{H}$ has same energy spectrum as H. It is therefore easier to work with $\tilde{H}$. Now we compute $\tilde{H}_{eff}$.

$$\begin{aligned} \tilde{H}_{eff} &= \tilde{H} + i\hbar(\frac{\partial}{\partial t}e^{-iS})e^{iS} \qquad (3.50) \\ &= \tilde{H} + \hbar\omega_1 c^\dagger c + \hbar\omega_2 d^\dagger d \\ &= (\alpha + \hbar\omega_1)c^\dagger c + (\beta + \hbar\omega_1)d^\dagger d + \lambda(c^\dagger d + d^\dagger c) - \hbar\omega d^\dagger d \end{aligned}$$

$$\boxed{\tilde{H}_{eff} = (\alpha + \hbar\omega_1)c^\dagger c + (\beta + \hbar\omega_1)d^\dagger d + \lambda(c^\dagger d + d^\dagger c) - \hbar\omega d^\dagger d} \tag{3.51}$$

Evolution of the wave function We discuss now the time evolution of the particle placed at level # 1 at $t = 0$. The Hamiltonian of the problem is given by Eq.(3.32). We thus have a time-dependent potential that connects the two energy eigenstates of H_0. In other words, we can have transition between the states $c^\dagger \rightarrow d^\dagger$. If initially at $t = 0$ only the lower level (state #1 with energy α) is populated then,

$$c_1(0) = 1 \tag{3.52}$$

$$c_2(0) = 0 \tag{3.53}$$

where c_1 and c_2 are the probability amplitude of being found in corresponding states. The time dependence of the amplitudes $c_m(t)$ are given [2] by the

Schrödinger equation:

$$i\hbar\frac{d}{dt}c_n(t) = \sum_m V_{nm}e^{i\omega_{nm}t}c_m(t) \tag{3.54}$$

where $\omega_{nm} \equiv \frac{(E_n - E_m)}{\hbar}$. Then the probability for being found in each of the two states is given by Rabi's formula [2] as

$$|c_2(t)|^2 = \frac{\lambda^2/\hbar^2}{\lambda^2/\hbar^2 + (\omega-\omega_{21})^2/4} sin^2\{[\frac{\lambda^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4}]^{1/2}t\} \tag{3.55}$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2 \tag{3.56}$$

We see that $|c_2|^2$,the probability for finding the particle in the upper state #2 exhibits an oscillatory time dependence with angular frequency, two times that of

$$\Omega = \sqrt{(\frac{\lambda^2}{\hbar^2}) + \frac{(\omega-\omega_{21})^2}{4}} \tag{3.57}$$

There is resonance when

$$\omega = \omega_{21} = \frac{(\beta-\alpha)}{\hbar} \tag{3.58}$$

So that at the resonance point:

$$\Omega = \frac{\lambda}{\hbar} \tag{3.59}$$

We plot in Fig.(3.4) $|c_1(t)|^2$ and $|c_2(t)|^2$ as function of time t exactly at resonance $\omega = \omega_{21}$ and $\Omega = \lambda/\hbar$. The graph also illustrates the back-and-forth behavior between $|1>$ and $|2>$. In Fig.(3.5), we also give the plot of $|c_2(t)|^2_{max}$ as function of ω, where $\omega = \omega_{21}$ corresponds to the resonant frequency. This plot shows the important point that even below the resonant frequency there is a finite transition probability. This is an important point, since this feature will give rise to subbandgap absorption in the photo-induced ferro-magnetism which we will discuss later.

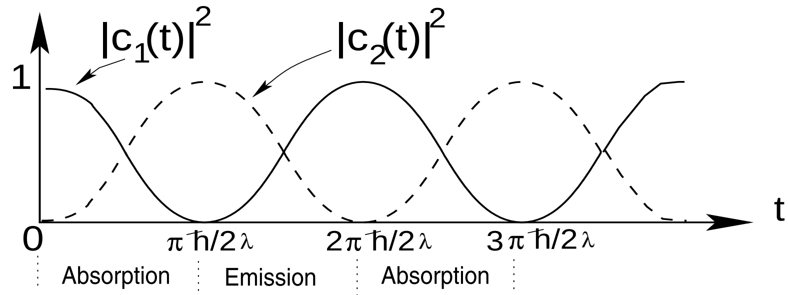

Figure 3.4: Plot of $|c_1(t)|^2$ and $|c_2(t)|^2$ as functions of time t exactly at resonance $\omega = \omega_{21}$ and $\Omega = \lambda/\hbar$. The graph also illustrates the oscillatory behavior between $|1>$ and $|2>$.

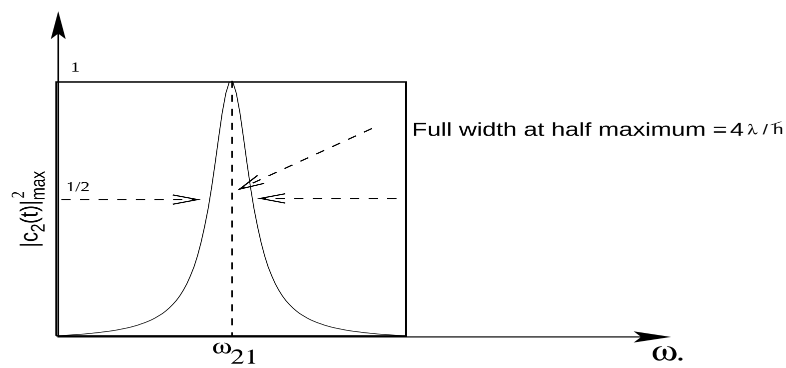

Figure 3.5: Plot of $|c_2(t)|^2_{max}$ as function of ω, where $\omega = \omega_{21}$ corresponds to the resonant frequency. This plot shows that even below the resonant condition there is a finite transition probability between the two states.

3.1.3 Hamiltonian for a single particle-hole pair

We now turn to the Hamiltonian which describes an electron-hole pair interacting with the classical light field . $c^\dagger$ is the creation operator for the electron in the conduction band, and $d^\dagger$, hole in valence band. This Hamiltonian resembles a single particle picture of our full Hamiltonian for describing the light induced particle-hole creation in diluted magnetic semiconductor.

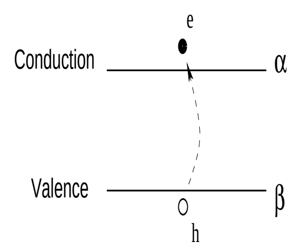

Figure 3.6: Plot of electron(e) in the conduction band and hole(h) in the valence band.

$$\boxed{H = \alpha c^\dagger c + \beta d^\dagger d + \lambda(c^\dagger d^\dagger e^{i\omega t} + dce^{-i\omega t})} \tag{3.60}$$

This Hamiltonian allows for creation and destruction of one electron and one hole simultaneously. The one hole and one electron state here are coupled to light. For the basis set $|1,0>$,$|0,1>$, $|1,1>$ and $|0,0>$, the above Hamiltonian can be written in matrix form as

$$H = \begin{pmatrix} \alpha & & & \\ & \beta & & \\ & & \alpha+\beta & \lambda e^{-i\omega t} \\ & & \lambda e^{i\omega t} & 0 \end{pmatrix} \tag{3.61}$$

By diagonalizing the above Hamiltonian , we get the eigenvalues E_i as:

$$E_1, E_2 = \alpha, \beta \tag{3.62}$$

$$E_3, E_4 = \frac{\alpha+\beta}{2} \pm \sqrt{(\frac{\alpha-\beta}{2})^2 + \lambda^2} \tag{3.63}$$

Energy of the two-level system is shifted by the coupling λ. In Fig(3.7), we give a plot of eigen energies of Hamiltonian Eq.(3.61) as given by Eq.(3.62) and Eq.(3.63). Now observe that even though the Hamiltonian is time dependent, the eigenvalues are not!

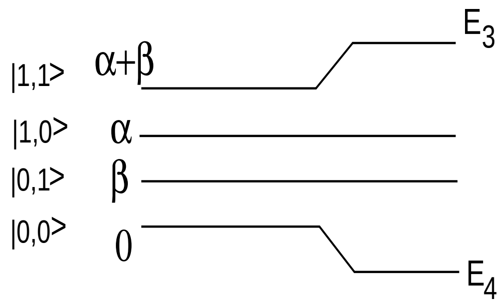

Figure 3.7: Eigen energies of Hamiltonian Eq.(3.61) as given by Eq.(3.62) and Eq.(3.63). $|n_e, n_h>$ denote the occupation number state of the electron and hole.

Note: E_4 the vacuum energy came down because of λ. E_3, the two particle state energy went up. We now make the unitary transformation e^{iS}, so that

$$\tilde{H} = e^{-iS} H e^{iS} \tag{3.64}$$

where

$$S = \omega_1 t c^\dagger c + \omega_2 t d^\dagger d \tag{3.65}$$

We write

$$H = H_1 + H_2 + H_3 \tag{3.66}$$

so that

$$\tilde{H}_1 = e^{-i\omega_1 c^\dagger c - i\omega_2 t d^\dagger d}(\alpha c^\dagger c) e^{i\omega_1 c^\dagger c + i\omega_2 t d^\dagger d} = \alpha c^\dagger c \tag{3.67}$$

Similarly we can evaluate

$$\tilde{H}_2 = \beta d^\dagger d \tag{3.68}$$

Now to compute $\tilde{H}_3$: we write

$$H_3 = T_1 + T_2 \tag{3.69}$$

wherer $T_1 = \lambda c^\dagger d^\dagger e^{i\omega t}$ and T_2 is its Hermitian conjugate. We write

$$\begin{aligned} \tilde{T}_1 &= e^{-i\omega_1 c^\dagger c - i\omega_2 t d^\dagger d}(\lambda c^\dagger d^\dagger e^{i\omega t}) e^{i\omega_1 c^\dagger c + i\omega_2 t d^\dagger d} && (3.70) \\ &= e^{itB} A e^{-itB} && (3.71) \end{aligned}$$

Now we require to calculate [B,A]. We know that $[c^\dagger c, c^\dagger] = c^\dagger$, and $[d^\dagger d, d] = -d$. Hence

$$\begin{aligned} [B, A] &= [-\omega_1 c^\dagger c - \omega_2 d^\dagger d, c^\dagger d^\dagger] \lambda e^{i\omega t} && (3.72) \\ &= (-\omega_1 c^\dagger d^\dagger + \omega_2 d^\dagger c^\dagger) \lambda e^{i\omega t} && (3.73) \\ &= (-\omega_1 + \omega_2) c^\dagger d^\dagger \lambda e^{i\omega t} && (3.74) \end{aligned}$$

$$[B, [B, A]] = (-\omega_1 + \omega_2)^2 c^\dagger d^\dagger \lambda e^{i\omega t} \tag{3.75}$$

So we have

$$\begin{aligned} \tilde{T}_1 &= A + it[B, A] + \frac{(it)^2}{2!}[B, [B, A]] + ... && (3.76) \\ &= \lambda c^\dagger d e^{i\omega t} + it(-\omega_1 + \omega_2)\lambda c^\dagger d^\dagger e^{i\omega t} + \frac{(it)^2}{2!}(-\omega_1 + \omega_2)^2 \lambda c^\dagger d^\dagger e^{i\omega t} + ...] \\ &= \lambda c^\dagger d^\dagger e^{i\omega t}[1 + it(-\omega_1 + \omega_2) + \frac{(it)^2}{2!}(-\omega_1 + \omega_2)^2 + ...] \\ &= \lambda c^\dagger d^\dagger e^{i\omega t} e^{it(\omega_1 - \omega_2)} \\ &= \lambda c^\dagger d^\dagger && (3.77) \end{aligned}$$

where we have taken $\omega = \omega_1 - \omega_2$. The transformed Hamiltonian is given as

$$\boxed{\tilde{H} = \tilde{H}_1 + \tilde{H}_2 + \tilde{H}_3 = \alpha c^\dagger c + \beta d^\dagger d + \lambda (c^\dagger d^\dagger + dc)} \tag{3.78}$$

We see that $\tilde{H}$ is independent of time. Notice once again that $\tilde{H}$ has same energy spectrum as H.

Similarly, if we are interested in the time evolution of the $\tilde{\Psi}(t)$then per section 3.1, we should calculate $\tilde{H}_{eff}$.

$$\begin{aligned}\tilde{H}_{eff} &= \tilde{H} + i\hbar(\frac{\partial}{\partial t}e^{-iS})e^{iS} \\ &= \tilde{H} + \hbar\omega_1 c^\dagger c + \hbar\omega_2 d^\dagger d \\ &= (\alpha + \hbar\omega_1)c^\dagger c + (\beta + \hbar\omega_1)d^\dagger d + \lambda(c^\dagger d^\dagger + dc) - \hbar\omega d^\dagger d\end{aligned} \tag{3.79}$$

$$\boxed{\tilde{H}_{eff} = (\alpha + \hbar\omega_1)c^\dagger c + (\beta + \hbar\omega_1)d^\dagger d + \lambda(c^\dagger d^\dagger + dc) - \hbar\omega d^\dagger d} \tag{3.80}$$

Note that $\tilde{H}_{eff}$ has a different spectrum than H or $\tilde{H}$.

3.2 Unitary transformation of the full Hamiltonian

In this section we will perform an unitary transformation on our many particle Hamiltonian of electrons and holes (Eq.(2.1-2.7)) interacting among themselves and with a time-dependent classical light field to get rid of the time.

$$H = H_{kin} + H_{ee} + H_{hh} + H_{eh} + H_L(t) \tag{3.81}$$

where

$$H_{kin} = \sum_{\vec{k},\sigma}(\epsilon_{c\vec{k}\sigma} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + \epsilon_{v\vec{k}\sigma} d^\dagger_{\vec{k}\sigma} d_{\vec{k}\sigma}) \tag{3.82}$$

$$H_{ee} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^\dagger_{\vec{k}+\vec{q}\sigma} c^\dagger_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{3.83}$$

$$H_{hh} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} d^\dagger_{\vec{k}+\vec{q}\sigma} d^\dagger_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} d_{\vec{k}\sigma} \tag{3.84}$$

$$H_{eh} = - \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^\dagger_{\vec{k}+\vec{q}\sigma} d^\dagger_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{3.85}$$

$$H_L(t) = \lambda \sum_{\vec{k}} \rho_k [(c^\dagger_{\vec{k}\uparrow} d^\dagger_{-\vec{k}\downarrow} + c^\dagger_{\vec{k}\downarrow} d^\dagger_{-\vec{k}\uparrow}) e^{-i\omega t} + h.c] \tag{3.86}$$

The Hamiltonian for the kinetic energy is given as

$$H_{kin} = \sum_{\vec{k}\sigma}(\epsilon_{c\vec{k}\sigma}c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \epsilon_{v\vec{k}\sigma}d^{\dagger}_{\vec{k}\sigma}d_{\vec{k}\sigma}) = H^{e}_{kin} + H^{h}_{kin} \tag{3.87}$$

The unitary transformation is given as

$$\tilde{H} = e^{-iS}He^{iS} = U^{\dagger}HU \tag{3.88}$$

where

$$S = -\omega_1 t\sum_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} - \omega_2 t\sum_{\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma}d_{\vec{k}\sigma} \tag{3.89}$$

We know

$$e^{itB}Ae^{-itB} = A + it[B,A] + \frac{(it)^2}{2!}[B,[B,A]] + ... \tag{3.90}$$

So we should evaluate

$$\tilde{H}_{kin} = e^{it(\omega_1 t\sum_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \omega_2 t\sum_{\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma}d_{\vec{k}\sigma})}(H^{e}_{k} + H^{h}_{k})e^{-it(\omega_1 t\sum_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \omega_2 t\sum_{\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma}d_{\vec{k}\sigma})} \tag{3.91}$$

We need to evaluate

$$[(\omega_1 t\sum_{\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \omega_2 t\sum_{\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma}d_{\vec{k}\sigma}), (\sum_{\vec{k}\sigma}\epsilon_{c\vec{k}\sigma}c^{\dagger}_{\vec{k}\sigma}c_{\vec{k}\sigma} + \sum_{\vec{k}\sigma}\epsilon_{v\vec{k}\sigma}d^{\dagger}_{\vec{k}\sigma}d_{\vec{k}\sigma})] \tag{3.92}$$

This commutator is of the form

$$[\mathcal{A}+\mathcal{B},\mathcal{C}+\mathcal{D}] = [\mathcal{A}+\mathcal{B},\mathcal{C}] + [\mathcal{A}+\mathcal{B},\mathcal{D}] = [\mathcal{A},\mathcal{C}] + [\mathcal{B},\mathcal{C}] + [\mathcal{A},\mathcal{D}] + [\mathcal{B},\mathcal{D}] \tag{3.93}$$

Out of all these four commutators, only $[\mathcal{A},\mathcal{C}]$ and $[\mathcal{B},\mathcal{D}]$ are to be calculated. $[\mathcal{A},\mathcal{D}]$, and $[\mathcal{B},\mathcal{C}]$ can be easily checked to be zero because $c^{\dagger}$, $d^{\dagger}$ refers to different particles. Now

$$[\mathcal{A},\mathcal{C}] = [\omega_1\sum_{k\sigma} c^{\dagger}_{k\sigma}c_{k\sigma}, \sum_{k'\sigma'}\epsilon_{ck'\sigma'}c^{\dagger}_{k'\sigma'}c_{k'\sigma'}] = \omega_1\sum_{k\sigma}\sum_{k'\sigma'}\epsilon_{ck',\sigma'}[c^{\dagger}_{k\sigma}c_{k\sigma}, c^{\dagger}_{k'\sigma'}c_{k'\sigma'}] \tag{3.94}$$

We know $[XY, Z] = X[Y, Z] + [X, Z]Y = X\{Y, Z\} - \{X, Z\}Y$. So

$$\begin{aligned}
[c^\dagger_{k\sigma}c_{k\sigma}, c^\dagger_{k'\sigma'}c_{k'\sigma'}] &= c^\dagger_{k\sigma}[c_{k\sigma}, c^\dagger_{k'\sigma'}c_{k'\sigma'}] + [c^\dagger_{k\sigma}, c^\dagger_{k'\sigma'}c_{k'\sigma'}]c_{k\sigma} \\
&= -c^\dagger_{k\sigma}[c^\dagger_{k'\sigma'}c_{k'\sigma'}, c_{k\sigma}] - [c^\dagger_{k'\sigma'}c_{k'\sigma'}, c^\dagger_{k\sigma}]c_{k\sigma} \\
&= -c^\dagger_{k\sigma}(c^\dagger_{k'\sigma'}\{c_{k'\sigma'}, c_{k\sigma}\} - \{c^\dagger_{k'\sigma'}, c_{k\sigma}\}c_{k'\sigma'}) \\
&- (c^\dagger_{k'\sigma'}\{c_{k'\sigma'}, c^\dagger_{k\sigma}\} - \{c^\dagger_{k'\sigma'}, c^\dagger_{k\sigma}\}c_{k'\sigma'})c_{k\sigma} \\
&= c^\dagger_{k\sigma}c_{k\sigma} - c^\dagger_{k\sigma}c_{k\sigma} \\
&= 0
\end{aligned} \tag{3.95}$$

Similarly it can be shown that

$$[d^\dagger_{k\sigma}d_{k\sigma}, d^\dagger_{k'\sigma'}d_{k'\sigma'}] = 0 \tag{3.96}$$

So $[B, A] = 0$ and also $[B, [B, A]] = 0$,... Hence

$$\tilde{H}_{kin} = H^e_{kin} + H^h_{kin} = \sum_{k\sigma}(\epsilon_{ck\sigma}c^\dagger_{ck\sigma}c_{ck\sigma} + \epsilon_{vk\sigma}d^\dagger_{vk\sigma}d_{vk\sigma}) \tag{3.97}$$

Now we transformation the electron-electron part of the Hamiltonian H_{ee}.

$$\tilde{H}_{ee} = e^{-iS}H_{ee}e^{iS} = U^\dagger H_{ee}U \tag{3.98}$$

Now we take

$$B = \omega_1\sum_{k\sigma}c^\dagger_{k\sigma}c_{k\sigma} + \omega_2\sum_{k\sigma}d^\dagger_{k\sigma}d_{k\sigma} \tag{3.99}$$

$$A = c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}c_{k',\sigma}c_{k,\sigma} \tag{3.100}$$

We need to calculate [B,A]

$$[A, B] = [c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}c_{k'\sigma}c_{k\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] \tag{3.101}$$

Since $[XY, Z] = X[Y, Z] + [X, Z]Y$, we have

$$\begin{aligned}
&[A, B] \\
&= c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}[c_{k'\sigma}c_{k\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] + [c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}, c^\dagger_{k''\sigma''}c_{k''\sigma''}]c_{k'\sigma'}c_{k\sigma} \\
&= 1^{st} + 2^{nd}
\end{aligned} \tag{3.102}$$

In the above expression the 1^{st} term is expanded as

$$\begin{aligned}
1^{st} &= c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}(c_{k'\sigma'}[c_{k\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] + [c_{k'\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}]c_{k\sigma}) \\
&= -c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}(c_{k'\sigma'}(c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c_{k''\sigma''}\} - \{c^\dagger_{k''\sigma''}, c_{k\sigma}\}c_{k''\sigma''}) \\
&+ (c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c_{k'\sigma'}\} - \{c^\dagger_{k''\sigma''}, c_{k'\sigma'}\}c_{k''\sigma''})c_{k\sigma}) \\
&= c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}c_{k'\sigma'}\delta_{k''k,\sigma''\sigma}c_{k''\sigma''} + c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}\delta_{k''k',\sigma''\sigma'}c_{k''\sigma''}c_{k\sigma} \\
&= c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}c_{k'\sigma'}c_{k\sigma} + c^\dagger_{k+q,\sigma}c^\dagger_{k'-q,\sigma'}c_{k'\sigma'}c_{k\sigma}
\end{aligned} \tag{3.103}$$

$$\begin{aligned}
2^{nd} &= (c^\dagger_{k+q,\sigma}[c^\dagger_{k'-q,\sigma'}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] + [c^\dagger_{k+q,\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}]c^\dagger_{k'-q,\sigma'})c_{k',\sigma'}c_{k,\sigma} \\
&= -(c^\dagger_{k+q,\sigma}(c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c^\dagger_{k'-q,\sigma'}\} - \{c^\dagger_{k''\sigma''}, c^\dagger_{k'-q\sigma'}\}c_{k''\sigma''}) \\
&+ (c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c^\dagger_{k+q,\sigma}\} - \{c^\dagger_{k''\sigma''}, c^\dagger_{k+q,\sigma}\}c_{k''\sigma''})c_{k',\sigma'})c_{k,\sigma} \\
&= -(c^\dagger_{k+q,\sigma}c^\dagger_{k''\sigma''}\delta_{k''k'-q;\sigma''\sigma'}c_{k',\sigma'}c_{k,\sigma} + c^\dagger_{k''\sigma''}\delta_{k''k+q;\sigma''\sigma'}c^\dagger_{k'-q,\sigma'}c_{k',\sigma'}c_{k,\sigma}) \\
&= -(c^\dagger_{k+q,\sigma}c^\dagger_{k'-q\sigma'}c_{k',\sigma'}c_{k,\sigma} + c^\dagger_{k+q,\sigma}c^\dagger_{k'-q\sigma'}c_{k',\sigma'}c_{k,\sigma})
\end{aligned} \tag{3.104}$$

We see that

$$[B, A] = -(1^{st} + 2^{nd}) = 0 \tag{3.105}$$

Hence [B,[B,A]], and all other higher order commutators are zero. Therefore,

$$\tilde{H}_{ee} = H_{ee} \tag{3.106}$$

Similarly it can be shown that

$$\tilde{H}_{hh} = H_{hh} \tag{3.107}$$

Now we transform the electron-hole ,H_{eh} part of the Hamiltonian

$$\tilde{H}_{eh} = e^{-iS}H_{eh}e^{iS} \tag{3.108}$$

As done before, we now evaluate [A,B]

$$
\begin{aligned}
[A,B] &= [c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}d_{k'\sigma'}c_{k\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] \\
&= c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}[d_{k'\sigma'}c_{k\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] \\
&+ [c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}, c^\dagger_{k''\sigma''}c_{k''\sigma''}]d_{k'\sigma'}c_{k\sigma}
\end{aligned} \tag{3.109}
$$

In the above expression the Ist term is expanded as

$$
\begin{aligned}
1^{st} &= c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}(d_{k'\sigma'}[c_{k\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}] \\
&+ [d_{k'\sigma'}, c^\dagger_{k''\sigma''}c_{k''\sigma''}]d^\dagger_{k'-q\sigma'}) \\
&= -c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}(d_{k'\sigma'}(c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c_{k'\sigma'}\} - \{c^\dagger_{k''\sigma''}, c_{k\sigma}\}c_{k''\sigma''}) \\
&+ (c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, d_{k'\sigma'}\} - \{c^\dagger_{k''\sigma''}, d_{k'\sigma'}\}c_{k''\sigma''})d_{k'-q,\sigma'}) \\
&= c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}d_{k'\sigma'}\delta_{k''k;\sigma''\sigma}c_{k''\sigma''} \\
&= c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}d_{k'\sigma'}c_{k\sigma}
\end{aligned} \tag{3.110}
$$

Similarly the 2^{nd} term can be expanded as

$$
\begin{aligned}
2^{nd} &= [c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}, c^\dagger_{k''\sigma''}, c_{k''\sigma''}]d_{k'\sigma'}c_{k\sigma}] \\
&= (c^\dagger_{k+q,\sigma}[d^\dagger_{k'-q,\sigma'}, (c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c_{k''\sigma''}\} - c^\dagger_{k''\sigma''}, c_{k''\sigma''}] \\
&+ [c^\dagger_{k+q\sigma}, c^\dagger_{k''\sigma''}c_{k''\sigma''}])d_{k'\sigma'}c_{k\sigma} \\
&= -(c^\dagger_{k+q,\sigma}(c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, d^\dagger_{k'-q,\sigma'}\} - \{c^\dagger_{k''\sigma''}, d^\dagger_{k'-q,\sigma'}\}c_{k''\sigma''}) \\
&+ (c^\dagger_{k''\sigma''}\{c_{k''\sigma''}, c^\dagger_{k+q\sigma}\} - \{c^\dagger_{k''\sigma''}, c^\dagger_{k-q\sigma}\}c_{k''\sigma''})d^\dagger_{k'-q,\sigma'})d_{k'\sigma'}c_{k\sigma} \\
&= -c^\dagger_{k+q,\sigma}c^\dagger_{k''\sigma''}\delta_{k''k+q;\sigma''\sigma}d^\dagger_{k'-q,\sigma'}d_{k'\sigma'}c_{k\sigma} \\
&= -c^\dagger_{k+q,\sigma}d^\dagger_{k'-q,\sigma'}d_{k'\sigma'}c_{k\sigma}
\end{aligned} \tag{3.111}
$$

We see that

$$[B,A] = -(1^{st} + 2^{nd}) = 0 \tag{3.112}$$

So it can be shown that [B,[B,A]] and all other higher order commutators vanish. So only the zero order term survives.

$$\tilde{H}_{eh} = H_{eh} \tag{3.113}$$

Now we transform the light term. We need to evaluate terms like [B,A].

$$\begin{aligned}
[B, A] &= [c^\dagger_{k\uparrow} c_{k\uparrow}, c^\dagger_{k'\uparrow} d^\dagger_{-k'\downarrow}] \\
&= c^\dagger_{k\uparrow}[c_{k\uparrow}, c^\dagger_{k'\uparrow} d^\dagger_{-k'\downarrow}] + [c^\dagger_{k\uparrow}, c^\dagger_{k'\uparrow} d^\dagger_{-k'\downarrow}] c_{k\uparrow} \\
&= -c^\dagger_{k\uparrow}[c^\dagger_{k'\uparrow} d^\dagger_{-k'\downarrow}, c_{k\uparrow}] + 0 \\
&= -c^\dagger_{k\uparrow}(c^\dagger_{k'\uparrow}\{d^\dagger_{-k'\downarrow}, c_{k\uparrow}\} - \{c^\dagger_{k'\uparrow}, c_{k\uparrow}\} d^\dagger_{-k'\downarrow}) \\
&= c^\dagger_{k\uparrow} d^\dagger_{-k\downarrow} \\
&= A
\end{aligned} \tag{3.114}$$

And so it can be shown that

$$[B, [B, A]] = [B, A] = \textit{all other higher order commutators} \tag{3.115}$$

Similarly it holds for the other terms. Therefore, the transformed light part of the Hamiltonian can be written to all orders as

$$\begin{aligned}
\tilde{H}_L &= H_L + \lambda \sum_k \rho_k c^\dagger_{k\uparrow} d^\dagger_{-k\downarrow} (i\omega_1 + i\omega_2) e^{-i\omega t} \\
&+ \lambda \sum_k c^\dagger_{k\uparrow} d^\dagger_{-k\downarrow} ((i\omega_1 + i\omega_2)^2/2!) e^{-i\omega t} + ... \\
&= \lambda \sum_k \rho_k c^\dagger_{k\uparrow} d^\dagger_{-k\downarrow} e^{-i\omega t} (1 + i(\omega_1 + \omega_2) + (i(\omega_1 + \omega_2))^2/2! + ...) \\
&= \lambda \sum_k \rho_k c^\dagger_{k\uparrow} d^\dagger_{-k\downarrow} e^{-i\omega t} e^{i(\omega_1 + \omega_2)t}
\end{aligned} \tag{3.116}$$

So it can be seen that if we take

$$\omega = \omega_1 + \omega_2 \tag{3.117}$$

then the above term of light interaction is independent of time. It can be shown from symmetry, all other terms in the light interaction Hamiltonian are independent of time if the above condition is satisfied. So the full light part of the transformed Hamiltonian can be written as:

$$\tilde{H}_L = \lambda \sum_k \rho_k [(c^\dagger_{k\uparrow} d^\dagger_{-k\downarrow} + c^\dagger_{k\downarrow} d^\dagger_{-k\uparrow}) + h.c] \tag{3.118}$$

So we can write the total transformed Hamiltonian as

$$\boxed{\tilde{H} = H_{kin} + H_{ee} + H_{hh} + H_{eh} + \tilde{H}_L} \tag{3.119}$$

We are interested only in the eigenenergies of the above Hamiltonian. So we do not construct the effective Hamiltonian, $\tilde{H}_{eff}$. Note that the transformation did not change any other part of the Hamiltonian except the $\tilde{H}_L$ making it time independent.

The system of electrons and holes are in a light bath. As discussed in Eq.(2.12) the free energy to be minimized is given as

$$\boxed{F = \tilde{H} - \frac{\mu}{2} \sum_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} - \frac{\mu}{2} \sum_{k\sigma} d^{\dagger}_{k\sigma} d_{k\sigma}} \tag{3.120}$$

where $\mu =$ chemical potential $= \hbar\omega$.

This is the Free energy we will use in our calculation.

Bibliography

[1] M. Wagner, *Unitary transformations in solid state physics* (Elsevier Science Publishers B.V., 1986, New York).

[2] J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, New York, 1994), p.320.

Chapter 4

Solution by Bogoliubov-Valatin transformation

In the last chapter we performed an unitary transformation on our many-particle Hamiltonian to get rid of the time and got the time-independent many-particle Hamiltonian Eq.(3.119) as,

$$\tilde{H} = H_{kin} + H_{ee} + H_{hh} + H_{eh} + \tilde{H}_L \tag{4.1}$$

and the Free energy as

$$\boxed{F = \tilde{H} - \frac{\mu}{2} \sum_{k\sigma} c^{\dagger}_{k\sigma} c_{k\sigma} - \frac{\mu}{2} \sum_{k\sigma} d^{\dagger}_{k\sigma} d_{k\sigma}} \tag{4.2}$$

where

$$H_{kin} = \sum_{\vec{k},\sigma} (\epsilon_{c\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \epsilon_{v\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma} d_{\vec{k}\sigma}) \tag{4.3}$$

$$H_{ee} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} c^{\dagger}_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{4.4}$$

$$H_{hh} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} d^{\dagger}_{\vec{k}+\vec{q}\sigma} d^{\dagger}_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} d_{\vec{k}\sigma} \tag{4.5}$$

$$H_{eh} = - \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} d^{\dagger}_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{4.6}$$

$$\tilde{H}_L = \lambda \sum_{\vec{k}} \rho_k [(c^{\dagger}_{\vec{k}\uparrow} d^{\dagger}_{-\vec{k}\downarrow} + c^{\dagger}_{\vec{k}\downarrow} d^{\dagger}_{-\vec{k}\uparrow}) + h.c] \tag{4.7}$$

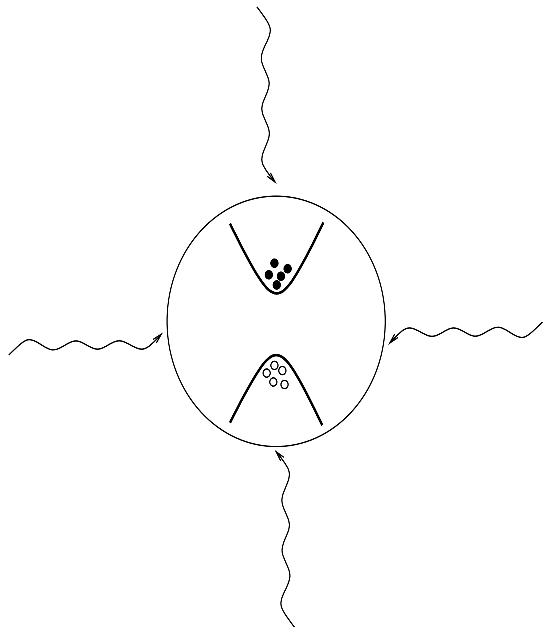

Figure 4.1: The system of electrons in the conduction band and holes in the valence band inside a light bath.

We in this chapter perform another transformation on our Hamiltonian i,e. we do Bogoliubov-Valatin (BV) transformation [3–5] on our Hamiltonian to treat the system of electrons and holes in terms of BV quasi particles, so that we can study the system in a mean field way. We need to find ground state energy and the excited state energy of the system. Bogoliubov and Valatin independently applied a quasi-particle picture to study the BCS-superconductivity and also Bogoliubov [5] studied Bose-Einstein Condensation in dilute Bose gas. We construct Bogoliubov-Valatin [3, 4] type quasi particles by constructing a canonical unitary transformation and transforming the total time-independent Hamiltonian of electrons and holes to that of quasi-particles.

4.1 Construction of the Bogoliubov-Valatin transformations

The Hamiltonian Eq.(4.1) consists of electron creation operators ($c^{\dagger}_{\vec{k}\uparrow}$,$c^{\dagger}_{\vec{k}\downarrow}$) and electron destruction operators($c_{\vec{k}\uparrow}$,$c_{\vec{k}\downarrow}$) and also consists of hole creation operators ($d^{\dagger}_{-\vec{k}\uparrow}$,$d^{\dagger}_{-\vec{k}\downarrow}$) and hole destruction operators ($d_{\vec{k}\uparrow}$,$d_{\vec{k}\downarrow}$). Let us define four new operators α,β,γ and δ in terms of the above operators *a la* Bogoliubov-Valatin.

$$\alpha_{\vec{k}} = u_{\vec{k}} c_{\vec{k}\uparrow} + v_{\vec{k}} d^{\dagger}_{-\vec{k}\downarrow} \tag{4.8}$$

$$\delta_{\vec{k}} = u_{\vec{k}} d_{\vec{k}\downarrow} - v_{\vec{k}} c^{\dagger}_{-\vec{k}\uparrow} \tag{4.9}$$

$$\beta_{\vec{k}} = \bar{u}_{\vec{k}} d_{\vec{k}\uparrow} - \bar{v}_{\vec{k}} c^{\dagger}_{-\vec{k}\downarrow} \tag{4.10}$$

$$\gamma_{\vec{k}} = \bar{u}_{\vec{k}} c_{\vec{k}\downarrow} + \bar{v}_{\vec{k}} d^{\dagger}_{-\vec{k}\uparrow} \tag{4.11}$$

Here the annihilation operator for a BV quasi particle $\alpha_{\vec{k}}$ is a linear combination of an annihilation operator for an electron with momentum $\vec{k}$ and spin up ($c_{\vec{k}\uparrow}$) in the conduction band with probability amplitude u_k and an creation operator for a hole ($d^{\dagger}_{-\vec{k}\downarrow}$) within the valence band with opposite momentum and spin with probability amplitude $v_{\vec{k}}$. Similarly one can interpret other three Bogoliubov operators. These are the new operators satisfying fermionic commutation relations provided the normalization conditions are satisfied. The normalization conditions are:

$$u^2_{\vec{k}} + v^2_{\vec{k}} = 1 \tag{4.12}$$

$$\bar{u}^2_{\vec{k}} + \bar{v}^2_{\vec{k}} = 1 \tag{4.13}$$

Here $u_{\vec{k}}(\bar{u}_{\vec{k}})$ and $v_{\vec{k}}(\bar{v}_{\vec{k}})$ are real.

The fermionic canonical commutation relations are given as

$$\delta_{\vec{k},\vec{k}'} = \{\alpha_{\vec{k}}, \alpha^{\dagger}_{\vec{k}}\} = \{\delta_{\vec{k}}, \delta^{\dagger}_{\vec{k}}\} = \{\beta_{\vec{k}}, \beta^{\dagger}_{\vec{k}}\} = \{\gamma_{\vec{k}}, \gamma^{\dagger}_{\vec{k}}\} \tag{4.14}$$

And also

$$0 = \{\alpha_{\vec{k}}, \alpha_{\vec{k}'}\} = \{\delta_{\vec{k}}, \delta_{\vec{k}'}\} = \{\beta_{\vec{k}}, \beta_{\vec{k}'}\} = \{\gamma_{\vec{k}}, \gamma_{\vec{k}'}\} \tag{4.15}$$

and special attention should be given to the following two commutators

$$0 = \{\alpha_{\vec{k}}, \delta_{\vec{k}'}\} = \{\beta_{\vec{k}}, \gamma_{\vec{k}'}\} \tag{4.16}$$

This is true since $u_{\vec{k}} = u_{-\vec{k}}$ and $v_{\vec{k}} = v_{-\vec{k}}$. Any other commutator is trivially zero. The operators defined in Eq.(4.8-4.11) are considered to destroy an excited state of the system(which consists of a correlated electron-hole pair). The hermitian conjugates of the corresponding operators create an excited state of the aforementioned system.

By inverting the Eqs.(4.8-4.11),we arrive at relations of electrons and holes in terms of the quasi particle operators. The new realtions are given as:

$$c_{\vec{k}\uparrow} = u_{\vec{k}}\alpha_{\vec{k}} - v_{\vec{k}}\delta^{\dagger}_{-\vec{k}} \tag{4.17}$$

$$c_{\vec{k}\downarrow} = \bar{u}_{\vec{k}}\gamma_{\vec{k}} - \bar{v}_{\vec{k}}\beta^{\dagger}_{-\vec{k}} \tag{4.18}$$

$$d_{\vec{k}\uparrow} = \bar{u}_{\vec{k}}\beta_{\vec{k}} + \bar{v}_{\vec{k}}\gamma^{\dagger}_{-\vec{k}} \tag{4.19}$$

$$d_{\vec{k}\downarrow} = u_{\vec{k}}\delta_{\vec{k}} + v_{\vec{k}}\alpha^{\dagger}_{-\vec{k}} \tag{4.20}$$

4.2 Transformed Free energy

Using Eq.(4.17-4.20) in Eq.(4.2), neglecting the products of four operators, we obtain, after a tedious algebra (the details are given in the Appendix A) the transformed Free energy as:

$$\begin{aligned} F_T = &\sum_k (\xi^+_{\vec{k}} v^2_{\vec{k}} + \xi^-_{\vec{k}} \bar{v}^2_{\vec{k}}) \\ -\sum_{k,k'}\{&V_{\vec{k}-\vec{k}'}(u_{\vec{k}}v_{\vec{k}}u_{\vec{k}'}v_{\vec{k}'} + \bar{u}_{\vec{k}}\bar{v}_{\vec{k}}\bar{u}_{\vec{k}'}\bar{v}_{\vec{k}'}) \\ &+V_{\vec{k}-\vec{k}'}(v^2_{\vec{k}}v^2_{\vec{k}'} + \bar{v}^2_{\vec{k}}\bar{v}^2_{\vec{k}'})\} \\ &-2\sum_k \lambda_k\rho_k(u_{\vec{k}}v_{\vec{k}} + \bar{u}_{\vec{k}}\bar{v}_{\vec{k}}) \end{aligned}$$

$$
\begin{aligned}
+\sum_{\vec{k}}[\{\epsilon_{c\vec{k}\omega} + J_e < M > +A_k\}\alpha_k^\dagger\alpha_k \\
+\{\epsilon_{v\vec{k}\omega} - J_h < M > +A_k\}\delta_k^\dagger\delta_k \\
+\{\epsilon_{c\vec{k}\omega} - J_e < M > +\bar{A}_k\}\gamma_k^\dagger\gamma_k \\
+\{\epsilon_{v\vec{k}\omega} + J_h < M > +\bar{A}_k\}\beta_k^\dagger\beta_k \\
+B_k(\alpha_{\vec{k}}^\dagger\delta_{-\vec{k}}^\dagger + \delta_{-\vec{k}}\alpha_{\vec{k}}) \\
+\bar{B}_k(\gamma_{\vec{k}}^\dagger\beta_{-\vec{k}}^\dagger + \beta_{-\vec{k}}\gamma_{\vec{k}}) \\
+O(\alpha_k^\dagger\beta_k^\dagger\gamma_k^\dagger\delta_k^\dagger + ...)] \\
= F_0 + H_2 + H_4
\end{aligned}
\tag{4.21}
$$

Note that the transformed Free energy is of the form

$$
F_T = F_0 + \sum_k a^\eta \eta_k^\dagger \eta_k + b^\eta \eta_k^\dagger \eta_k^{'\dagger} + c^\eta \eta_k \eta_k' + O(\eta^4) \tag{4.22}
$$

where $\eta = \alpha, \beta, \gamma, \delta$ and H_4 contains many terms; each one is a product of four Bogoliubov operators such that the destruction operators are on the right-hand side (Appendix A). H_2 describes the sum of the terms containing two operators and F_0 is the constant terms involving $u_{\vec{k}}$ and $v_{\vec{k}}$.

In the transformed Free energy F_T we have

$$
A_k = \{\frac{1}{2}\Omega_{\vec{k}} - (\xi_{\vec{k}+} + \Omega_{\vec{k}})v_{\vec{k}}^2 + \Delta_{\vec{k}}u_{\vec{k}}v_{\vec{k}}\} \tag{4.23}
$$

$$
B_k = \{\frac{1}{2}\Delta_{\vec{k}}(u_{\vec{k}}^2 - v_{\vec{k}}^2) - u_{\vec{k}}v_{\vec{k}}(\xi_{\vec{k}}^+ + \Omega_{\vec{k}})\} \tag{4.24}
$$

and similarly for $\bar{A}_k$ and $\bar{B}_k$ we have expressions where all unbarred quantities are replaced by barred quantities and $\xi_{\vec{k}}^+$ by $\xi_{\vec{k}}^-$. The symbols used here are as follows

$$
\xi_{\vec{k}}^\pm = \xi_{\vec{k}}^0 \pm J < M > \tag{4.25}
$$

$$
J = J_e - J_h \tag{4.26}
$$

$$\xi^0_{\vec{k}} = E_g + \frac{\hbar^2 k^2}{2m^*} - \hbar\omega \tag{4.27}$$

$$m^{*-1} = m_e^{-1} + m_h^{-1} \tag{4.28}$$

$$\epsilon_{ck\omega} = E_g + E_c - \frac{\hbar\omega}{2} \tag{4.29}$$

$$\epsilon_{vk\omega} = E_v - \frac{\hbar\omega}{2} \tag{4.30}$$

$$\Delta_{\vec{k}} = \Delta^0_{\vec{k}} + 2\lambda\rho_{\vec{k}} \tag{4.31}$$

$$\Delta^0_{\vec{k}} = 2\sum_{\vec{k}'} V_{\vec{k}-\vec{k}'} u_{\vec{k}'} v_{\vec{k}'} \tag{4.32}$$

$$\bar{\Delta}_{\vec{k}} = \bar{\Delta}^0_{\vec{k}} + 2\lambda\rho_{\vec{k}} \tag{4.33}$$

$$\bar{\Delta}^0_{\vec{k}} = 2\sum_{\vec{k}'} V_{\vec{k}-\vec{k}'} \bar{u}_{\vec{k}'} \bar{v}_{\vec{k}'} \tag{4.34}$$

$$\Omega_{\vec{k}} = -2\sum_{\vec{k}'} V_{\vec{k}-\vec{k}'} v^2_{\vec{k}'} \tag{4.35}$$

$$\bar{\Omega}_{\vec{k}} = -2\sum_{\vec{k}'} V_{\vec{k}-\vec{k}'} \bar{v}^2_{\vec{k}'} \tag{4.36}$$

4.3 The Free energy F_0

Since we are interested in the ground state energy of the system, after neglecting H_4 which is small [3, 6], we take the condition that the off diagonal terms in H_2 vanish so that our Free energy is diagonalized. So we have

$$B_k \equiv \frac{1}{2}\Delta_{\vec{k}}(u^2_{\vec{k}} - v^2_{\vec{k}}) - u_{\vec{k}} v_{\vec{k}}(\xi^+_{\vec{k}} + \Omega_{\vec{k}}) = 0 \tag{4.37}$$

$$\bar{B}_k \equiv \frac{1}{2}\bar{\Delta}_{\vec{k}}(\bar{u}^2_{\vec{k}} - \bar{v}^2_{\vec{k}}) - \bar{u}_{\vec{k}} \bar{v}_{\vec{k}}(\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}}) = 0 \tag{4.38}$$

The first of the above two equations with the help of the normalization condition,

$$u^2_k + v^2_k = 1 \tag{4.39}$$

leads to

$$u^2_{\vec{k}} = \frac{1}{2}[1 + \frac{\xi^+_{\vec{k}} + \Omega_{\vec{k}}}{\sqrt{\Delta^2_{\vec{k}} + (\xi^+_{\vec{k}} + \Omega_{\vec{k}})^2}}] \tag{4.40}$$

and

$$v^2_{\vec{k}} = \frac{1}{2}[1 - \frac{\xi^+_{\vec{k}} + \Omega_{\vec{k}}}{\sqrt{\Delta^2_{\vec{k}} + (\xi^+_{\vec{k}} + \Omega_{\vec{k}})^2}}] \tag{4.41}$$

Similarly one can find expressions for $\bar{u}^2_k$ and $\bar{v}^2_k$. The Eq.(4.38) with the unitary condition

$$\bar{u}^2_k + \bar{v}^2_k = 1 \tag{4.42}$$

leads to

$$\bar{u}^2_{\vec{k}} = \frac{1}{2}[1 + \frac{\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}}}{\sqrt{\bar{\Delta}^2_{\vec{k}} + (\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}})^2}}] \tag{4.43}$$

and

$$\bar{v}^2_{\vec{k}} = \frac{1}{2}[1 - \frac{\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}}}{\sqrt{\bar{\Delta}^2_{\vec{k}} + (\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}})^2}}] \tag{4.44}$$

We see from Eq.(4.31,4.33,4.35, 4.36), that when $V_{k-k'} = 0, \lambda = 0$, then $\Delta_k,\ \bar{\Delta}_k$, Ω_k *and* $\bar{\Omega}_k$ are zero for all k. So Eq.(4.41) for v^2_k simplifies as,

$$v^2_k = \frac{1}{2}[1 - \frac{\xi_k}{|\xi_k|}] \tag{4.45}$$

So

$$\begin{aligned} \xi_k > 0 &: v_k = 0 \\ \xi_k < 0 &: v_k = 1 \end{aligned} \tag{4.46}$$

So v^2_k behaves as a theta function,$\theta(\xi_k)$ or $\theta(\xi'_k - \hbar\omega)$, since

$$\xi_k = E_g + \frac{\hbar^2 k^2}{2m^*} + J < M > -\hbar\omega \tag{4.47}$$

Similarly one can show that $\bar{v}^2_k$ also behaves as a theta function under similar conditions.

The Free energy can be obtained from Eq.(4.21) and is $< F_0 >$, the constant terms. In terms of the sysmbols defined we can write the Free energy as

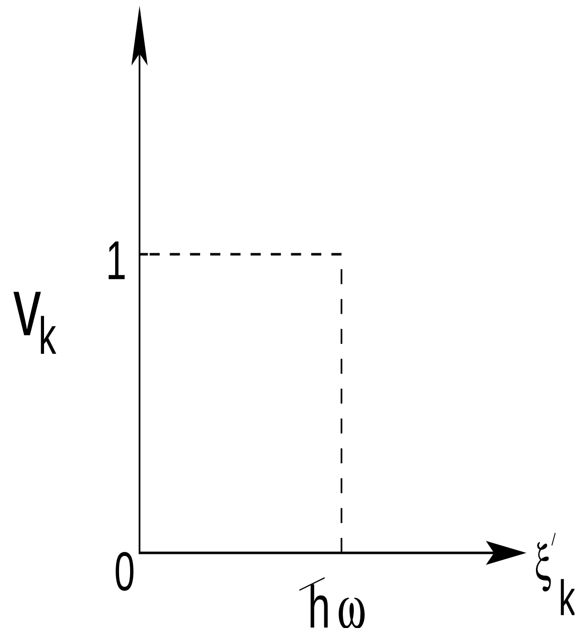

Figure 4.2: The probability amplitude of creation of an electron-hole pair as a step function at zero temperature given by Eq.(4.46).

$$\begin{aligned} F_0(<M>) \quad &= \sum_{\vec{k}}[(\xi^+_{\vec{k}} + \Omega_{\vec{k}}/2)v^2_{\vec{k}} + (\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}}/2)\bar{v}^2_{\vec{k}} \\ &-\Delta_{\vec{k}}u_{\vec{k}}v_{\vec{k}} - \bar{\Delta}_{\vec{k}}\bar{u}_{\vec{k}}\bar{v}_{\vec{k}} \\ &+\frac{\Delta^0_{\vec{k}}}{2}u_{\vec{k}}v_{\vec{k}} + \frac{\bar{\Delta}^0_{\vec{k}}}{2}\bar{u}_{\vec{k}}\bar{v}_{\vec{k}}] \end{aligned} \tag{4.48}$$

where $u_{\vec{k}}$ and $v_{\vec{k}}$ are given by Eq.(4.40-4.41) and $\bar{u}_{\vec{k}}$ and $\bar{v}_{\vec{k}}$ are given by Eq.(4.43-4.44). The remaining symbols are defined previously.

4.4 Contact interaction

4.4.1 Case(i): $\rho(k) = 1$

We assume a contact-type of interaction for the Coulomb terms such that Δ's and Ω's are independent of $\vec{k}$. The amplitude ρ_k is assumed to be independent of $\vec{k}$ and is taken as $\rho_0 = 1$ and $\lambda = \lambda_0$. Within the above approximations, we obtain two sets of equations from Eq.(4.31) and Eq.(4.35) respectively as

$$\frac{\Delta - 2\lambda_0}{2U_0} = \sum_k u_k v_k \tag{4.49}$$

and

$$\frac{-\Omega}{2U_0} = \sum_k v_k^2 \tag{4.50}$$

where U_0 is the strength of Dirac delta function replacing the Coulomb interaction between electrons, holes and electron-electron and hole-hole interactions. The strength U_0 is estimated in section 6.2 of chapter 6 Similarly we have another two equations for $\bar{u}_k$ *and* $\bar{v}_k$. The ground state energy $F_0(M)$ can be written as

$$\begin{aligned} F_0(< M >) = {} & (E_g - \hbar\omega + \Omega/2 + J < M >)\frac{-\Omega}{2U_0} \\ & (E_g - \hbar\omega + \bar{\Omega}/2 - J < M >)\frac{-\bar{\Omega}}{2U_0} \\ & -\frac{1}{4U_0}(\Delta^2 - 4\lambda_0^2) - \frac{1}{4U_0}(\bar{\Delta}^2 - 4\lambda_0^2) \\ & + \frac{\hbar^2}{2m^*}\sum_{\vec{k}} k^2(v_k^2 + \bar{v}_k^2) \end{aligned} \tag{4.51}$$

4.4.2 Analytical expression for F_0 when $U_0 = 0, \lambda_0 = 0$

When $U_0 = 0, \lambda_0 = 0$, the two-particle energies ξ_1 *and* ξ_2 given in chapter 2 are

$$\begin{aligned} \xi_1 &= E_g + \frac{\hbar^2 k^2}{2m^*} + J < M > \\ \xi_2 &= E_g + \frac{\hbar^2 k^2}{2m^*} - J < M > \end{aligned} \tag{4.52}$$

We find that using Eq.(3.33) of chapter 3 that the new two particle energies remain unchanged if $\lambda_0 = 0$.

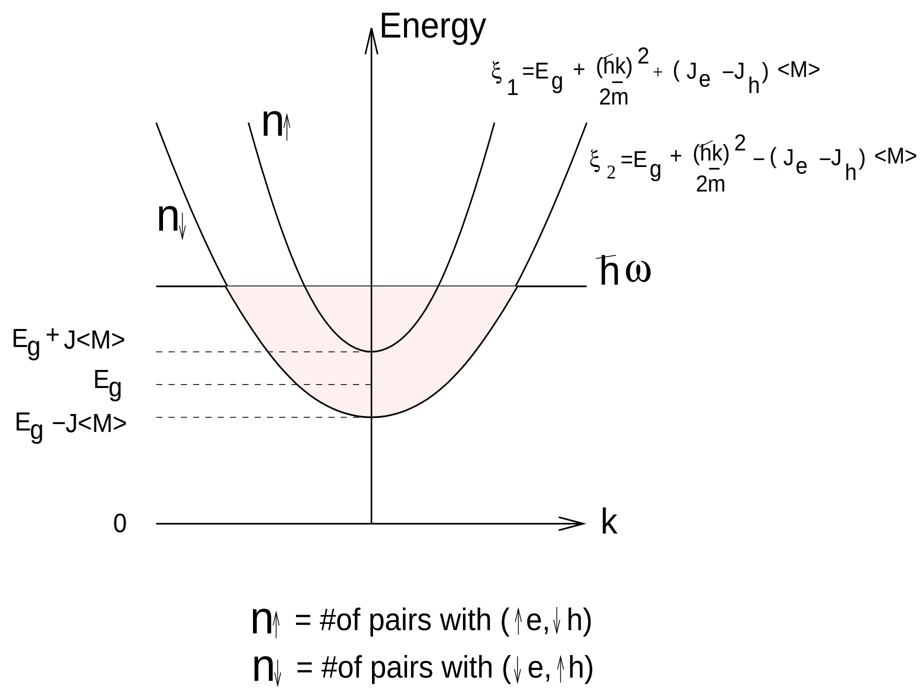

Figure 4.3: The two-particle energy band when light coupling $\lambda_0 = 0$ given by Eq.(4.52). Energy ξ_1 corresponds to $n \uparrow$ which refers to number of pairs with electron with up spin and hole with down spin and energy ξ_2 corresponds to $n \downarrow$ which refers to number of pairs with electron with down spin and hole with up spin. E_g refers to the highest position of the band gap. $E_g + J < M >$ and $E_g - J < M >$ refers to the highest positions of up and down two particle band split by the magnetic interaction energy $J < M >$.

For ξ_1, the minimum and maximum are given as,

$$\xi_1^{min} = E_g + J < M >$$

$$\xi_1^{max} = \hbar\omega = \xi_1^{min} + \frac{\hbar^2 k_{max1}^2}{2m^*}$$

$$\hbar\omega = E_g + J < M > + \frac{\hbar^2 k_{max1}^2}{2m^*}$$

$$k_{max1} = \sqrt{(\frac{2m^*}{\hbar^2}(\hbar\omega - E_g - J < M >))} \tag{4.53}$$

Similarly we can get for ξ_2

$$\begin{aligned} \xi_2^{min} &= E_g - J < M > \\ \xi_2^{max} = \hbar\omega &= \xi_2^{min} + \frac{\hbar^2 k_{max2}^2}{2m^*} \\ \hbar\omega &= E_g - J < M > + \frac{\hbar^2 k_{max2}^2}{2m^*} \\ k_{max2} &= \sqrt{(\frac{2m^*}{\hbar^2}(\hbar\omega - E_g + J < M >))} \end{aligned} \tag{4.54}$$

Refering to the Fig.4.3, we calculate the free energy for this two-particle energy system as

$$\begin{aligned} F_0 &= \frac{1}{2\pi^2}[\int_0^{kmax1} \xi_k^1 k^2 dk + \int_0^{kmax2} \xi_k^2 k^2 dk] - \hbar\omega(\int_0^{kmax1} k^2 dk + \int_0^{kmax2} k^2 dk)] \\ &= \frac{1}{2\pi^2}[\int_0^{kmax1} (\xi_{min}^1 + \frac{\hbar^2 k^2}{2m^*})k^2 dk + \int_0^{kmax2} (\xi_{min}^2 + \frac{\hbar^2 k^2}{2m^*})k^2 dk \\ &- \hbar\omega(\int_0^{kmax1} k^2 dk + \int_0^{kmax2} k^2 dk)] \\ &= (\frac{2m^*}{\hbar^2})^{3/2} \frac{1}{2\pi^2}((((\mu' - J < M >)^{5/2} + (\mu' + J < M >)^{5/2})/5 \\ &+ ((\hbar\omega - \mu' + J < M >)(\mu' - J < M >)^{3/2} \\ &+ (\hbar\omega - \mu' - J < M >)(\mu' + J < M >)^{3/2})/3 \\ &- \hbar\omega((\mu' - J < M >)^{3/2} + (\mu' + J < M >)^{3/2})/3) \end{aligned} \tag{4.55}$$

where $\mu' = \hbar\omega - E_g$ and $2m^*/\hbar^2 = \frac{2m_e}{\hbar^2} \times \tilde{m} = 0.1/3.81\ eV.A^2$.

4.4.3 Case(ii): $\rho(k) = \frac{1}{(1+(a_{ex}k)^2)^2}$

We also calculate energy taking $\rho(k) = \frac{1}{(1+(a_{ex}k)^2)^2}$ and a contact interaction. We take the above k-dependent $\rho(k)$ due to the fact that this is the Fourier transform [7] of the 1s hydrogen wave function which describes an exciton of electron and hole of our system. For $GaAs$ $a_{ex} \approx 100a_B,\ a_B = 0.529$ Å. Eqs.(4.49) and (4.50) are solved numerically by using Eq.(4.40) and (4.41). Numerical Results will be discussed in Chapter.6.

We in the next chapter calculate the energy of the system using another well known technique that is by constructing an appropriate many-body BCS type wavefunction for our system.

We here summarize the equations that we use to evaluate numerically the free energy F_0.

$$F_0(< M >) = \sum_{\vec{k}}[(\xi^+_{\vec{k}} + \Omega_{\vec{k}}/2)v^2_{\vec{k}} - \Delta_{\vec{k}}u_{\vec{k}}v_{\vec{k}} + \frac{\Delta^0_{\vec{k}}}{2}u_{\vec{k}}v_{\vec{k}}] + \sum_{\vec{k}}[(\xi^-_{\vec{k}} + \bar{\Omega}_{\vec{k}}/2)\bar{v}^2_{\vec{k}} - \bar{\Delta}_{\vec{k}}\bar{u}_{\vec{k}}\bar{v}_{\vec{k}} + \frac{\bar{\Delta}^0_{\vec{k}}}{2}\bar{u}_{\vec{k}}\bar{v}_{\vec{k}}] \tag{4.56}$$

where

$$\xi^{\pm}_k = \frac{\hbar^2 k^2}{2m^*} + E_g - \hbar\omega \pm J < M > \tag{4.57}$$

$$\Omega_k = -2\sum_{k'} V_{k-k'}v^2_{k'} \tag{4.58}$$

$$\Delta_k = \Delta^0_k + 2\lambda\rho_k \tag{4.59}$$

$$\Delta^0_k = 2\sum_{k'} V_{k-k'}u_{k'}v_{k'} \tag{4.60}$$

$$u^2_{\vec{k}} = \frac{1}{2}[1 + \frac{\xi^+_{\vec{k}} + \Omega_{\vec{k}}}{\sqrt{\Delta^2_{\vec{k}} + (\xi^+_{\vec{k}} + \Omega^2_{\vec{k}})}}] \tag{4.61}$$

$$v^2_{\vec{k}} = \frac{1}{2}[1 - \frac{\xi^+_{\vec{k}} + \Omega_{\vec{k}}}{\sqrt{\Delta^2_{\vec{k}} + (\xi^+_{\vec{k}} + \Omega^2_{\vec{k}})}}] \tag{4.62}$$

We use u *and* v in equations for Δ, *and* Ω and guess some value for Δ, *and* Ω and solve these two equations self-consistently till it converges and thereby determine Δ, Ω, u, *and* v for each k. We have also a similar set of equations for the barred quantities, where ξ^+, Δ, Ω, u *and* v are replaced by ξ^-, $\bar{\Delta}$, $\bar{\Omega}$, $\bar{u}$, $\bar{v}$. As above we solve them self-consistently to get $\bar{\Delta}$, $\bar{\Omega}$, $\bar{u}$, *and* $\bar{v}$. We use these values to calculate F_0.

Bibliography

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. B.**108**,1175 (1957).

[2] J. R. Schrieffer, *Theory of Superconductivity*, (Perseus Books, Massachusetts, 1983) p.40.

[3] N. N. Bogoliubov, V. V. Tolmachov, and D. V. Sirkov, Fortschritte der Physik, **6**, 605 (1958). [*The theory of Superconductivity*, Ed. N. N. Bogoliubov, The international science review series, Vol. IV, (Gordon and Breach, New York) 1962].

[4] J. G. Valatin, Il Nuovo Cimento, **VII**, 843, (1958).

[5] N. N. Bogoliubov, J. Phys. USSR, **9**, 23,(1947).

[6] L. V. Kjeldysh and A. N. Kozlov, Zh. Eksp. Teor. Fiz. **54**, 978 (1968)[Sov. Phys.-JETP **27**, 521 (1968)].

[7] F. Bassani and G. P. Parravicini, *Electronic states and optical transitions in solids*, (Pergamon, New York, 1975),p.188.

Chapter 5

The BCS wave function

In this chapter we study the problem of photo-induced ferro-magnetism in Dilute Magnetic Semiconductors using the famous BCS [1] wave function approach. We construct a many-body wave function for the problem and calculate the ground state energy using the variational technique. We find that this method exactly reproduces the ground state energy calculated using the Bogoliubov-Valatin approach [2–4] as done in the last chapter. But in the BCS approach we miss the excitations that we get directly in the Bogoliubov-Valatin approach.

5.1 Construction of the BCS wave function and calculation of ground state energy

We construct the wave function as

$$\boxed{|\Psi >= \prod_{k,\sigma}(u_{k\sigma} + v_{k\sigma} c^{\dagger}_{k\sigma} d^{\dagger}_{-k-\sigma})|0 >} \tag{5.1}$$

where $|\Psi >$ is the ground state of electron and hole pair and $|0 >$ is the vaccum state for the electron and hole. The amplitudes are defined as:

$$u_{k\downarrow} \equiv u_k \tag{5.2}$$

$$v_{k\downarrow} \equiv v_k$$

$$u_{k\uparrow} \equiv \bar{u}_k$$
$$v_{k\uparrow} \equiv \bar{v}_k$$

The wavefunction $|\Psi>$ can be written more explicitly as

$$|\Psi>=\prod_{k,k'}(\bar{u}_{k'}+\bar{v}_{k'}c^\dagger_{k'\uparrow}d^\dagger_{-k'\downarrow})(u_k+v_kc^\dagger_{k\downarrow}d^\dagger_{-k\uparrow})|0> \tag{5.3}$$

We now show below that the above wave function is normalized.

Let $A^\dagger_k = u_k + v_kc^\dagger_{k\downarrow}d^\dagger_{-k\uparrow}$ and $B^\dagger_{k'} = \bar{u}_{k'} + \bar{v}_{k'}c^\dagger_{k'\uparrow}d^\dagger_{-k'\downarrow}$ then

$$\begin{aligned}
<\Psi|\Psi> &=< 0|(\prod_{k'',k'''} A_{k'''}B_{k''})(\prod_{k,k'} B^\dagger_{k'}A^\dagger_k)|0> \\
&=< 0|(\prod_{k',k''} B_{k''}B^\dagger_{k'})(\prod_{k,k'''} A_{k'''}A^\dagger_k)|0> \\
&=< 0|(\prod_{k'',k'''} B_{k'''}B^\dagger_{k''})(\prod_{k,k'} A_{k'}A^\dagger_k)|0> \\
&=< 0|(\prod_{k'',k'''} B_{k'''}B^\dagger_{k''})((\prod_{k'\neq k} A_{k'}A^\dagger_{k'})A_kA^\dagger_k)|0> \\
&=< 0|(\prod_{k'',k'''} B_{k'''}B^\dagger_{k''})(\prod_{k'\neq k} A_{k'}A^\dagger_{k'})[u_k^2+v_k^2d_{-k\uparrow}c_{k\downarrow}c^\dagger_{k\downarrow}d^\dagger_{-k\uparrow} \\
&\quad +u_kv_kc^\dagger_{k\downarrow}d^\dagger_{-k\uparrow}+u_kv_kd_{-k\uparrow}c_{k\downarrow}]|0> \\
&=< 0|(\prod_{k'',k'''} B_{k'''}B^\dagger_{k''})(\prod_{k'\neq k} A_{k'}A^\dagger_{k'})[u_k^2+v_k^2]|0> \\
&= (u_k^2+v_k^2) < 0|(\prod_{k'',k'''} B_{k'''}B^\dagger_{k''})(\prod_{k'\neq k} A_{k'}A^\dagger_{k'})|0>
\end{aligned} \tag{5.4}$$

By repeating the same calculation for other terms of the product and taking into account that $u_k^2 + v_k^2 = 1$ and $\bar{u}_k^2 + \bar{v}_k^2 = 1$, one verifies that $|\Psi>$ is normalized to 1. One can easily see that the BCS state $|\Psi>$ plays the role of vacuum for the $\alpha_k,\ \beta_k,\ \gamma_k,\ \delta_k$, defined in chapter 4 by Eq.(4.8,4.9,4.10,4.11), that is

$$\alpha_k|\Psi>=\beta_k|\Psi>=\gamma_k|\Psi>=\delta_k|\Psi>=0 \tag{5.5}$$

Let us check it for α_k.

$$\alpha_k|\Psi> \;=\; (u_kc_{k\uparrow}+v_kd^\dagger_{-k\downarrow})\prod_{k',k''}(u_{k''}+v_{k''}c^\dagger_{k''\uparrow}d^\dagger_{-k''\downarrow})(\bar{u}_{k'}+\bar{v}_{k'}c^\dagger_{k'\downarrow}d^\dagger_{-k'\uparrow})|0>$$

$$
\begin{aligned}
&= [\prod_{k',k''}(\bar{u}_{k'} + \bar{v}_{k'}c^{\dagger}_{k'\downarrow}d^{\dagger}_{-k'\uparrow})](u_k c_{k\uparrow} + v_k d^{\dagger}_{-k\downarrow})(u_{k''} + v_{k''}c^{\dagger}_{k''\uparrow}d^{\dagger}_{-k''\downarrow})|0> \\
&= [\prod_{k',k''\neq k}(\bar{u}_{k'} + \bar{v}_{k'}c^{\dagger}_{k'\downarrow}d^{\dagger}_{-k'\uparrow})(u_{k''} + v_{k''}c^{\dagger}_{k''\uparrow}d^{\dagger}_{-k''\downarrow}] \\
&\quad (u_k c_{k\uparrow} + v_k d^{\dagger}_{-k\downarrow})(u_k - v_k c^{\dagger}_{k\uparrow}d^{\dagger}_{-k\downarrow})|0> \\
&= 0 \qquad (5.6)
\end{aligned}
$$

where we have taken $v_{k''} = -v_k$ for $k^{''} = k$ without loss of generality. We have the total Hamiltonian given by Eq.(4.1) as

$$
\tilde{H} = H_{kin} + H_{ee} + H_{hh} + H_{eh} + \tilde{H}_L \qquad (5.7)
$$

where the each individual part of the Hamiltonian is discussed in beginning of the previous chapter. Now we calculate the expectation value of the above Hamiltonian with our constructed wave function, that is we calculate

$$
< \Psi|\tilde{H}|\Psi > \qquad (5.8)
$$

We calculate the expectation value term by term explicitly. First we work with kinetic part of the Hamiltonian of electrons with spin up. We use the values of commutations evaluated in Apppendix B.

$$
\begin{aligned}
< \Psi|H^T_{ke1}|\Psi > &= < \Psi|\sum_k \epsilon_{ck\uparrow}c^{\dagger}_{k\uparrow}c_{k\uparrow}|\Psi > \\
&= \sum_k \epsilon_{ck\uparrow}v^2_k \qquad (5.9)
\end{aligned}
$$

Similarly we will get

$$
\begin{aligned}
< \Psi|H^T_{ke2}|\Psi > &= < \Psi|\sum_k \epsilon_{ck\downarrow}c^{\dagger}_{k\downarrow}c_{k\downarrow}]|\Psi > \\
&= \sum_k \epsilon_{ck\downarrow}\bar{v}^2_k \qquad (5.10)
\end{aligned}
$$

$$
\begin{aligned}
< \Psi|H^T_{ke3}|\Psi > &= < \Psi|\epsilon_{vk\uparrow}\sum_k d^{\dagger}_{k\uparrow}d_{k\uparrow}|\Psi > \\
&= \sum_k \epsilon_{vk\uparrow}\bar{v}^2_k \qquad (5.11)
\end{aligned}
$$

$$< \Psi|H_{ke4}^T|\Psi > \ = \ < \Psi|\sum_k \epsilon_{vk\downarrow} d_{k\downarrow}^\dagger d_{k\downarrow}|\Psi >$$
$$= \ \sum_k \epsilon_{vk\downarrow} v_k^2 \qquad (5.12)$$

We want to calculate the energy with the light part of the Hamiltonian

$$< \Psi|H_L^T|\Psi > \ = \ < \Psi|\lambda \sum_k \rho_k c_{k\uparrow}^\dagger d_{-k\downarrow}^\dagger|\Psi >$$
$$= \ -\lambda \sum_k \rho_k u_k v_k \qquad (5.13)$$

Similarly the other term is $-\lambda \sum_k \rho_k \bar{u}_k \bar{v}_k$. So the total light term gives

$$E_L = -2\lambda \sum_k \rho_k (u_k v_k + \bar{u}_k \bar{v}_k) \qquad (5.14)$$

The factor 2 is due to the fact each of the above light term has a complex conjugate term. Now we want to find the expectation value of H_{eh}^T.

$$H_{eh}^T \ = \ - \sum_{kk'q,\sigma\sigma',\sigma\neq\sigma'} V_q c_{k+q,\sigma}^\dagger d_{k'-q,\sigma'}^\dagger d_{k',\sigma'} c_{k,\sigma} \qquad (5.15)$$
$$= \ - \sum_{kk'q} V_q \{ c_{k+q,\uparrow}^\dagger d_{k'-q,\downarrow}^\dagger d_{k',\downarrow} c_{k,\uparrow} + c_{k+q,\downarrow}^\dagger d_{k'-q,\uparrow}^\dagger d_{k',\uparrow} c_{k,\downarrow} \}$$

Now using the normal ordering technique of the Wick theorem, we have

$$< \Psi| \sum_{k,k',q} V_q c_{k+q,\uparrow}^\dagger d_{k'-q,\downarrow}^\dagger d_{k',\downarrow} c_{k,\uparrow} |\Psi >$$
$$= \ \sum_{k,k'} V_q (< c_{k+q,\uparrow}^\dagger d_{k'-q,\downarrow}^\dagger >< d_{k',\downarrow} c_{k,\uparrow} >$$
$$+ \ < c_{k+q,\uparrow}^\dagger c_{k,\uparrow} >< d_{k'-q,\downarrow}^\dagger d_{k',\downarrow} > - < c_{k+q,\uparrow}^\dagger d_{k',\downarrow} >< d_{k'-q,\downarrow}^\dagger c_{k,\uparrow} >)$$
$$= \ \sum_{k,k',q} V_q (-v_{k+q} u_{k'-q} \delta_{-k-q,k'-q})(-u_{k'} v_k \delta_{k',-k}) + V_{q=0}\ term - 0$$
$$= \ \sum_{k,q} V_q (v_{k+q} u_{-k-q} \delta_{-k-q,-k-q})(u_{-k} v_k)$$

$$
\begin{aligned}
&= \sum_{k,k'} V_{k'-k}(v_{k'}u_{-k'}\delta_{-k',-k'})(u_{-k}v_k) \\
&= \sum_{k,k'} V_{k'-k}(v_{k'}u_{-k'})(u_{-k}v_k) \\
&= \sum_{k,k'} V_{k'-k}(u_{k'}v_{k'}u_k v_k)
\end{aligned} \tag{5.16}
$$

In the above expression second term gives $q = 0$ term which is not included, and third term gives terms identically equal to zero.

Similarly the other term gives

$$
< \Psi|\sum_{k,k'} V_{k'-k} c^{\dagger}_{k+q,\downarrow} d^{\dagger}_{k'-q,\uparrow} d_{k',\uparrow} c_{k,\downarrow}|\Psi >= \sum_{k,k'} V(k'-k)\bar{u}_{k'}\bar{v}_{k'}\bar{u}_k\bar{v}_k \tag{5.17}
$$

So the total energy from the electron-hole part of the Hamiltonian is

$$
E^{eh} = -\sum_{k,k'} V_{k-k'}(u_{k'}v_{k'}u_k v_k + \bar{u}_{k'}\bar{v}_{k'}\bar{u}_k\bar{v}_k) \tag{5.18}
$$

Now we calculate the energy due to e-e interaction.

$$
H^{T}_{ee} = \frac{1}{2}\sum_{kk',\sigma\sigma'} V_q c^{\dagger}_{k+q,\sigma} c^{\dagger}_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma} \tag{5.19}
$$

Again using the normal ordering technique of the Wick theorem, we have

$$
\begin{aligned}
& \sum_{k,k',q,\sigma,\sigma'} V_q < \Psi|c^{\dagger}_{k+q,\sigma} c^{\dagger}_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma}|\Psi > \\
= & \sum_{k,k',q,\sigma,\sigma'} V_q(< c^{\dagger}_{k+q,\sigma} c^{\dagger}_{k'-q,\sigma'} >< c_{k',\sigma'} c_{k,\sigma} > + < c^{\dagger}_{k+q,\sigma} c_{k,\sigma} >< c^{\dagger}_{k'-q,\sigma'} c_{k',\sigma'} > \\
- & < c^{\dagger}_{k+q,\sigma} c_{k',\sigma'} >< c^{\dagger}_{k'-q,\sigma'} c_{k,\sigma} >)
\end{aligned} \tag{5.20}
$$

In the above expression the first term, since it contains two electron creation terms its value is zero. The second term gives $V(q = 0)$ terms which we do not include. Only third term survives. Hence,

$$
\begin{aligned}
& < \Psi|\sum_{k,k',q,\sigma,\sigma'} V_q c^{\dagger}_{k+q,\sigma} c^{\dagger}_{k'-q,\sigma'} c_{k',\sigma'} c_{k,\sigma}|\Psi > \\
= & -\sum_{k,k',q,\sigma,\sigma'} V_q < c^{\dagger}_{k+q,\sigma} c_{k',\sigma'} >< c^{\dagger}_{k'-q,\sigma'} c_{k,\sigma} >
\end{aligned}
$$

$$
\begin{aligned}
&= -\sum_{k,k',q} V_q(< c^{\dagger}_{k+q,\uparrow} c_{k',\uparrow} >< c^{\dagger}_{k'-q,\uparrow} c_{k,\uparrow} > + < c^{\dagger}_{k+q,\downarrow} c_{k',\downarrow} >< c^{\dagger}_{k'-q,\downarrow} c_{k,\downarrow} >) \\
&= -\sum_{k,k',q} V_q(v_{k+q} v_{k'} \delta_{k+q,k'} v_{k'-q} v_k \delta_{k'-q,k} + \bar{v}_{k+q} \bar{v}_{k'} \delta_{k+q,k'} \bar{v}_{k'-q} \bar{v}_k \delta_{k'-q,k}) \\
&= -\sum_{k,k',q} V_q(v_{k+q} v_{k'} v_{k'-q} v_k \delta_{q,k'-k} + \bar{v}_{k+q} \bar{v}_{k'} \bar{v}_{k'-q} \bar{v}_k \delta_{q,k'-k}) \\
&= -\sum_{k,k'} V_{k'-k}(v_{k'} v_{k'} v_k v_k + \bar{v}_{k'} \bar{v}_{k'} \bar{v}_k \bar{v}_k) \\
&= -\sum_{k,k'} V_{k'-k}(v^2_{k'} v^2_k + \bar{v}^2_{k'} \bar{v}^2_k) \qquad (5.21)
\end{aligned}
$$

In the above expansion, terms like $< c^{\dagger}_{k+q,\uparrow} c_{k',\downarrow} >$ are not taken into accout since those terms are zero due to the fact that they contain one spin up operator and one spin down operator of the same kind of particles.

The the hole-hole interaction term will contribute

$$
< \Psi| \sum_{k,k',q} V_q d^{\dagger}_{k+q,\sigma} d^{\dagger}_{k'-q,\sigma'} d_{k',\sigma'} d_{k,\sigma} |\Psi >= -\sum_{k,k'} V_{k'-k}(v^2_{k'} v^2_k + \bar{v}^2_{k'} \bar{v}^2_k) \qquad (5.22)
$$

Collecting all the energy terms, we get the total free energy as

$$
\begin{aligned}
F_0 &= \sum_k (\xi^+_k v^2_k + \xi^-_k \bar{v}^2_k) \\
&- \sum_{k,k'} \{V_{k-k'}(u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'} + v^2_{k'} v^2_k + \bar{v}^2_{k'} \bar{v}^2_k)\} \\
&- 2\sum_k \lambda \rho_k (u_k v_k + \bar{u}_k \bar{v}_k) \qquad (5.23)
\end{aligned}
$$

This is exactly the constant term F_0 in Eq.(4.21) of chapter 4 of the Free energy expression. All $V(q=0)$ terms cancel each other.

5.2 Minimization of Free energy

Using

$$
\begin{aligned}
u^2_k + v^2_k &= 1 \\
\bar{u}^2_k + \bar{v}^2_k &= 1, \qquad (5.24)
\end{aligned}
$$

we write the Free energy expression as

$$
\begin{aligned}
F_0 &= \sum_k (\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2) \\
&- \sum_{k,k'} V_{k-k'} (v_k \sqrt{1-v_k} v_{k'} \sqrt{1-v_{k'}} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'} \\
&+ v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2) - 2\sum_k \lambda_k \rho_k (\sqrt{1-v_k^2} v_k + \bar{u}_k \bar{v}_k) \\
&= \sum_k (\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2) \\
&- \sum_{k,k'} V_{k-k'} (\sqrt{v_k^2 - v_k^4} \sqrt{v_{k'}^2 - v_{k'}^4} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'} \\
&+ v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2) - 2\sum_k \lambda_k \rho_k (\sqrt{v_k^2 - v_k^4} + \bar{u}_k \bar{v}_k)
\end{aligned} \tag{5.25}
$$

Now we minimize the energy with respect to v_k, that is

$$
\frac{\partial F_0}{\partial v_k} = 0 \tag{5.26}
$$

We get,

$$
\begin{aligned}
0 &= \sum_k 2\xi_k^+ 2v_k \\
&- 2\sum_{kk'} V_{k,k'} [\sqrt{v_{k'}^2 - v_{k'}^4} \frac{1}{2} (v_k^2 - v_k^4)^{-1/2} (2v_k - 4v_k^3) \\
&+ \sqrt{v_k^2 - v_k^4} \frac{1}{2} (v_{k'}^2 - v_{k'}^4)^{-1/2} (2v_{k'} - 4v_{k'}^3) \delta_{k,k'} \\
&+ 2v_k v_{k'}^2 + 2v_k^2 v_{k'} \delta_{v_k, v_{k'}}] - 2\sum_k \lambda_k \rho_k \frac{1}{2} (v_k^2 - v_k^4)^{-1/2} (2v_k - 4v_k^3) \\
&= \sum_k 2\xi_k^+ v_k - 2\sum_{kk'} V_{k,k'} [v_{k'} \sqrt{1 - v_{k'}^2} \frac{(1-2v_k^2)}{\sqrt{(1-v_k^2)}} + 2v_k v_{k'}^2] - 2\sum_k \lambda_k \rho_k \frac{(1-2v_k^2)}{\sqrt{(1-v_k^2)}} \\
&= \sum_k 2\xi_k^+ v_k - 2\sum_{kk'} V_{k,k'} [u_{k'} v_{k'} \frac{(u_k^2 - v_k^2)}{u_k} + 2v_k v_{k'}^2] - 2\sum_k \lambda_k \rho_k \frac{(u_k^2 - v_k^2)}{u_k}
\end{aligned} \tag{5.27}
$$

Multipling the above equation by u_k, we get

$$
0 = \sum_k 2\xi_k^+ u_k v_k - 2\sum_{kk'} V_{k,k'} [u_{k'} v_{k'} (u_k^2 - v_k^2) + 2u_k v_k v_{k'}^2] - 2\sum_k \lambda_k \rho_k (u_k^2 - v_k^2)
$$

$$
\begin{aligned}
&= 2[\sum_k 2u_k v_k(\xi_k^+ - 2\sum_{kk'} V_{k,k'} v_{k'}^2) - \sum_{kk'} V_{k,k'} u_{k'} v_{k'}(u_k^2 - v_k^2) - \sum_k \lambda_k \rho_k (u_k^2 - v_k^2)] \\
&= 2[\sum_k u_k v_k(\xi_k^+ - 2\sum_{k,k'} V_{k,k'} v_{k'}^2) - \sum_k \lambda \rho_k (u_k^2 - v_k^2) - \sum_{k,k'} V_{k,k'} u_{k'} v_{k'}(u_k^2 - v_k^2)] \\
&= 2[\sum_k u_k v_k(\xi_k^+ + \Omega_k) - \frac{1}{2}\sum_k (u_k^2 - v_k^2)(2\lambda\rho_k + 2\sum_{k'} V_{k,k'} u_{k'} v_{k'})] \\
&= 2[\sum_k u_k v_k(\xi_k^+ + \Omega_k) - \frac{1}{2}\sum_k (u_k^2 - v_k^2)(2\lambda\rho_k + 2\sum_{k'} V_{k,k'} u_{k'} v_{k'})] \\
&= 2[\sum_k u_k v_k(\xi_k^+ + \Omega_k) - \frac{1}{2}\sum_k (u_k^2 - v_k^2)(2\lambda\rho_k + \Delta_k^0)] \\
&= 2\sum_k [u_k v_k(\xi_k^+ + \Omega_k) - \frac{1}{2}\Delta_k (u_k^2 - v_k^2)] \qquad (5.28)
\end{aligned}
$$

So we have

$$
\frac{1}{2}\Delta_k(u_k^2 - v_k^2) - u_k v_k(\xi_k^+ + \Omega_k) = 0 \qquad (5.29)
$$

Now if we minimize the energy with respect to $\bar{v}_k$, we have

$$
\frac{\partial F_0}{\partial \bar{v}_k} = 0 \qquad (5.30)
$$

We will get the other condition as

$$
\frac{1}{2}\bar{\Delta}_k(\bar{u}_k^2 - \bar{v}_k^2) - \bar{u}_k \bar{v}_k(\xi_k^- + \bar{\Omega}_k) = 0 \qquad (5.31)
$$

These are the conditions for the off diagonal term Eq.(4.37-4.38)to be zero in B-V energy expression for diagonalization. So as done before together with the unitary condition, we can solve for $u_k,\ v_k,\ \bar{u}_k, \bar{v}_k$ and get Free energy.

Bibliography

[1] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. B. **108**, 1175 (1957).

[2] N. N. Bogoliubov, V. V. Tolmachov, and D. V. Sirkov, Fortschritte der Physik, **6**, 605 (1958).

[3] J. G. Valatin, Il Nuovo Cimento, **VII**, 843, (1958).

[4] N. N. Bogoliubov, J. Phys. USSR, **9**,23 (1947).

Chapter 6

Results and Discussions

In this Chapter we study para to ferro-magnetic transition of magnetic moments by the incident light by calculating the magnetization in a mean-field way by using the free energy expression Eq.(4.48) of chapter 4 and study different scenarios of dependences of transition on various physical quantities. We generally consider a contact interaction between electrons and holes and k-independent ρ (probability of light coupling to particles). We have also studied more general case of a k-dependent $\rho(k)$.

6.1 Calculation of magnetization in a mean-field way

In our system the light induced free carriers such as electrons and holes interact with the localized moments antiferromagnetically and there by induce a ferromagnetic interaction between impurity magnetic moments. These moments themselves constitute a many-body magnetic system. We replace this interacting magnetic moments in a mean-field way. The main idea is to replace all many-body interactions to any one body with an average or effective interaction. This reduces the many-body problem into an effective one-body problem of magnetic moments. Each magnetic moment feels a mean-field of the other magnetic moments. In Fig.6.1, we give the picture of mean-field [1–3] representation of a magnetic moment.

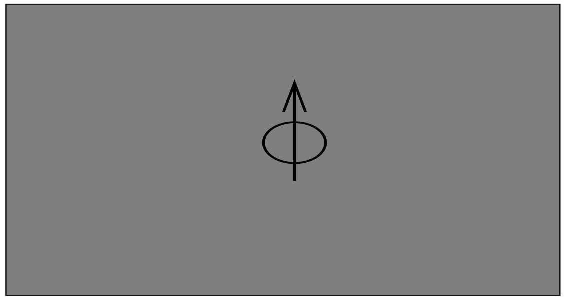

Figure 6.1: Mean-field representation of interaction of impurity moment. The figure shows that the many body system is represented by a single body feeling the mean field of other N-1 moments in an average way.

The effective magnetic field experienced by a single magnetic moment M due to the rest of the moments is given as

$$H_{eff} = -\frac{\partial F_0(M)}{\partial M} \tag{6.1}$$

Thus the self-consistent equation for magnetization to be solved is :

$$< M(T) >= (\sum_{m=-5/2}^{+5/2} me^{-\beta H_{eff}(M)m})/(\sum_{m=-5/2}^{+5/2} e^{-\beta H_{eff}(M)m}) \tag{6.2}$$

where $\beta = (k_\beta T)^{-1}$ and $m = 5/2$ because Ga has 5 d-electrons. In order to solve self consistently $M(T)$, we use the free energy expression F_0 from Eq.(4.48) and calculate H_{eff}. Given a temperature, guess a value for the M and solve the Eq.(6.2) self-consistently, till it converges. Then that is the mean field value of M for that given temperature. Similarly we solve for magnetization for a range of temperatures.

6.2 Parameters, Results and Discussions

The following parameters are taken in our calculation [4].

$$
\begin{aligned}
&\mu' = \hbar\omega - E_g = 0.1 - 1.8eV \\
&\lambda = strength\ of\ the\ coupling\ of\ light\ to\ electron\ or\ hole\ = 0.1 - 2.8eV \\
&J = J_e - J_h = 30eV.\mathring{A}^3 \\
&x = concentration\ of\ Mn\ atoms \approx 0.1 \\
&lattice\ constant\ of\ GaMnAs\ = a = 5.65\mathring{A} \\
&c = concentration\ of\ Mn/\mathring{A}^3 = \frac{x}{a^3/4} = 0.022x/\mathring{A}^3 \\
&m^* = (m_e^{-1} + m_h^{-1})^{-1} \approx 0.1\ m
\end{aligned} \tag{6.3}
$$

If $x = 0.01$ then the zeeman splitting of conduction band electron is

$\Delta = 2J_eMc = 2(4eV.\mathring{A}^3)(\frac{5}{2})(\frac{0.022\times 0.01}{\mathring{A}^3}) = 4meV$

Since splitting energy of a hole (concentration $x = 1$) with five d-electrons is $5 \times 0.9eV = 4.5eV$, this is consistent with the above result because J_h is $\approx 10J_e$ and concentration is also 0.1, hence the zeeman splitting is $100 \times 4meV = 0.4eV$.

Estimation of U_0 We in our final calculation take a contact interaction [5, 6] of strength U_0 for $V_{k-k'}$. We find that since the density of photo-generated carriers is very small, the critical temperature T_c is unchanged within a range of values $0.1\ eV.\mathring{A}^3 \leq U_0 \leq 1200\ eV.\mathring{A}^3$. We want to estimate the U_0. We proceed as follows. The Coulomb interaction in the real space is given as $\frac{e^2}{4\pi\epsilon_0\epsilon_r r}$. Since we have roughly 8×10^{-6} number of particles per $\mathring{A}^3$, average inter-particle separation is $a_0 = ((3/4\pi)8^{-1} \times 10^6\mathring{A}^3)^{1/3} = 0.31 \times 10^2\mathring{A}$. Using for GaAs $\epsilon_r = 13.13,\ \epsilon_0 = 8.85 \times 10^{-12}C^2/N.m^2,\ and\ e = 1.6 \times 10^{-19}C$, we estimate that the interaction strength is 0.035eV. Since we will replace the Coulomb interaction by a contact interaction, we have

$$< \psi|U_0\delta(\vec{r})|\psi >= U_0eV.\mathring{A}^3|\psi(0)|^2 = U_0eV.\mathring{A}^3.\frac{N}{\mathring{A}^3} = 0.035eV \tag{6.4}$$

So we get

$$U_0 = 0.035/N = 0.035/(8 \times 10^{-6}) \approx 4000 \ eV.\mathring{A}^3 \tag{6.5}$$

This value is an approximate estimation and it is order of thousand ,roughly 3.5 times the value 1200 $eV.\mathring{A}^3$ up to which T_c does not change. We take $U_0 = 1200 \ eV.\mathring{A}^3$ in all our calculation.

We study the effect of light coupling λ on free energy as a function of magnetic moment, other parameters of the system remaining constant. In Fig.6.2, we give a plot of free energy as given by Eq.(4.51) of chapter 4 as a function of magnetic moment M for different values of light coupling λ. We have taken $U_0 = 1200 \ eV.\mathring{A}^3, \ \mu' = \hbar\omega - E_g = 0.1eV, \ J = 30eV, \ m^* = 0.1, \ concentration = c = 0.022x/\mathring{A}^3, \ and \ x = 0.1$. The plot shows that for a given value of light coupling free energy increases with increase of magnetic moment and also for a given value of magnetic moment, with increase in light coupling free energy increases. When $\lambda = 0$ (no coupling of light to particles) and $\mu' = -10.0eV$, that is when energy of the light is below the energy gap there is no excitation of electron and hole.

We study the effect of energy of the light above the gap, on free energy as function of magnetic moment, in the special case of light coupling $\lambda = 0, \ and \ U_0 = 0$. In Fig.6.3 we give a plot of free energy as a function of magnetic moment M for different values of $\mu' = \hbar\omega - E_g$, for light coupling $\lambda = 0, \ U_0 = 0$. The plot shows with increase in the value of light energy above the gap, free energy F increases as magnetic moment is increased. When $\lambda = 0, \ U_0 = 0$ we have derived an analytical expression for the free energy as given by the Eq.(4.55) of the chapter 4. Our calculated values for free energy using the expression Eq.(4.51) matches exactly with the value calculated using Eq.(4.55). Our system of electrons and holes in the light bath is in a state of equilibrium. So even if there is no light signing on the system, there are electrons and holes. It is like taking limit of $\lambda \to 0$ when the system is in equilibrium with the light bath. The plot shows

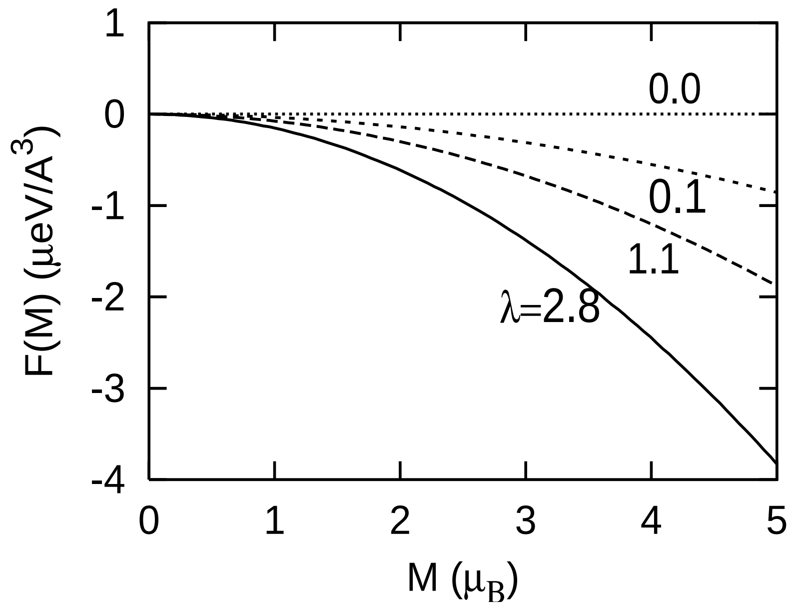

Figure 6.2: Free energy as a function of magnetic moment M for different values of light coupling λ evaluated using the expression for magnetization dependent free energy Eqs.(4.56-62) and magnetization Eq.(6.2). The parameters are $U_0 = 1200\ eV.\AA^3,\ \mu' = \hbar\omega - E_g = 0.1eV$. Other parameters are given in Eq.(6.3). The plot shows with increase in light coupling free energy F increases as magnetic moment is increased. When $\lambda = 0$ (no coupling of light to particles) and $\mu' = -10.0eV$, that is when energy of the light is below the energy gap there is no excitation of electron and hole and the free energy is zero. The top most line corresponds to this situation.

with increase in the value of light energy above the gap, free energy F increases as magnetization is increased.

Next we study the effect of light coupling λ on the critical temperature of phase transition provided other parameters of the system remain unchanged. In Fig.6.4, we give a plot of Magnetization M(T) as a function of Temperature T for different values of light coupling λ as solved self consistently using Eq.(6.2). Here we have taken $U_0 = 1200\ eV.\AA^3,\ \mu' = 0.1eV$. The plot shows a phase transition from para to ferromagnetic state as temperature is decreased. With increase

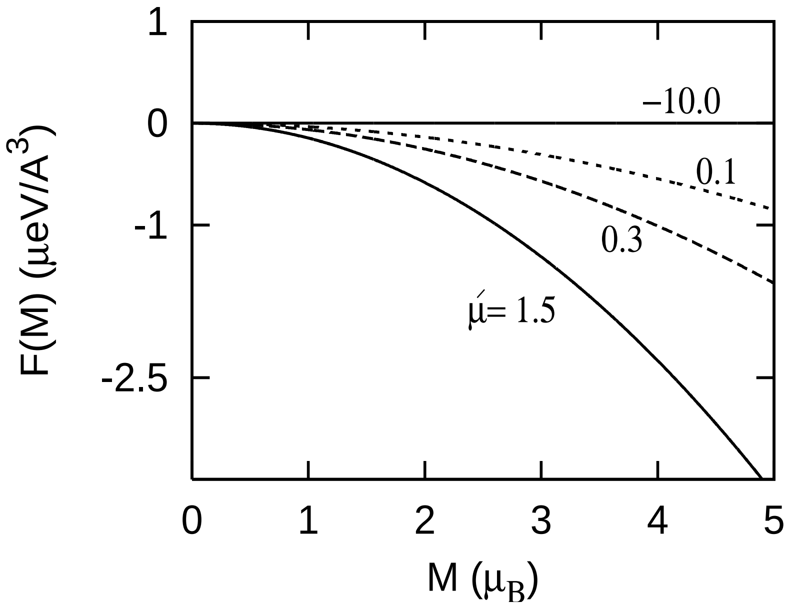

Figure 6.3: Free energy as a function of magnetic moment M for different values of $\mu' = \hbar\omega - E_g$ for light coupling $\lambda = 0$ $U_0 = 0$ evaluated using the expression for magnetization dependent free energy Eqs.(4.56-62) and magnetization Eq.(6.2). Other parameters are given in Eq.(6.3). The plot shows with increase in the value of light energy above the gap, free energy F increases as magnetic moment is increased. When energy of the light is below the gap $\mu' = \hbar\omega - E_g = -10eV$, there is no magnetization for any value of magnetic moment.

in the light coupling λ, more and more electron-hole pairs are created, thereby increasing the magnetization and hence the critical temperature is increased.

We examine the variation of critical temperature on light coupling. In Fig.6.5, we give a plot of Critical temperature T_c as a function of light coupling λ evaluated using Eq.(6.2). The plot shows an increase in critical temperature with increased value of light coupling. But with increase of $\lambda > 2.43eV$ there is an decrease in the critical temperature. This is due to the competition between particle-particle interaction and the light energy of the system.

We want to study how the number of spin up electron and spin down hole pairs

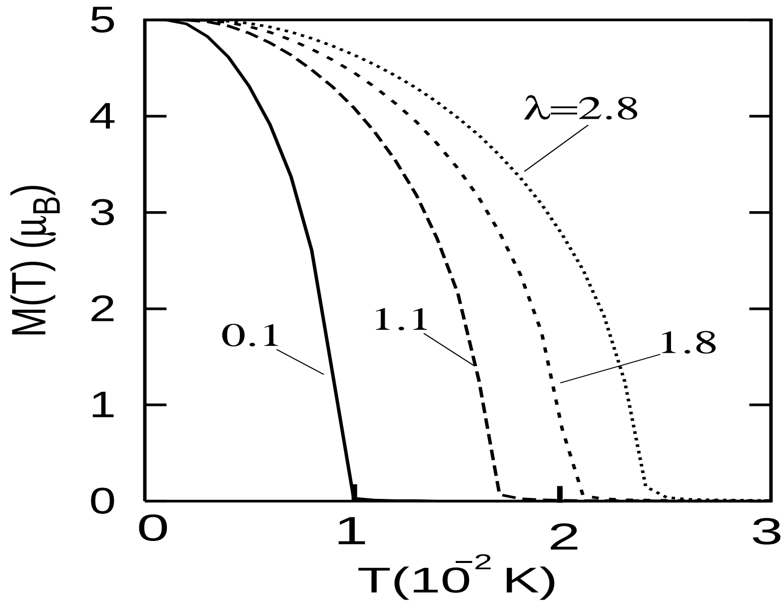

Figure 6.4: Magnetization M(T) as a function of Temperature T for different values of light coupling λ evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). The parameters are $U_0 = 1200\ eV.\AA^3\ \mu' = 0.1eV$. Other parameters are given in Eq.(6.3). The plot shows a phase transition from paramagnetic to ferromagnetic state as temperature is lowered. With increase in the light coupling λ, more and more electron-hole pairs are created, thereby increasing the magnetization and hence the critical temperature is increased.

$n_\uparrow$ and spin down electron and spin up hole pairs $n_\downarrow$ vary with the temperature of the system as system changes its phase from paramagnetic to ferromagnetic state. In Fig.6.6, we give a plot of number of spin up electron and spin down hole pairs $n_\uparrow$ and spin down electron and spin up hole pairs $n_\downarrow$ as a function of temperature T. Here we have taken $U_0 = 1200\ eV.\AA^3,\ \mu' = 0.1eV,\ \lambda = 0.1$. The plot shows below the critical temperature the number of spin up electron and spin down hole pairs $n_\uparrow$ is different than the number of spin down electron and spin up holes $n_\downarrow$. This shows the onset of ferromagnetic phase.

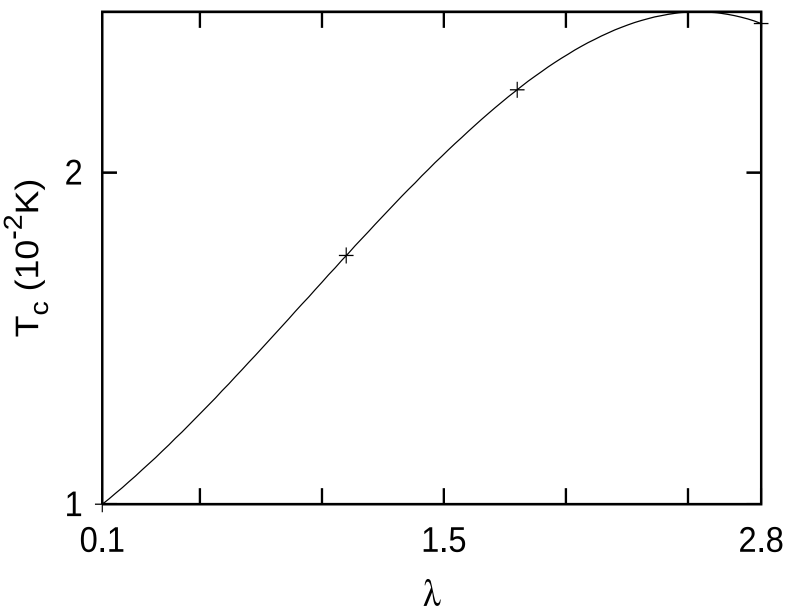

Figure 6.5: Critical temperature T_c as a function of light coupling λ evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). The parameters are $U_0 = 1200\ eV.A\mathring{A}^3\ \mu' = 0.1eV$.Other parameters are given in Eq.(6.3). The plot shows an increase in critical temperature with increased value of light coupling. With increase in the light coupling λ, more and more electron-hole pairs are created, thereby increasing the magnetization and hence the critical temperature is increased. With increase of $\lambda > 2.43eV$ there is an decrease in the critical temperature. This is due to the competition between particle-particle interaction and the light energy of the system

We want to examine how in the para to ferromagnetic phase change, magnetization and the number of spin up electron and spin down hole pairs $n_\uparrow$ and spin down electron and spin up hole pairs $n_\downarrow$ vary with temperature. Here we have taken $U_0 = 1200\ eV.\mathring{A}^3,\ \mu' = 0.1eV,\ \lambda = 0.1$. In Fig.6.7, we give a plot of variation magnetization with temperature in the upper panel and how at that temperatures the number of spin up electron and spin down hole pairs $n_\uparrow$ and spin down electron and spin up hole pairs $n_\downarrow$ vary in the lower panel. This clearly shows that below the critical temperature the number of spin up electron and

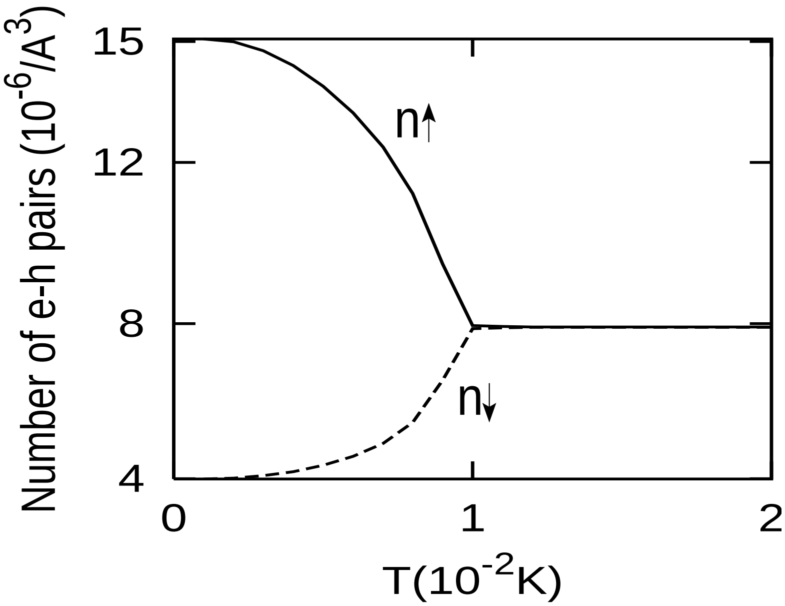

Figure 6.6: Number of pairs of spin up electrons and down hole $n_\uparrow$ and spin down electrons and spin up holes $n_\downarrow$ as a function of temperature T. The parameters are $U_0 = 1200\ eV.\AA^3$ $\mu' = 0.1eV$ $\lambda = 0.1eV$ Other parameters are given in Eq.(6.3). The plot shows below the critical temperature the number of spin up electron and down hole pairs $n_\uparrow$ is different than the number of spin down electron and spin up holes $n_\downarrow$. This shows the onset of ferromagnetic phase.

down hole pairs $n_\uparrow$ is different than the number of spin down electron and spin up holes $n_\downarrow$. This shows the onset of ferromagnetic phase.

We want to study effect of energy of the incident light on the magnetization of the system that is on the critical temperature when system changes from para to ferro magnetic state provided other parameters of the system remain unchanged. In Fig.6.8, we give a plot of magnetization M(T) as a function of temperature T for different values of μ for a given value of light coupling λ. Here we have taken $U_0 = 1200\ eV.\AA^3,\ \lambda = 0.1$. The plot shows a phase transition from paramagnetic to ferromagnetic state as temperature is decreased. With increase in the value of the light energy $\mu = \hbar\omega$, there is an increase in the value of the critical temperature. This is due to the fact that increase of light energy produces more and more of electron-hole pairs and there by aligning the magnetic moments more and more and hence the critical temperature is increased.

Now we examine the nature of variation of critical temperature on the energy of the incident light provided other parameters of the system remains constant. In Fig.6.9, we give a plot of critical temperature T_c as a function of chemical potential $\mu = \hbar\omega$. The plot shows increase in critical temperature with increased value of chemical potential.This is due to the fact that increase of light energy produces more and more of electron-hole pairs and there by aligning the magnetic moments more and more and hence the critical temperature is increased.

Here we examine the nature of variation of critical temperature on the energy of the incident light when the interaction among particles is taken to be zero, $U_0 = 0.0\ eV.\AA^3$. In Fig.6.10, we give a plot of critical temperature T_c as a function of chemical potential $\mu = \hbar\omega$. The plot shows increase in critical temperature with increased value of chemical potential.This is due to the fact that increase of light energy produces more and more of electron-hole pairs and there by aligning the magnetic moments more and more and hence the critical temperature varies as the density of states which goes as $\sim \mu^{1/2}$. The solid line is a fit with $3.5\mu^{1/2}$ of the four data points. The fit is exact.

Next we study the effect of temperature on the magnetization of the system as a function of chemical potential $\mu = \hbar\omega$. Here we have taken $U_0 = 1200\ eV.\AA^3,\ \lambda = 0.1$. In Fig.6.11, we give a plot of magnetization M as a function of chemical potential μ for two different values of temperature T. The plot shows that for lower temperature magnetization increases more rapidly with μ when value of light energy crosses the gap value.

We want to study sub-band gap Magnetization M as a function of chemical potential $\mu = \hbar\omega$ for two different values of temperature T evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy

Eqs.(4.56-62). The parameters are $U_0 = 1200\ eV.\AA^3$, $\lambda = 0.1eV$ and broken line and solid line are for temperature 0.005K and 0.008K respectively. The Fig.6.12 shows that there is finite magnetization for photon energy bellow the band gap value. The band gap is at $\mu = 0.0$ on the x-axis. This clearly indicates that even if energy of the light is below the band gap, there is small but finite magnetization. This is due to the virtual electron-hole pair excitation.

We study the effect of k-dependence of light coupling ρ_k on the critical temperature for two different light coupling strengths λ_0 provided other parameters of the system remain unchanged. In Fig.6.13, we give a plot of magnetization M(T) as a function of temperature T for different values of light coupling λ as solved self consistently using Eq.(6.2). Here we have taken $U_0 = 1200\ eV.\AA^3$ and $\rho_k = 1$ for the solid line and $\rho_k = \frac{1}{(1+(a_{ex}k)^2)^2}$ for the broken line. Other parameters are given in Eq.(6.3).The plot shows phase transition temperature is decreased with the k-dependent coupling.

We examine in Fig.6.14 occupation of pair-particles as a function of energy. The left lines are for up-electron and down-hole and right lines are for down-electron and up-hole pairs. Energy supplied to the system is 1.1 eV. One can see that the two theta functions are zero at $E = 1.1 - J < M >$ and $E = 1.1 + J < M >$ where $J = 0.067$ and $M = 5/2$. As light coupling is included with $\lambda = 0.1$ the functions deviate from theta functions. These are all calculated at zero temperature.

In Fig.6.15 we plot amplitude of occupation of pair-particles as a function of energy. The solid line is u for down-electron and up-hole pair and broken line is for amplitude v for the same pair. We find that $u^2 + v^2 = 1$, as it should be.

We want to study the dependence of critical temperature T_c on the net anti-ferromagnetic coupling strength $J = J_e - J_h$ of particles to the magnetic moment.The parameters are $U_0 = 1200\ eV.\AA^3$, $\lambda = 0.1eV$. In Fig.6.16, we give a plot of critical temperature T_c as a function of $J^2 = (J_e - J_h)^2$. We see a linear behavior. This is expected. Since the basic origin of exchange Hamiltonian goes as $H = JS.s\delta(r)$, so the effective exchange between magnetic moments is $J_{eff} = J^2$ and according to Heisenberg model critical temperature $T_c \sim J_{eff} \sim J^2$. This linear behavior has been predicted by Piermarochhi et al [7] based on a diagrammatic calculation of a mechanism of coupling of spins localized in neighboring quantum dots by virtual excitation of delocalized exciton states in the host material by light field. This is termed as ORKKY interaction.

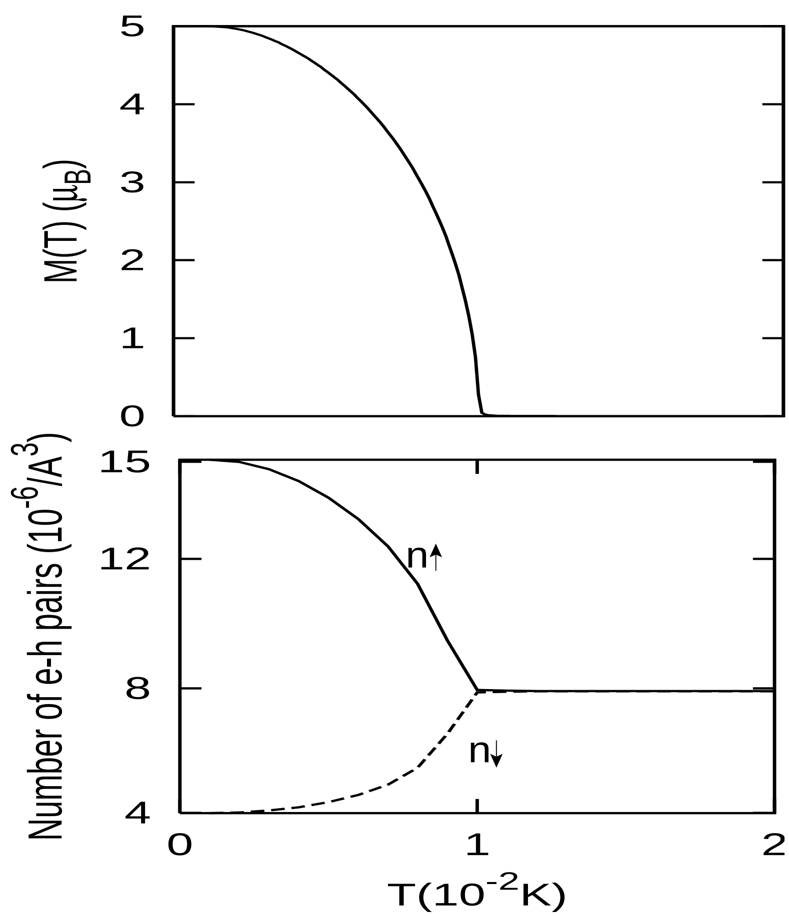

Figure 6.7: Magnetization and number of pairs of spin up electrons and spin down holes $n_\uparrow$ and spin down electrons and spin up holes $n_\downarrow$ as a function of temperature T evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). Here we have taken $U_0 = 1200\ eV.\AA^3$, $\mu' = 0.1eV\ \lambda = 0.1$. Other parameters are given in Eq.(6.3). In Fig.6.7, we give plot of variation magnetization with temperature in the upper panel and how at that temperatures the number of spin up electron and spin down hole pairs $n_\uparrow$ and spin down electron and spin up hole pairs $n_\downarrow$ vary in the lower panel. This clearly shows that below the critical temperature the number of spin up electron and down hole pairs $n_\uparrow$ is different than the number of spin down electron and spin up holes $n_\downarrow$. This shows the onset of ferromagnetic phase.

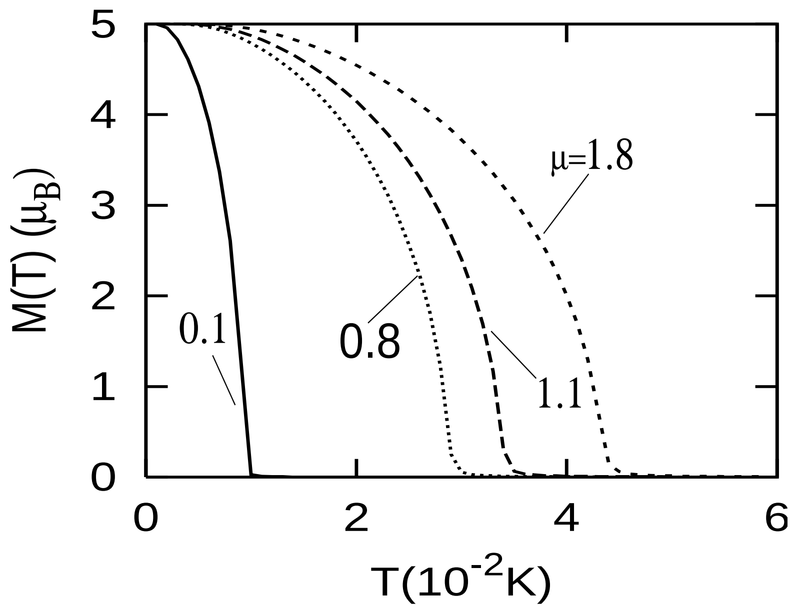

Figure 6.8: Magnetization M(T) as a function of temperature T for different values of μ for a given value of light coupling λ evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). The parameters are $U_0 = 1200\ eV.\mathring{A}^3,\ \lambda = 0.1$. Other parameters are given in Eq.(6.3). The plot shows a phase transition from paramagnetic to ferromagnetic state as temperature is decreased. With increase in the value of the light energy $\mu = \hbar\omega$, there is an increase in the value of the critical temperature. This is due to the fact that increase value of light energy produces more and more of electron-hole pairs and there by aligning the magnetic moments more and more and hence the critical temperature is increased.

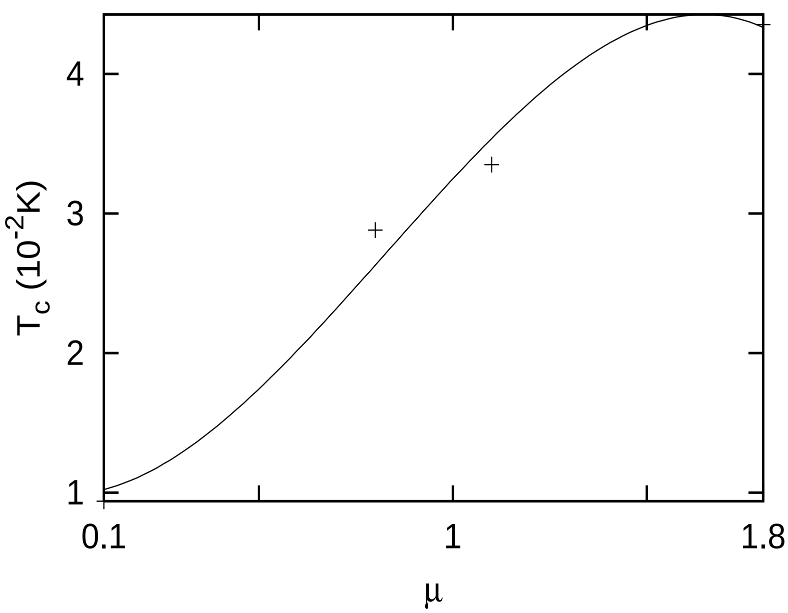

Figure 6.9: Critical temperature T_c as a function of chemical potential $\mu = \hbar\omega$. The parameters are $U_0 = 1200\ eV.\AA^3,\ \lambda = 0.1$. Other parameters are given in Eq.(6.3). The plot shows increase in critical temperature with increased value of chemical potential. This is due to the fact that increase in light energy produces more and more of electron-hole pairs and there by aligning the magnetic moments more and more and hence the critical temperature is increased.

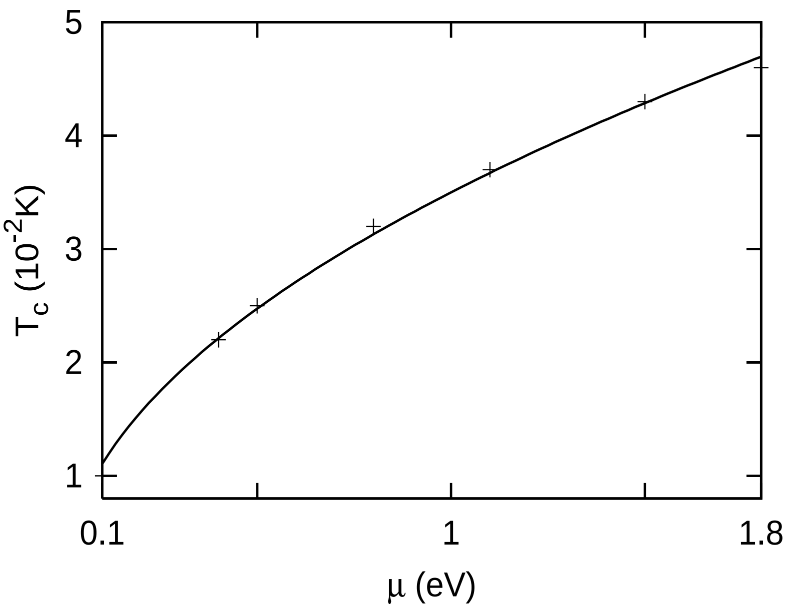

Figure 6.10: Critical temperature T_c as a function of chemical potential $\mu = \hbar\omega$. The parameters are $U_0 = 0.0\ eV.\AA^3,\ \lambda = 0.1$. Other parameters are given in Eq.(6.3). The plot shows increase in critical temperature with increased value of chemical potential. This is due to the fact that increase in light energy produces more and more of electron-hole pairs and there by aligning the magnetic moments more and more and hence the critical temperature varies as the density of states which goes as $\sim \mu^{1/2}$. The solid line is a fit with $3.5\mu^{1/2}$ of the four data points. The fit is exact.

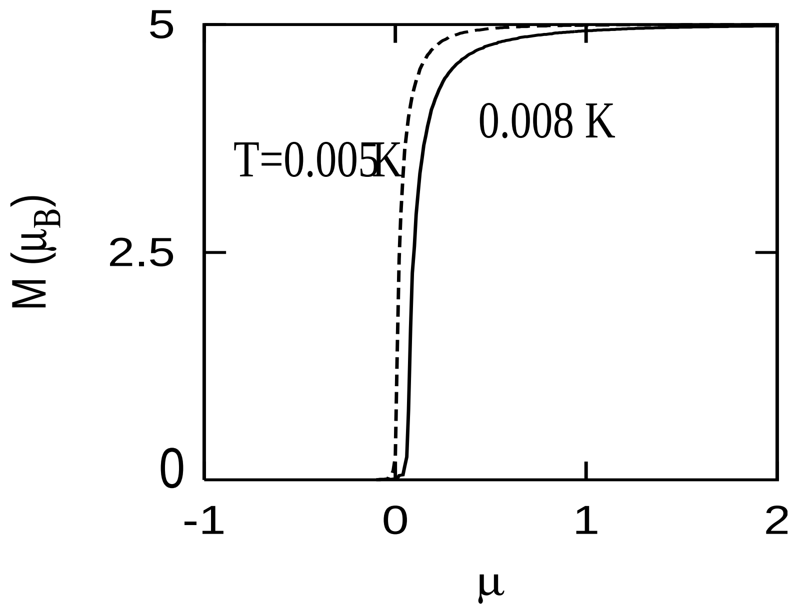

Figure 6.11: Magnetization M as a function of chemical potential $\mu = \hbar\omega$ for two different values of temperature T evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). The parameters are $U_0 = 1200\ eV.\AA^3$, $\lambda = 0.1$. Other parameters are given in Eq.(6.3). The plot shows that for lower temperature magnetization increases more rapidly with μ when value of light energy crosses the band-gap. The band gap is at zero of the x-axis.

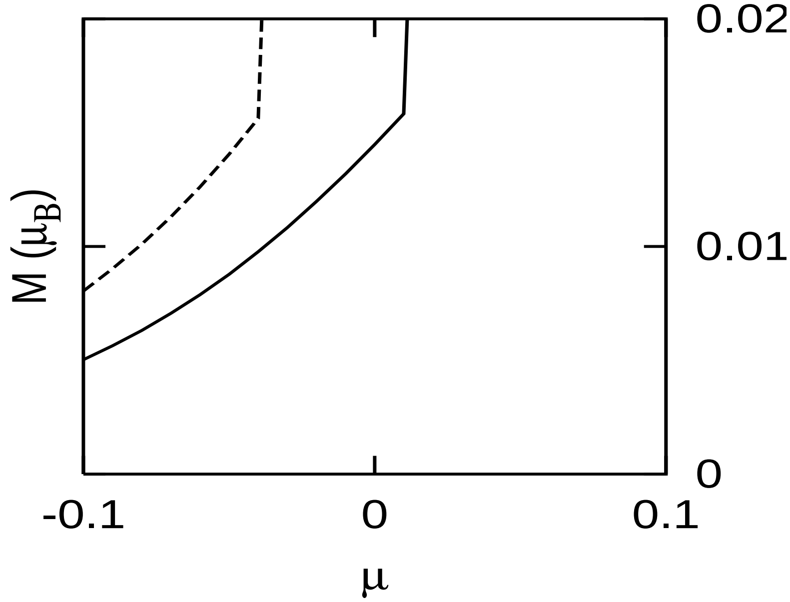

Figure 6.12: Sub-band gap Magnetization M as a function of chemical potential $\mu = \hbar\omega$ for two different values of temperature T evaluated using the expression for magnetization Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). The parameters are $U_0 = 1200\ eV.\mathring{A}^3,\ \lambda = 0.1$. Other parameters are given in Eq.(6.3). Broken line and solid line are for temperature 0.005K and 0.008K respectively. The plot shows that there is finite magnetization for photon energy bellow the band gap value. The band gap is at $\mu = 0.0$ on the x-axis. This clearly indicates that even if energy of the light is below the band gap, there is small but finite magnetization. This is due to the virtual electron-hole pair excitations.

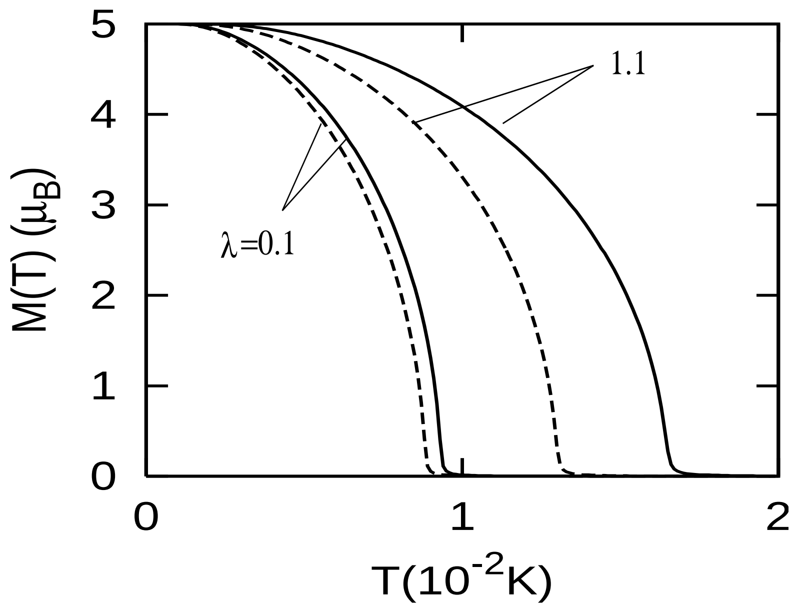

Figure 6.13: Magnetization M(T) as a function of temperature T for different values of light coupling λ as given by Eq.(6.2) and magnetization dependent free energy Eqs.(4.56-62). Here we have taken $U_0 = 1200\ eV.\mathring{A}^3$ and $\rho_k = 1$ for the solid line and $\rho_k = \frac{1}{(1+(a_{ex}k)^2)^2}$ for the broken line. Other parameters are given in Eq.(6.3). The plot shows phase transition temperature is decreased with the k-dependent coupling.

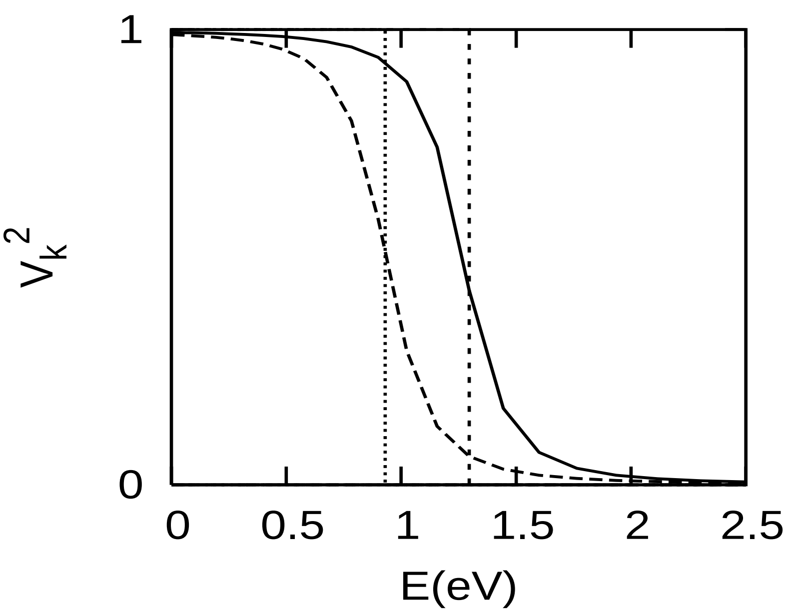

Figure 6.14: Occupation of pair-particles as a function of energy ξ^+ *or* ξ^- using Eqs.(4.56-62) and Eq.(6.2). The left lines are for up-electron and down-hole and right lines are for down-electron and up-hole pairs. Energy supplied to the system is 1.1 eV. Other parameters are given in Eq.(6.3). One can see that the two theta functions are zero at $E = 1.1 - J < M >$ and $E = 1.1 + J < M >$ where $J = 0.067$ and $M = 5/2$. As light coupling is included with $\lambda = 0.1$ the functions deviate from theta functions. These are all calculated at zero temperature.

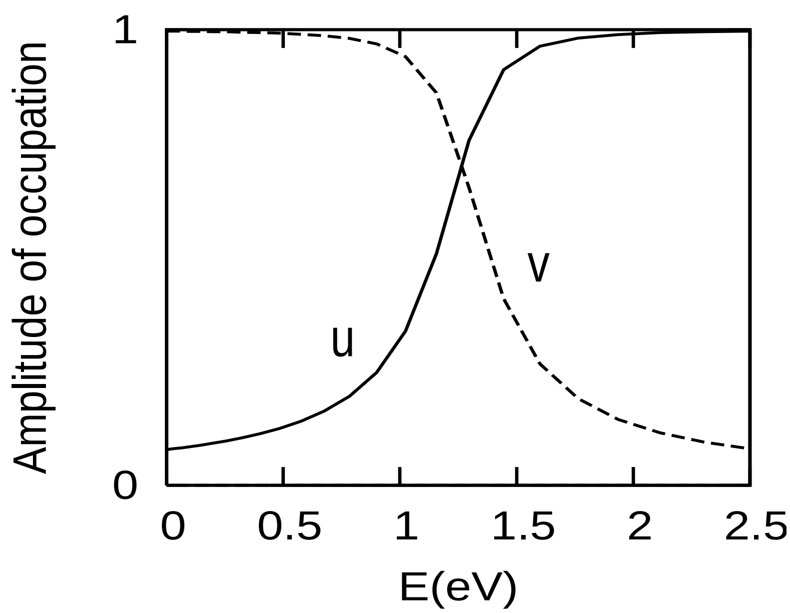

Figure 6.15: Amplitude of occupation of pair-particles as a function of energy using Eqs.(4.56-62) and Eq.(6.2). Parameters are given in Eq.(6.3). The solid line is u for down-electron and up-hole pair and broken line is for amplitude v for the same pair.

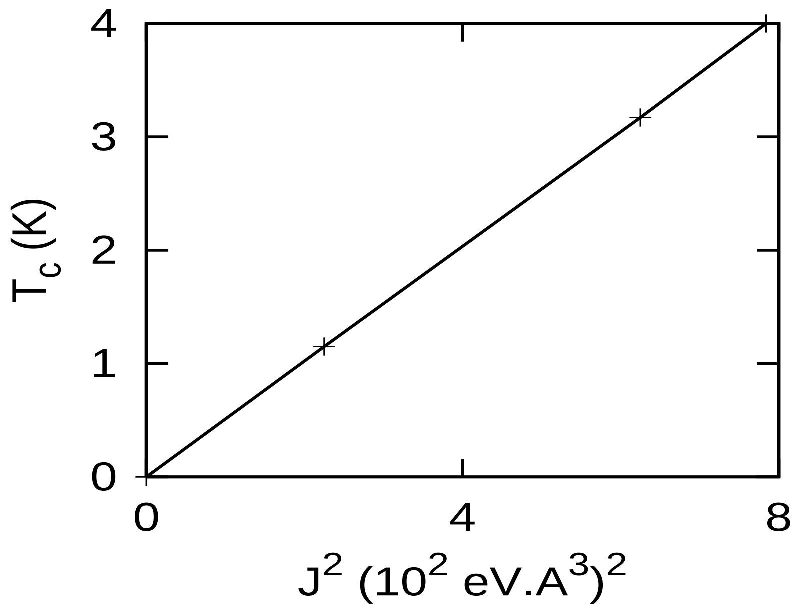

Figure 6.16: Critical temperature T_c as a function of $J^2 = (J_e - J_h)^2$. The parameters are $U_0 = 1200\ eV.\mathring{A}^3$, $\lambda = 0.1$. Other parameters are given in Eq.(6.3). We give a plot of critical temperature T_c using Eq.(6.2) and Eqs.(4.56-62) as a function of $J^2 = (J_e - J_h)^2$. We see a linear behavior. This is expected. Since the basic origin of exchange Hamiltonian goes as $H = JS.s\delta(r)$, so the effective exchange between magnetic moments is $J_{eff} = J^2$ and according to Heisenberg model critical temperature $T_c \sim J_{eff} \sim J^2$.

Bibliography

[1] H. Bruss & K. Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics* (Oxford, New York, 2004) p.67.

[2] R. Kubo, *Statistical Mechanics* (North-Holland, Amsterdam, 1993), p.51.

[3] G. Rickayzen,*Green's Functions and Condensed Matter* (Academic Press, New York, 1980) p.268.

[4] J. Fernandez-Rossier, C. Piermarocchi, P. Chen, A. H. MacDonald and L. J. Sham, Phys. Rev. Lett. **93**, 127201 (2004).

[5] G. D. Mahan, *Many-Particle Physics*,(Kluwer Academic, 3rd Ed. New York,,2000) p.607.

[6] P. Gosdzinsky and R. Tarrach, Am. J. Phys. **59**, 70 (1991).

[7] C. Peirmarocchi, P. Chen, L. J. Sham and D. G. Steel, Phys. Rev. Lett. **89**, 167402-1 (2002).

Chapter 7

Summary and Conclusions

We developed a model many-body theory for the para to ferro-magnetic transition in Dilute Magnetic Semiconductors when light signs on it. When light is incident on these systems, electron and holes are created across the band gap. These particles interact with the impurity magnetic moments and mediate ferro-magnetism when temperature is lowered. This is a situation similar to the famous Rabi problem of a two state system coupled to time-dependent oscillating electric field. Ours is a multi-state system with electrons and holes coupled to an oscillating electric field. This is a generalization of the Rabi problem which shows also a phase transition from para to ferromagnetic state.

We first studied some model one and two state systems including the Rabi problem. We showed by performing appropriate unitary transformations, it is possible to eliminate the time from the time-dependent Hamiltonian and get the eigen energies. Since our system of electron and holes in contact with the photon bath is in a steady state, we calculated the free energy of the system. We studied the problem of phase transition in two different ways , one by constructing Bogoliubov-Valatin quasi particles and the other by BCS wave function approach as in the low-temperature superconducting phenomenon.

Our time-independent Hamiltonian was transformed by the B-V transformations. We got the ground state energy and the excitations also. We then constructed a BCS-type wave function and calculated the expectation value of the time-independent Hamiltonian. In this procedure we get the ground state energy of the system identical to the energy calculated in BV way without the excitations. This also establishes that BCS and BV approaches are equivalent mean-field methods.

We then use a mean-field way of calculating the partition function and hence the ensemble average of a magnetic moment which gives the magnetization of the system. The magnetization and thereby the critical temperature is dependent on the photon energy incident on the system. By increasing the light coupling λ to the particles the transition temperature increases. Also by increasing the frequency of the light, the transition temperature is increased. Since more and more of the electron and holes are created, these carriers mediate more with the magnetic moment and flip their moments into the ferro-magnetic state. It was also found that even when light energy is below the band-gap there is still magnetization and a ferro-magnetic state is still possible. The effect of Coulomb interaction was found to be not much. It was interesting to find a linear dependence of critical temperature T_c on the coupling J^2.

In our system prior to the signing of light there are no extra electrons or holes. It will be interesting to include extra particles into the system by modifying the Hamiltonian and BCS wave function.

Appendix A

Bogoliubov-Valatin transformation

In this appendix we perform the Bogoliubov-Valatin transformation on our time-independent total Hamiltonian Eq.(3.119). The Hamiltonian is given as

$$\boxed{\tilde{H} = H_{kin} + H_c + \tilde{H}_L} \tag{A.1}$$

where

$$H_{kin} = \sum_{\vec{k},\sigma} (\epsilon_{c\vec{k}\sigma} c^{\dagger}_{\vec{k}\sigma} c_{\vec{k}\sigma} + \epsilon_{v\vec{k}\sigma} d^{\dagger}_{\vec{k}\sigma} d_{\vec{k}\sigma}) \tag{A.2}$$

$$H_c = H_{ee} + H_{hh} + H_{eh}$$

$$H_{ee} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} c^{\dagger}_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{A.3}$$

$$H_{hh} = \frac{1}{2} \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} d^{\dagger}_{\vec{k}+\vec{q}\sigma} d^{\dagger}_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} d_{\vec{k}\sigma} \tag{A.4}$$

$$H_{eh} = - \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} d^{\dagger}_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \tag{A.5}$$

$$\tilde{H}_L = \lambda \sum_{\vec{k}} \rho_k [(c^{\dagger}_{\vec{k}\uparrow} d^{\dagger}_{-\vec{k}\downarrow} + c^{\dagger}_{\vec{k}\downarrow} d^{\dagger}_{-\vec{k}\uparrow}) + h.c.] \tag{A.6}$$

$$\begin{aligned}
H_{ee} &= \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} c^{\dagger}_{\vec{k}+\vec{q}\sigma} c^{\dagger}_{\vec{k}'-\vec{q}\sigma'} c_{\vec{k}'\sigma'} c_{\vec{k}\sigma} \\
&= \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}} (c^{\dagger}_{\vec{k}+\vec{q},\uparrow} c^{\dagger}_{\vec{k}'-\vec{q}\uparrow} c_{\vec{k}'\uparrow} c_{\vec{k}\uparrow} \\
&+ \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}} (c^{\dagger}_{\vec{k}+\vec{q},\uparrow} c^{\dagger}_{\vec{k}'-\vec{q}\downarrow} c_{\vec{k}'\downarrow} c_{\vec{k}\uparrow} \\
&+ \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}} (c^{\dagger}_{\vec{k}+\vec{q},\downarrow} c^{\dagger}_{\vec{k}'-\vec{q}\uparrow} c_{\vec{k}'\uparrow} c_{\vec{k}\downarrow} \\
&+ \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}} (c^{\dagger}_{\vec{k}+\vec{q},\downarrow} c^{\dagger}_{\vec{k}'-\vec{q}\downarrow} c_{\vec{k}'\downarrow} c_{\vec{k}\downarrow}) \qquad \text{(A.7)}
\end{aligned}$$

We have

$$c_{k+q,\uparrow} = u_{k+q}\alpha_{k+q} - v_{k+q}\delta^{\dagger}_{-k-q} \qquad \text{(A.8)}$$

$$c^{\dagger}_{k+q,\uparrow} = u_{k+q}\alpha^{\dagger}_{k+q} - v_{k+q}\delta_{-k-q} \qquad \text{(A.9)}$$

$$c^{\dagger}_{k'-q,\uparrow} = u_{k'-q}\alpha^{\dagger}_{k'-q} - v_{k'-q}\delta_{-k'+q} \qquad \text{(A.10)}$$

$$c_{k',\uparrow} = u_{k'}\alpha_{k'} - v_{k'}\delta^{\dagger}_{-k'} \qquad \text{(A.11)}$$

$$c_{k,\uparrow} = u_{k}\alpha_{k} - v_{k}\delta^{\dagger}_{-k} \qquad \text{(A.12)}$$

After substituting the above creation and annhilation operators, the 1^{st} term of H_{ee} is given as

$$\begin{aligned}
1^{st} = \sum_{kk'q} V_q (u_{k+q}\alpha^{\dagger}_{k+q} - v_{k+q}\delta_{-k-q}) \\
\times(u_{k'-q}\alpha^{\dagger}_{k'-q} - v_{k'-q}\delta_{-k'+q}) \\
\times(u_{k'}\alpha_{k'} - v_{k'}\delta^{\dagger}_{-k'}) \\
\times(u_{k}\alpha_{k} - v_{k}\delta^{\dagger}_{-k}) \qquad \text{(A.13)}
\end{aligned}$$

$$= \sum_{kk'q} V_q (u_{k+q}u_{k'-q}\alpha^{\dagger}_{k+q}\alpha^{\dagger}_{k'-q} + v_{k+q}v_{k'-q}\delta_{-k-q}\delta_{-k'+q}$$

$$
\begin{aligned}
- & \quad u_{k'-q}v_{k+q}\delta_{-k-q}\alpha^{\dagger}_{k'-q} - u_{k+q}v_{k'-q}\alpha^{\dagger}_{k+q}\delta_{-k'+q}) \\
& \times(u_{k'}u_k\alpha_{k'}\alpha_k + v_{k'}v_k\delta^{\dagger}_{-k'}\delta^{\dagger}_{-k} - u_{k'}v_k\alpha_{k'}\delta^{\dagger}_{-k} - v_{k'}u_k\delta^{\dagger}_{-k'}\alpha_k) \quad \text{(A.14)}
\end{aligned}
$$

$$
\begin{aligned}
= & \quad \sum_{kk'q} V_q\{[u_{k+q}u_{k'-q}u_{k'}u_k\alpha^{\dagger}_{k+q}\alpha^{\dagger}_{k'-q}\alpha_{k'}\alpha_k \quad 1 \\
+ & \quad u_{k+q}u_{k'-q}v_{k'}v_k\alpha^{\dagger}_{k+q}\alpha^{\dagger}_{k'-q}\delta^{\dagger}_{-k'}\delta^{\dagger}_{-k} \quad 2 \\
- & \quad u_{k+q}u_{k'-q}u_{k'}v_k\alpha^{\dagger}_{k+q}\alpha^{\dagger}_{k'-q}\alpha_{k'}\delta^{\dagger}_{-k} \quad 3 \\
- & \quad u_{k+q}u_{k'-q}v_{k'}u_k\alpha^{\dagger}_{k+q}\alpha^{\dagger}_{k'-q}\delta^{\dagger}_{-k'}\alpha_k] \quad 4 \\
+ & \quad [v_{k+q}v_{k'-q}u_{k'}u_k\delta_{-k-q}\delta_{-k'+q}\alpha_{k'}\alpha_k \quad 5 \\
+ & \quad v_{k+q}v_{k'-q}v_{k'}v_k\delta_{-k-q}\delta_{-k'+q}\delta^{\dagger}_{-k'}\delta^{\dagger}_{-k} \quad 6 \\
- & \quad v_{k+q}v_{k'-q}u_{k'}v_k\delta_{-k-q}\delta_{-k'+q}\alpha_{k'}\delta^{\dagger}_{-k} \quad 7 \\
- & \quad v_{k+q}v_{k'-q}v_{k'}u_k\delta_{-k-q}\delta_{-k'+q}\delta^{\dagger}_{-k'}\alpha_k] \quad 8 \\
+ & \quad [-u_{k'-q}v_{k+q}u_{k'}u_k\delta_{-k-q}\alpha^{\dagger}_{k'-q}\alpha_{k'}\alpha_k \quad 9 \\
- & \quad u_{k'-q}v_{k+q}v_{k'}v_k\delta_{-k-q}\alpha^{\dagger}_{k'-q}\delta^{\dagger}_{-k'}\delta^{\dagger}_{-}k \quad 10 \\
+ & \quad u_{k'-q}v_{k+q}u_{k'}v_k\delta_{-k-q}\alpha^{\dagger}_{k'-q}\alpha_{k'}\delta^{\dagger}_{-}k \quad 11 \\
+ & \quad u_{k'-q}v_{k+q}v_{k'}u_k\delta_{-k-q}\alpha^{\dagger}_{k'-q}\delta^{\dagger}_{-k'}\alpha_k] \quad 12 \\
+ & \quad [-u_{k+q}v_{k'-q}v_{k'}u_k\alpha^{\dagger}_{k+q}\delta_{-k'+q}\alpha_{k'}\alpha_k \quad 13 \\
- & \quad u_{k+q}v_{k'-q}v_{k'}v_k\alpha^{\dagger}_{k+q}\delta_{-k'+q}\delta^{\dagger}_{-k'}\delta^{\dagger}_{-k} \quad 14 \\
+ & \quad u_{k+q}v_{k'-q}u_{k'}v_k\alpha^{\dagger}_{k+q}\delta_{-k'+q}\alpha_{k'}\delta^{\dagger}_{-k} \quad 15 \\
+ & \quad u_{k+q}v_{k'-q}v_{k'}u_k\alpha^{\dagger}_{k+q}\delta_{-k'+q}\delta^{\dagger}_{-k'}\alpha_k]\} \quad 16 \qquad \text{(A.15)}
\end{aligned}
$$

It can be easily seen that terms 7=8, 10=14,11=16,12=15. These terms along with term 6 are non zero. Other terms trivially give zero contribution. So

$$
\begin{aligned}
1^{st} = & \quad 2\sum_{kk'q} V_q\{u_{k'-q}v_{k+q}u_{k'}v_k\delta_{-k-q}\alpha^{\dagger}_{k'-q}\alpha_{k'}\delta^{\dagger}_{-k} \quad 11 = 16 \\
+ & \quad u_{k'-q}v_{k+q}v_{k'}u_k\delta_{-k-q}\alpha^{\dagger}_{k'-q}\delta^{\dagger}_{-k'}\alpha_k \quad 12 = 15
\end{aligned}
$$

$$
\begin{aligned}
&- \quad u_{k'-q}v_{k+q}v_{k'}v_k\delta_{-k-q}\alpha^\dagger_{k'-q}\delta^\dagger_{-k'}\delta^\dagger_{-k} \quad 10=14\\
&- \quad v_{k+q}v_{k'-q}v_{k'}u_k\delta_{-k-q}\delta_{-k'+q}\delta^\dagger_{-k'}\alpha_k \quad 7=8\\
&+ \quad \frac{1}{2}v_{k+q}v_{k'-q}v_{k'}v_k\delta_{-k-q}\delta_{-k'+q}\delta^\dagger_{-k'}\delta^\dagger_{-k}\} \quad 6\\
= \quad & 2\sum_{kk'q}V_q\{u_{k'-q}u_{k'}v_{k+q}v_k\delta_{-k-q}\delta^\dagger_{-k}\alpha^\dagger_{k'-q}\alpha_{k'}\\
&- \quad u_{k'-q}u_kv_{k+q}v_{k'}\delta_{-k-q}\delta^\dagger_{-k'}\alpha^\dagger_{k'-q}\alpha_k\\
&- \quad u_{k'-q}v_{k+q}v_{k'}v_k\delta_{-k-q}\alpha^\dagger_{k'-q}\delta^\dagger_{-k'}\delta^\dagger_{-k}\\
&- \quad v_{k+q}v_{k'-q}v_{k'}u_k\delta_{-k-q}\delta_{-k'+q}\delta^\dagger_{-k'}\alpha_k\\
&+ \quad \frac{1}{2}v_{k+q}v_{k'-q}v_{k'}v_k\delta_{-k-q}\delta_{-k'+q}\delta^\dagger_{-k'}\delta^\dagger_{-k}\}
\end{aligned}
\tag{A.16}
$$

$$
\begin{aligned}
= \quad & 2\sum_{kk'q}V_q\{u_{k'-q}u_{k'}v_{k+q}v_k(\delta_{k,k+q}-\delta^\dagger_{-k}\delta_{-k-q})\alpha^\dagger_{k'-q}\alpha_{k'}\\
&- \quad u_{k'-q}u_kv_{k+q}v_{k'}(\delta_{k',k+q}-\delta^\dagger_{-k'}\delta_{-k-q})\alpha^\dagger_{k'-q}\alpha_k\\
&+ \quad u_{k'-q}v_{k+q}v_{k'}v_k\alpha^\dagger_{k'-q}(\delta_{-k-q,-k'}-\delta^\dagger_{-k'}\delta_{-k-q})\delta^\dagger_{-k}\\
&- \quad v_{k+q}v_{k'-q}v_{k'}u_k\delta_{-k-q}(\delta_{k',k'-q}-\delta^\dagger_{-k'}\delta_{-k'+q})\alpha_k\\
&+ \quad \frac{1}{2}v_{k+q}v_{k'-q}v_{k'}v_k\delta_{-k-q}(\delta_{-k'+q,-k'-k'}-\delta^\dagger_{-k'}\delta_{-k'+q})\delta^\dagger_{-k}\}
\end{aligned}
\tag{A.17}
$$

First we simplify the first two terms. Then we simplify other three terms individually and then add them together. Then

$$
\begin{aligned}
1^{st} = \quad & 2(\sum_{kk'q}V_q\{u_{k'-q}u_{k'}v_{k+q}v_k\alpha^\dagger_{k'-q}\alpha_{k'}\delta_{k,k+q}\\
&- \quad u_{k'-q}u_kv_{k+q}v_{k'}\alpha^\dagger_{k'-q}\alpha_k\delta_{k',k+q}\}\\
&+ \quad \sum_{kk'q}V_q\{-u_{k'-q}u_{k'}v_{k+q}v_k\delta^\dagger_{-k}\delta_{-k-q}\alpha^\dagger_{k'-q}\alpha_{k'}\\
&+ \quad u_{k'-q}u_kv_{k+q}v_{k'}\delta^\dagger_{-k'}\delta_{-k-q}\alpha^\dagger_{k'-q}\alpha_k\\
&+ \quad Term3+Term4+\frac{1}{2}Term5\})\\
= \quad & 2\sum_{kk'}\{V_0u^2_{k'}v^2_k\alpha^\dagger_{k'}\alpha_{k'}
\end{aligned}
$$

$$
\begin{aligned}
&- \quad V_{k'-k} u_k^2 v_{k'}^2 \alpha_k^\dagger \alpha_k \\
&+ \quad Term3 + Term4 + \frac{1}{2} Term5\} \\
= \quad & 2 \sum_{kk'} \{ V_0 u_k^2 v_{k'}^2 \alpha_k^\dagger \alpha_k \\
&- \quad V_{k'-k} u_k^2 v_{k'}^2 \alpha_k^\dagger \alpha_k \\
&+ \quad Term3 + Term4 + \frac{1}{2} Term5\} \\
= \quad & 2 (\sum_{kk'} (V_0 - V_{k'-k}) \alpha_k^\dagger \alpha_k u_k^2 v_{k'}^2 \\
&+ \quad Term3 + Term4 + \frac{1}{2} Term5)
\end{aligned}
\tag{A.18}
$$

$$
\begin{aligned}
Term3 = \quad & 2 \sum_{kk'q} V_q u_{k'-q} v_{k+q} v_{k'} v_k \alpha_{k'-q}^\dagger (\delta_{-k-q,-k'} - \delta_{-k'}^\dagger \delta_{-k-q}) \delta_{-k}^\dagger \\
= \quad & 2 \sum_{kk'q} V_q \{ u_k v_{k'} v_{k'} v_k \alpha_k^\dagger \delta_{-k}^\dagger \\
+ \quad & u_{k'-q} v_{k+q} v_{k'} v_k \alpha_{k'-q}^\dagger \delta_{-k'}^\dagger (\delta_{-k-q,-k} - \delta_{-k}^\dagger \delta_{-k-q}) \} \\
= \quad & 2 \{ \sum_{kk'q} V_q v_{k'}^2 u_k v_k \alpha_k^\dagger \delta_{-k}^\dagger + \sum_{kk'} V_0 u_{k'} v_k v_{k'} v_k \alpha_{k'}^\dagger \delta_{-k'}^\dagger \} \\
= \quad & 2 \sum_{kk'q} V_q v_{k'}^2 u_k v_k \alpha_k^\dagger \delta_{-k}^\dagger
\end{aligned}
\tag{A.19}
$$

$$
\begin{aligned}
Term4 = \quad & -2 \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} u_k \{ \delta_{-k-q} (\delta_{k',k'-q} - \delta_{-k'}^\dagger \delta_{-k'+q}) \alpha_k \} \\
= \quad & 2 \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} u_k \{ -\delta_{-k-q} \alpha_k \delta_{k',k'-q} + \delta_{-k-q} \delta_{-k'}^\dagger \delta_{-k'+q} \alpha_k \} \\
= \quad & -2 \sum_{kk'} V_0 v_{k'}^2 u_k v_k \delta_{-k} \alpha_k \\
+ \quad & 2 \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} u_k (\delta_{k',k+q} - \delta_{-k'}^\dagger \delta_{-k-q}) \delta_{-k'+q} \alpha_k \\
= \quad & -2 \sum_{kk'} V_0 v_{k'}^2 u_k v_k \delta_{-k} \alpha_k \\
+ \quad & 2 \sum_{kk'q} V_{k,k'} v_{k'}^2 u_k v_k \delta_{-k} \alpha_k
\end{aligned}
$$

$$
\begin{aligned}
& - \quad 2\sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} u_k \delta^\dagger_{-k'} \delta_{-k-q} \delta_{-k'-q} \alpha_k \\
= & \quad 2\sum_{kk'} V_{k,k'} v^2_{k'} u_k v_k \delta_{-k} \alpha_k
\end{aligned} \tag{A.20}
$$

$$
\begin{aligned}
Term5 = & \quad \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} v_k \delta_{-k-q} \delta_{-k'+q} \delta^\dagger_{-k'} \delta^\dagger_{-k} \\
= & \quad \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} v_k \delta_{-k-q} (\delta_{-k'+q,-k'} - \delta^\dagger_{-k'} \delta_{-k'+q}) \delta^\dagger_{-k} \\
= & \quad \sum_{kk'q} V_0 v^2_k v^2_{k'} \delta_{-k} \delta^\dagger_{-k} \\
& - \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} v_k \delta_{-k-q} \delta^\dagger_{-k'} \delta_{-k'+q} \delta^\dagger_{-k} \\
= & \quad \sum_{kk'q} V_0 v^2_k v^2_{k'} \delta_{-k} \delta^\dagger_{-k} \\
& - \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} v_k (\delta_{-k-q,k'} - \delta^\dagger_{-k'} \delta_{-k-q}) \delta_{-k'+q} \delta^\dagger_{-k} \\
= & \quad \sum_{kk'q} V_0 v^2_k v^2_{k'} \delta_{-k} \delta^\dagger_{-k} \\
& - \sum_{kk'} V_{k,k'} v^2_{k'} v^2_k \delta_{-k} \delta^\dagger_{-k} \\
& + \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_{k'} v_k \delta^\dagger_{-k'} \delta_{-k-q} \delta_{-k'+q} \delta^\dagger_{-k} \\
= & \quad \sum_{kk'q} V_0 v^2_k v^2_{k'} \delta_{-k} \delta^\dagger_{-k} \\
& - \sum_{kk'} V_{k,k'} v^2_{k'} v^2_k \delta_{-k} \delta^\dagger_{-k} \\
& + \sum_{kk'} V_{k,k'} v_{k+q} v_{k'-q} v_{k'} v_k \delta^\dagger_{-k'} \delta_{-k-q} (\delta_{-k'+q,-k} - \delta^\dagger_{-k} \delta_{-k'+q}) \\
= & \quad \sum_{kk'q} V_0 v^2_k v^2_{k'} \delta_{-k} \delta^\dagger_{-k} \\
& - \sum_{kk'} V_{k,k'} v^2_{k'} v^2_k \delta_{-k} \delta^\dagger_{-k} \\
& + \sum_{kk'} V_{k,k'} v^2_{k'} v^2_k \delta^\dagger_{-k'} \delta_{-k'} \\
& - \sum_{kk'q} V_{k,k'} v_{k+q} v_{k'-q} v_{k'} v_k \delta^\dagger_{-k'} \delta_{-k-q} \delta^\dagger_{-k} \delta_{-k'+q}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \sum_{kk'q} V_0 v_k^2 v_{k'}^2 \delta_{-k}\delta^{\dagger}_{-k} \\
- \quad & \sum_{kk'} V_{k,k'} v_{k'}^2 v_k^2 \delta_{-k}\delta^{\dagger}_{-k} \\
+ \quad & \sum_{kk'} V_{k,k'} v_{k'}^2 v_k^2 \delta^{\dagger}_{-k'}\delta_{-k'} \\
- \quad & \sum_{kk'q} V_{k,k'} v_{k+q} v_{k'-q} v_{k'} v_k \delta^{\dagger}_{-k'}(\delta_{-k-q,-k} - \delta^{\dagger}_{-k}\delta_{-k-q})\delta_{-k'+q} \\
= \quad & \sum_{kk'q} V_0 v_k^2 v_{k'}^2 \delta_{-k}\delta^{\dagger}_{-k} \\
- \quad & \sum_{kk'} V_{k,k'} v_{k'}^2 v_k^2 (1 - \delta^{\dagger}_{-k}\delta_{-k}) \\
+ \quad & \sum_{kk'} V_{k,k'} v_{k'}^2 v_k^2 \delta^{\dagger}_{-k}\delta_{-k} \\
- \quad & \sum_{kk'q} V_0 v_k^2 v_{k'}^2 \delta^{\dagger}_{-k'}\delta_{-k'} \\
+ \quad & \sum_{kk'q} V_{k,k'} v_{k+q} v_{k'-q} v_{k'} v_k \delta^{\dagger}_{-k'}\delta^{\dagger}_{-k}\delta_{-k-q}\delta_{-k'+q} \\
= \quad & -\sum_{kk'} V_{k,k'} v_k^2 v_{k'}^2 \{1 - 2\delta^{\dagger}_{-k}\delta_{-k}\} \qquad \text{(A.21)}
\end{aligned}
$$

Therefore adding the terms we get

$$
1^{st} = -\sum_{kk'} V_{k,k'} \{ v_k^2 v_{k'}^2 + 2(u_k^2 v_{k'}^2 \alpha_k^{\dagger}\alpha_k - v_k^2 v_{k'}^2 \delta_k^{\dagger}\delta_k - v_{k'}^2 u_k v_k \alpha_k^{\dagger}\delta^{\dagger}_{-k} - v_{k'}^2 u_k v_k \delta_{-k}\alpha_k)\} \qquad \text{(A.22)}
$$

We do not write the V_0 terms. Since all the $V(q = 0)$ terms cancel each other. In our calculation we also do not write explicitely the four operator product terms when they are of the form $\alpha^{\dagger}\beta^{\dagger}\gamma\delta$ which we neglect.

We have

$$c_{k+q,\uparrow} = u_{k+q}\alpha_{k+q} - v_{k+q}\delta^{\dagger}_{-k-q} \tag{A.23}$$

$$c^{\dagger}_{k+q,\uparrow} = u_{k+q}\alpha^{\dagger}_{k+q} - v_{k+q}\delta_{-k-q} \tag{A.24}$$

$$c_{k'-q,\downarrow} = \bar{u}_{k'-q}\gamma_{k'-q} - \bar{v}_{k'-q}\beta^{\dagger}_{-k'+q} \tag{A.25}$$

$$c^{\dagger}_{k'-q,\downarrow} = \bar{u}_{k'-q}\gamma^{\dagger}_{k'-q} - \bar{v}_{k'-q}\beta_{-k'+q} \tag{A.26}$$

$$c_{k',\downarrow} = \bar{u}_{k'}\gamma_{k'} - \bar{v}_{k'}\beta^{\dagger}_{-k'} \tag{A.27}$$

$$c_{k,\uparrow} = u_k\alpha_k - v_k\delta^{\dagger}_{-k} \tag{A.28}$$

The 2^{nd} term of H_{ee} is given as

$$\begin{aligned} 2^{nd} = \sum_{kk'q} V_q(u_{k+q}\alpha^{\dagger}_{k+q} - v_{k+q}\delta_{-k-q}) \\ \times(\bar{u}_{k'-q}\gamma^{\dagger}_{k'-q} - \bar{v}_{k'-q}\beta_{-k'+q}) \\ \times(\bar{u}_{k'}\gamma_{k'} - \bar{v}_{k'}\beta^{\dagger}_{-k'}) \\ \times(u_k\alpha_k - v_k\delta^{\dagger}_{-k}) \end{aligned} \tag{A.29}$$

$$\begin{aligned} = & \sum_{kk'q} V_q(u_{k+q}\bar{u}_{k'-q}\alpha^{\dagger}_{k+q}\gamma^{\dagger}_{k'-q} + v_{k+q}\bar{v}_{k'-q}\delta_{-k-q}\beta_{-k'+q} \\ - & u_{k+q}\bar{v}_{k'-q}\alpha^{\dagger}_{k+q}\beta_{-k'+q} - \bar{u}_{k'-q}v_{k+q}\delta_{-k-q}\gamma^{\dagger}_{k'-q}) \\ & (\bar{u}_{k'}u_k\gamma_{k'}\alpha_k + \bar{v}_{k'}v_k\beta^{\dagger}_{-k'}\delta^{\dagger}_{-k} - \bar{u}_{k'}v_k\gamma_{k'}\delta^{\dagger}_{-k} - u_k\bar{v}_{k'}\beta^{\dagger}_{-k'}\alpha_k) \end{aligned} \tag{A.30}$$

$$\begin{aligned} = & \sum_{kk'q} V_q\{[u_{k+q}\bar{u}_{k'-q}\bar{u}_{k'}u_k\alpha^{\dagger}_{k+q}\gamma^{\dagger}_{k'-q}\gamma_{k'}\alpha_k \\ + & u_{k+q}\bar{u}_{k'-q}\bar{v}_{k'}v_k\alpha^{\dagger}_{k+q}\gamma^{\dagger}_{k'-q}\beta^{\dagger}_{-k'}\delta^{\dagger}_{-k} \\ - & u_{k+q}\bar{u}_{k'-q}\bar{u}_{k'}v_k\alpha^{\dagger}_{k+q}\gamma^{\dagger}_{k'-q}\gamma_{k'}\delta^{\dagger}_{-k} \\ - & u_{k+q}\bar{u}_{k'-q}u_k\bar{v}_{k'}\alpha^{\dagger}_{k+q}\gamma^{\dagger}_{k'-q}\beta^{\dagger}_{-k'}\alpha_k] \\ + & [v_{k+q}\bar{v}_{k'-q}\bar{u}_{k'}u_k\delta_{-k-q}\beta_{-k'+q}\gamma_{k'}\alpha_k \end{aligned}$$

$$
\begin{aligned}
&+ \quad v_{k+q}\bar{v}_{k'-q}\bar{v}_{k'}v_k\delta_{-k-q}\beta_{-k'+q}\beta^\dagger_{-k'}\delta^\dagger_{-k} \\
&- \quad v_{k+q}\bar{v}_{k'-q}\bar{u}_{k'}v_k\delta_{-k-q}\beta_{-k'+q}\gamma_{k'}\delta^\dagger_{-k} \\
&- \quad v_{k+q}\bar{v}_{k'-q}u_k\bar{v}_{k'}\delta_{-k-q}\beta_{-k'+q}\beta^\dagger_{-k'}\alpha_k] \\
&+ \quad [-u_{k+q}\bar{v}_{k'-q}\bar{u}_{k'}u_k\alpha^\dagger_{k+q}\beta_{-k'+q}\gamma_{k'}\alpha_k \\
&- \quad u_{k+q}\bar{v}_{k'-q}\bar{v}_{k'}v_k\alpha^\dagger_{k+q}\beta_{-k'+q}\beta^\dagger_{-k'}\delta^\dagger_{-k} \\
&+ \quad u_{k+q}\bar{v}_{k'-q}\bar{u}_{k'}v_k\alpha^\dagger_{k+q}\beta_{-k'+q}\gamma_{k'}\delta^\dagger_{-k} \\
&+ \quad u_{k+q}\bar{v}_{k'-q}u_k\bar{v}_{k'}\alpha^\dagger_{k+q}\beta_{-k'+q}\beta^\dagger_{-k'}\alpha_k] \\
&+ \quad [-\bar{u}_{k'-q}v_{k+q}\bar{u}_{k'}u_k\delta_{-k-q}\gamma^\dagger_{k'-q}\gamma_{k'}\alpha_k \\
&- \quad \bar{u}_{k'-q}v_{k+q}\bar{v}_{k'}v_k\delta_{-k-q}\gamma^\dagger_{k'-q}\beta^\dagger_{-k'}\delta^\dagger_{-k} \\
&+ \quad \bar{u}_{k'-q}v_{k+q}\bar{u}_{k'}v_k\delta_{-k-q}\gamma^\dagger_{k'-q}\gamma_{k'}\delta^\dagger_{-k} \\
&+ \quad \bar{u}_{k'-q}v_{k+q}u_k\bar{v}_{k'}\delta_{-k-q}\gamma^\dagger_{k'-q}\beta^\dagger_{-k'}\alpha_k]\} \qquad \text{(A.31)}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \sum_{kk'q} V_q[v_{k+q}\bar{v}_{k'-q}\bar{v}_{k'}v_k\delta_{-k-q}\beta_{-k'+q}\beta^\dagger_{-k'}\delta^\dagger_{-k} \\
&- \quad v_{k+q}\bar{v}_{k'-q}\bar{u}_{k'}v_k\delta_{-k-q}\beta_{-k'+q}\gamma_{k'}\delta^\dagger_{-k} \\
&- \quad v_{k+q}\bar{v}_{k'-q}u_k\bar{v}_{k'}\delta_{-k-q}\beta_{-k'+q}\beta^\dagger_{-k'}\alpha_k \\
&- \quad u_{k+q}\bar{v}_{k'-q}\bar{v}_{k'}v_k\alpha^\dagger_{k+q}\beta_{-k'+q}\beta^\dagger_{-k'}\delta^\dagger_{-k} \\
&+ \quad u_{k+q}\bar{v}_{k'-q}u_k\bar{v}_{k'}\alpha^\dagger_{k+q}\beta_{-k'+q}\beta^\dagger_{-k'}\alpha_k \\
&- \quad \bar{u}_{k'-q}v_{k+q}\bar{v}_{k'}v_k\delta_{-k-q}\gamma^\dagger_{k'-q}\beta^\dagger_{-k'}\delta^\dagger_{-k} \\
&+ \quad \bar{u}_{k'-q}v_{k+q}\bar{u}_{k'}v_k\delta_{-k-q}\gamma^\dagger_{k'-q}\gamma_{k'}\delta^\dagger_{-k}] \qquad \text{(A.32)}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \sum_{kk'q} V_q[v_{k+q}\bar{v}_{k'-q}\bar{v}_{k'}v_k(\delta_{-k-q,-k} - \delta^\dagger_{-k}\delta_{-k-q})(\delta_{-k'+q,-k'} - \beta^\dagger_{-k'}\beta_{-k'+q}) \\
- \quad & v_{k+q}\bar{v}_{k'-q}\bar{u}_{k'}v_k(\delta_{-k-q,-k} - \delta^\dagger_{-k}\delta_{-k-q})\beta_{-k'+q}\gamma_{k'} \\
- \quad & v_{k+q}\bar{v}_{k'-q}u_k\bar{v}_{k'}(\delta_{-k'+q,-k'} - \beta^\dagger_{-k'}\beta_{-k'+q})\delta_{-k-q}\alpha_k \\
- \quad & u_{k+q}\bar{v}_{k'-q}\bar{v}_{k'}v_k(\delta_{-k'+q,-k'} - \beta^\dagger_{-k'}\beta_{-k'+q})\alpha^\dagger_{k+q}\delta^\dagger_{-k} \\
+ \quad & u_{k+q}\bar{v}_{k'-q}u_k\bar{v}_{k'}(\delta_{-k'+q,-k'} - \beta^\dagger_{-k'}\beta_{-k'+q})\alpha^\dagger_{k+q}\alpha_k
\end{aligned}
$$

$$
\begin{aligned}
- \quad & \bar{u}_{k'-q} v_{k+q} \bar{v}_{k'} v_k (\delta_{-k-q,-k} - \delta^\dagger_{-k} \delta_{-k-q}) \gamma^\dagger_{k'-q} \beta^\dagger_{-k'} \\
+ \quad & \bar{u}_{k'-q} v_{k+q} \bar{u}_{k'} v_k (\delta_{-k-q,-k} - \delta^\dagger_{-k} \delta_{-k-q}) \gamma^\dagger_{k'-q} \gamma_{k'}]
\end{aligned} \tag{A.33}
$$

We can easily see that all these terms contribute terms with $V_{q=0}$. We do not include these terms.

Since the 3^{rd} term in H_{ee} is structurally similar to the 2^{nd} term this will also contribute terms with $V_{q=0}$. We again do not include these terms.

The 4^{th} term in H_{ee} is given as

$$
\sum_{kk'q} V(q) c^\dagger_{k+q,\downarrow} c^\dagger_{k'-q,\downarrow} c_{k',\downarrow} c_{k,\downarrow} \tag{A.34}
$$

where

$$
c^\dagger_{k+q,\downarrow} = \bar{u}_{k+q} \gamma^\dagger_{k+q} - \bar{v}_{k+q} \beta_{-k-q} \tag{A.35}
$$

$$
c^\dagger_{k'-q,\downarrow} = \bar{u}_{k'-q} \gamma^\dagger_{k'-q} - \bar{v}_{k'-q} \beta_{-k'+q} \tag{A.36}
$$

$$
c_{k',\downarrow} = \bar{u}_{k'} \gamma_{k'} - \bar{v}_{k'} \beta^\dagger_{-k'} \tag{A.37}
$$

$$
c_{k,\downarrow} = \bar{u}_k \gamma_k - \bar{v}_k \beta^\dagger_{-k} \tag{A.38}
$$

If we compare with the 1^{st} term of the H_{ee} interaction we will see that in the above equation the structure is same. To get the transformed terms , we have to identify $u \to \bar{u}, \;\; v \to \bar{v}, \;\; \alpha \to \gamma, \;\; and \;\; \delta \to \beta$. Then it is easy to write down the transformed 4^{th} term as

$$
4^{th} = -\sum_{kk'} V_{k,k'} \{ \bar{v}_k^2 \bar{v}_{k'}^2 + 2(\bar{u}_k^2 \bar{v}_{k'}^2 \gamma^\dagger_k \gamma_k - \bar{v}_k^2 \bar{v}_{k'}^2 \beta^\dagger_k \beta_k - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k \gamma^\dagger_k \beta^\dagger_{-k} - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k \beta_{-k} \gamma_k) \} \tag{A.39}
$$

Now adding all the H_{ee} terms, that is the 1^{st} term and 4^{th} term we get

$$
\begin{aligned}
H^T_{ee} = \quad & -\sum_{kk'} V_{k,k'} \{ v_k^2 v_{k'}^2 + 2(u_k^2 v_{k'}^2 \alpha^\dagger_k \alpha_k - v_k^2 v_{k'}^2 \delta^\dagger_k \delta_k - v_{k'}^2 u_k v_k \alpha^\dagger_k \delta^\dagger_{-k} - v_{k'}^2 u_k v_k \delta_{-k} \alpha_k) \} \\
& -\sum_{kk'} V_{k,k'} \{ \bar{v}_k^2 \bar{v}_{k'}^2 + 2(\bar{u}_k^2 \bar{v}_{k'}^2 \gamma^\dagger_k \gamma_k - \bar{v}_k^2 \bar{v}_{k'}^2 \beta^\dagger_k \beta_k - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k \gamma^\dagger_k \beta^\dagger_{-k} - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k \beta_{-k} \gamma_k) \}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & -2\sum_{kk'} V_{k,k'}\{\frac{1}{2}(v_k^2 v_{k'}^2 + \bar{v}_k^2\bar{v}_{k'}^2) + u_k^2 v_{k'}^2 \alpha_k^\dagger\alpha_k + \bar{u}_k^2\bar{v}_{k'}^2\gamma_k^\dagger\gamma_k - v_k^2 v_{k'}^2\delta_k^\dagger\delta_k - \bar{v}_k^2\bar{v}_{k'}^2\beta_k^\dagger\beta_k \\
& -v_{k'}^2 u_k v_k(\delta_{-k}\alpha_k + \alpha_k^\dagger\delta_{-k}^\dagger) - \bar{v}_{k'}^2\bar{u}_k\bar{v}_k(\beta_{-k}\gamma_k + \gamma_k^\dagger\beta_{-k}^\dagger)\} \qquad (A.40)
\end{aligned}
$$

Now the hole-hole interaction part of Hamiltonian is given as

$$
\begin{aligned}
H_{hh} &= \sum_{\vec{k},\vec{k}',\vec{q},\sigma,\sigma'} V_{\vec{q}} d^\dagger_{\vec{k}+\vec{q}\sigma} d^\dagger_{\vec{k}'-\vec{q}\sigma'} d_{\vec{k}'\sigma'} d_{\vec{k}\sigma} \\
&= \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}}(d^\dagger_{\vec{k}+\vec{q},\uparrow} d^\dagger_{\vec{k}'-\vec{q}\uparrow} d_{\vec{k}'\uparrow} d_{\vec{k}\uparrow} \\
&+ \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}}(d^\dagger_{\vec{k}+\vec{q},\uparrow} d^\dagger_{\vec{k}'-\vec{q}\downarrow} d_{\vec{k}'\downarrow} d_{\vec{k}\uparrow} \\
&+ \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}}(d^\dagger_{\vec{k}+\vec{q},\downarrow} d^\dagger_{\vec{k}'-\vec{q}\uparrow} d_{\vec{k}'\uparrow} d_{\vec{k}\downarrow} \\
&+ \sum_{\vec{k},\vec{k}',\vec{q}} V_{\vec{q}}(d^\dagger_{\vec{k}+\vec{q},\downarrow} d^\dagger_{\vec{k}'-\vec{q}\downarrow} d_{\vec{k}'\downarrow} c_{\vec{k}\downarrow}) \qquad (A.41)
\end{aligned}
$$

Let us now transform the first term of H_{hh} interaction. We have

$$d_{k+q,\uparrow} = \bar{u}_{k+q}\beta_{k+q} + \bar{v}_{k+q}\gamma^\dagger_{-k-q} \qquad (A.42)$$

$$d^\dagger_{k+q,\uparrow} = \bar{u}_{k+q}\beta^\dagger_{k+q} + \bar{v}_{k+q}\gamma_{-k-q} \qquad (A.43)$$

$$d^\dagger_{k'-q,\uparrow} = \bar{u}_{k'-q}\beta^\dagger_{k'-q} + \bar{v}_{k'-q}\gamma_{-k'+q} \qquad (A.44)$$

$$d_{k',\uparrow} = \bar{u}_{k'}\beta_{k'} + \bar{v}_{k'}\gamma^\dagger_{-k'} \qquad (A.45)$$

$$d_{k,\uparrow} = \bar{u}_k\beta_k + \bar{v}_k\gamma^\dagger_{-k} \qquad (A.46)$$

If we compare with the 1^{st} term of the H_{ee} interaction we will see that in the above equation the structure is same. To get the transfromed terms , we have to identify $u \to \bar{u}, \quad v \to -\bar{v}, \quad \alpha \to \beta, \quad and \quad \delta \to \gamma$. Then it is easy to write down the transformed 1^{st} term as

$$1^{st} = -\sum_{kk'} V_{k,k'}\{\bar{v}_k^2\bar{v}_{k'}^2 + 2(\bar{u}_k^2\bar{v}_{k'}^2\beta_k^\dagger\beta_k - \bar{v}_k^2\bar{v}_{k'}^2\gamma_k^\dagger\gamma_k + \bar{v}_{k'}^2\bar{u}_k\bar{v}_k\beta_k^\dagger\gamma_{-k}^\dagger + \bar{v}_{k'}^2\bar{u}_k\bar{v}_k\gamma_{-k}\beta_k)\} \qquad (A.47)$$

As in the electron-electron part here in the hole-hole part the second and third terms will give $V_{q=0}$ terms which we will discard.

Let us now transform the 4^{th} term of H_{hh} interaction. We have

$$d_{k+q,\downarrow} = u_{k+q}\delta_{k+q} + v_{k+q}\alpha^{\dagger}_{-k-q} \tag{A.48}$$

$$d^{\dagger}_{k+q,\downarrow} = u_{k+q}\delta^{\dagger}_{k+q} + v_{k+q}\alpha_{-k-q} \tag{A.49}$$

$$d^{\dagger}_{k'-q,\downarrow} = u_{k'-q}\delta^{\dagger}_{k'-q} + v_{k'-q}\alpha_{-k'+q} \tag{A.50}$$

$$d_{k',\downarrow} = u_{k'}\delta_{k'} + v_{k'}\alpha^{\dagger}_{-k'} \tag{A.51}$$

$$d_{k,\downarrow} = u_{k}\delta_{k} + v_{k}\alpha^{\dagger}_{-k} \tag{A.52}$$

If we compare with the 4^{th} term of the H_{ee} interaction we will see that in the above equation the structure is same. To get the transformed terms , we have to identify $\bar{u} \to u, \quad \bar{v} \to -v, \quad \gamma \to \delta, \quad and \quad \beta \to \alpha$. Then it is easy to write down the transformed 4^{th} term as

$$4^{th} = -\sum_{kk'} V_{k,k'}\{v_k^2 v_{k'}^2 + 2(u_k^2 v_{k'}^2 \delta^{\dagger}_k \delta_k - v_k^2 v_{k'}^2 \alpha^{\dagger}_k \alpha_k + v_{k'}^2 u_k v_k \delta^{\dagger}_k \alpha^{\dagger}_{-k} + v_{k'}^2 u_k v_k \alpha_{-k}\delta_k)\} \tag{A.53}$$

Now adding all the H_{hh} terms, that is the I^{st} term and 4^{th} term we get

$$\begin{aligned}
H_{hh}^T = & -\sum_{kk'} V_{k,k'}\{\bar{v}_k^2\bar{v}_{k'}^2 + 2(\bar{u}_k^2\bar{v}_{k'}^2\beta_k^\dagger\beta_k - \bar{v}_k^2\bar{v}_{k'}^2\gamma_k^\dagger\gamma_k + \bar{v}_{k'}^2\bar{u}_k\bar{v}_k\beta_k^\dagger\gamma_{-k}^\dagger + \bar{v}_{k'}^2\bar{u}_k\bar{v}_k\gamma_{-k}\beta_k)\} \\
- & \sum_{kk'} V_{k,k'}\{v_k^2 v_{k'}^2 + 2(u_k^2 v_{k'}^2\delta_k^\dagger\delta_k - v_k^2 v_{k'}^2\alpha_k^\dagger\alpha_k + v_{k'}^2 u_k v_k\delta_k^\dagger\alpha_{-k}^\dagger + v_{k'}^2 u_k v_k\alpha_{-k}\delta_k)\} \\
= & -2\sum_{kk'} V_{k,k'}\{\frac{1}{2}(\bar{v}_k^2\bar{v}_{k'}^2 + v_k^2 v_{k'}^2) + \bar{u}_k^2\bar{v}_{k'}^2\beta_k^\dagger\beta_k + u_k^2 v_{k'}^2\delta_k^\dagger\delta_k - \bar{v}_k^2\bar{v}_{k'}^2\gamma_k^\dagger\gamma_k - v_k^2 v_{k'}^2\alpha_k^\dagger\alpha_k \\
& +\bar{v}_{k'}^2\bar{u}_k\bar{v}_k(\beta_k^\dagger\gamma_{-k}^\dagger + \gamma_{-k}\beta_k) + v_{k'}^2 u_k v_k(\delta_k^\dagger\alpha_{-k}^\dagger + \alpha_{-k}\delta_k)\} \qquad \text{(A.54)}
\end{aligned}$$

Now let us write down the electron-hole part of the interaction. It is given as

$$\begin{aligned}
H_{eh} &= -2\sum_{kk'q,\sigma\sigma'} V_q c_{k+q,\sigma}^\dagger d_{k'-q,\sigma'}^\dagger d_{k',\sigma'} c_{k\sigma} \\
&= -2\sum_{kk'q,\sigma\sigma'} V_q\{c_{k+q,\uparrow}^\dagger d_{k'-q,\downarrow}^\dagger d_{k'\downarrow} c_{k\uparrow} + c_{k+q,\downarrow}^\dagger d_{k'-q,\uparrow}^\dagger d_{k'\uparrow} c_{k\downarrow}\} \qquad \text{(A.55)}
\end{aligned}$$

We know that

$$c_{k+q,\uparrow}^\dagger = u_{k+q}\alpha_{k+q}^\dagger - v_{k+q}\delta_{-k-q} \qquad \text{(A.56)}$$

$$d_{k'-q,\downarrow}^\dagger = u_{k'-q}\delta_{k'-q}^\dagger + v_{k'-q}\alpha_{-k'+q} \qquad \text{(A.57)}$$

$$d_{k',\downarrow} = u_{k'}\delta_{k'}^\dagger + v_{k'}\alpha_{-k'} \qquad \text{(A.58)}$$

$$c_{k,\uparrow} = u_k\alpha_k - v_k\delta_{-k}^\dagger \qquad \text{(A.59)}$$

Let us transform the 1^{st} term of the electron-hole part of interaction.

$$\begin{aligned}
1^{st} &= \sum_{kk'q,\sigma\sigma'} V_q c_{k+q,\uparrow}^\dagger d_{k'-q,\downarrow}^\dagger d_{k'\downarrow} c_{k\uparrow} \\
&= \sum_{kk'q} V_q(u_{k+q}\alpha_{k+q}^\dagger - v_{k+q}\delta_{-k-q}) \\
&\times(u_{k'-q}\delta_{k'-q}^\dagger + v_{k'-q}\alpha_{-k'+q}) \\
&\times(u_{k'}\delta_{k'} + v_{k'}\alpha_{-k'}^\dagger) \\
&\times(u_k\alpha_k - v_k\delta_{-k}^\dagger) \qquad \text{(A.60)}
\end{aligned}$$

$$
\begin{aligned}
= \quad & \sum_{kk'q} V_q (u_{k+q} u_{k'-q} \alpha^\dagger_{k+q} \delta^\dagger_{k'-q} - v_{k+q} v_{k'-q} \delta_{-k-q} \alpha_{-k'+q} \\
& - u_{k'-q} v_{k+q} \delta_{-k-q} \delta^\dagger_{k'-q} + u_{k+q} v_{k'-q} \alpha^\dagger_{k+q} \alpha_{-k'+q}) \\
& \times (u_k u_{k'} \delta_{k'} \alpha_k - v_k v_{k'} \alpha^\dagger_{-k'} \delta^\dagger_{-k} + u_k v_{k'} \alpha^\dagger_{-k'} \alpha_k - u_{k'} v_k \delta_{k'} \delta^\dagger_{-k}) \qquad \text{(A.61)}
\end{aligned}
$$

$$
\begin{aligned}
= \quad & \sum_{kk'q} V_q \{ [u_{k+q} u_{k'-q} u_k u_{k'} \alpha^\dagger_{k+q} \delta^\dagger_{k'-q} \delta_{k'} \alpha_k \\
& - u_{k+q} u_{k'-q} v_k v_{k'} \alpha^\dagger_{k+q} \delta^\dagger_{k'-q} \alpha^\dagger_{-k'} \delta^\dagger_{-k} \\
& + u_{k+q} u_{k'-q} u_k v_{k'} \alpha^\dagger_{k+q} \delta^\dagger_{k'-q} \alpha^\dagger_{-k'} \alpha_k \\
& - u_{k+q} u_{k'-q} u_{k'} v_k \alpha^\dagger_{k+q} \delta^\dagger_{k'-q} \delta_{k'} \delta^\dagger_{-k}] \\
& + [- v_{k+q} v_{k'-q} u_k u_{k'} \delta_{-k-q} \alpha_{-k'+q} \delta_{k'} \alpha_k \\
& + v_{k+q} v_{k'-q} v_k v_{k'} \delta_{-k-q} \alpha_{-k'+q} \alpha^\dagger_{-k'} \delta^\dagger_{-k} \\
& - v_{k+q} v_{k'-q} u_k v_{k'} \delta_{-k-q} \alpha_{-k'+q} \alpha^\dagger_{-k'} \alpha_k \\
& + v_{k+q} v_{k'-q} u_{k'} v_k \delta_{-k-q} \alpha_{-k'+q} \delta_{k'} \delta^\dagger_{-k}] \\
& + [- u_{k'-q} v_{k+q} u_k u_{k'} \delta_{-k-q} \delta^\dagger_{k'-q} \delta_{k'} \alpha_k \\
& + u_{k'-q} v_{k+q} v_k v_{k'} \delta_{-k-q} \delta^\dagger_{k'-q} \alpha^\dagger_{-k'} \delta^\dagger_{-k} \\
& - u_{k'-q} v_{k+q} u_k v_{k'} \delta_{-k-q} \delta^\dagger_{k'-q} \alpha^\dagger_{-k'} \alpha_k \\
& + u_{k'-q} v_{k+q} u_{k'} v_k \delta_{-k-q} \delta^\dagger_{k'-q} \delta_{k'} \delta^\dagger_{-k}] \\
& + [+ u_{k+q} v_{k'-q} u_k u_{k'} \alpha^\dagger_{k+q} \alpha_{-k'+q} \delta_{k'} \alpha_k \\
& - u_{k+q} v_{k'-q} v_k v_{k'} \alpha^\dagger_{k+q} \alpha_{-k'+q} \alpha^\dagger_{-k'} \delta^\dagger_{-k} \\
& + u_{k+q} v_{k'-q} u_k v_{k'} \alpha^\dagger_{k+q} \alpha_{-k'+q} \alpha^\dagger_{-k'} \alpha_k \\
& - u_{k+q} v_{k'-q} u_{k'} v_k \alpha^\dagger_{k+q} \alpha_{-k'+q} \delta_{k'} \delta^\dagger_{-k}] \} \qquad \text{(A.62)}
\end{aligned}
$$

$$
= \quad \sum_{kk'q} V_q (- u_{k+q} u_{k'-q} u_{k'} v_k \alpha^\dagger_{k+q} \delta^\dagger_{k'-q} \delta_{k'} \delta^\dagger_{-k}
$$

$$+v_{k+q}v_{k'-q}v_kv_{k'}\delta_{-k-q}\alpha_{-k'+q}\alpha^\dagger_{-k'}\delta^\dagger_{-k}$$
$$+v_{k+q}v_{k'-q}u_{k'}v_k\delta_{-k-q}\alpha_{-k'+q}\delta_{k'}\delta^\dagger_{-k}$$
$$-u_{k'-q}v_{k+q}u_ku_{k'}\delta_{-k-q}\delta^\dagger_{k'-q}\delta_{k'}\alpha_k$$
$$+u_{k'-q}v_{k+q}v_kv_{k'}\delta_{-k-q}\delta^\dagger_{k'-q}\alpha^\dagger_{-k'}\delta^\dagger_{-k}$$
$$-u_{k'-q}v_{k+q}u_kv_{k'}\delta_{-k-q}\delta^\dagger_{k'-q}\alpha^\dagger_{-k'}\alpha_k$$
$$+u_{k'-q}v_{k+q}u_{k'}v_k\delta_{-k-q}\delta^\dagger_{k'-q}\delta_{k'}\delta^\dagger_{-k}$$
$$-u_{k+q}v_{k'-q}u_{k'}v_k\alpha^\dagger_{k+q}\alpha_{-k'+q}\delta_{k'}\delta^\dagger_{-k}) \tag{A.63}$$

$$\begin{aligned} = \quad & \sum_{kk'q} V_q\{-u_{k+q}u_{k'-q}u_{k'}v_k\alpha^\dagger_{k+q}\delta^\dagger_{k'-q}(\delta_{k',-k}-\delta^\dagger_{-k}\delta_{k'}) \\ & +v_{k+q}v_{k'-q}v_kv_{k'}\delta_{-k-q}\delta^\dagger_{-k}\alpha_{-k'+q}\alpha^\dagger_{-k'} \\ & +v_{k+q}v_{k'-q}u_{k'}v_k\delta_{-k-q}\alpha_{-k'+q}(\delta_{k',-k}-\delta^\dagger_{-k}\delta_{k'}) \\ & -u_{k'-q}v_{k+q}u_ku_{k'}(\delta_{-k,k'}-\delta^\dagger_{k'-q}\delta_{-k-q})\delta_{k'}\alpha_k \\ & +u_{k'-q}v_{k+q}v_kv_{k'}(\delta_{-k,k'}-\delta^\dagger_{k'-q}\delta_{-k-q})(-\delta^\dagger_{-k}\alpha^\dagger_{-k'}) \\ & -u_{k'-q}v_{k+q}u_kv_{k'}(\delta_{-k,k'}-\delta^\dagger_{k'-q}\delta_{-k-q})\alpha^\dagger_{-k'}\alpha_k \\ & +u_{k'-q}v_{k+q}u_{k'}v_k(\delta_{-k,k'}-\delta^\dagger_{k'-q}\delta_{-k-q})\delta_{k'}\delta^\dagger_{-k} \\ & -u_{k+q}v_{k'-q}u_{k'}v_k\alpha^\dagger_{k+q}\alpha_{-k'+q}(\delta_{-k,k'}-\delta^\dagger_{k'}\delta_{-k}) \end{aligned} \tag{A.64}$$

Now let us simplify term by term individually,

$$\begin{aligned} Term1 = \quad & -\sum_{kk'q} V_q u_{k+q}u_{k'-q}u_{k'}v_k\alpha^\dagger_{k+q}\delta^\dagger_{k'-q}(\delta_{k',-k}-\delta^\dagger_{-k}\delta_{k'}) \\ = \quad & -\sum_{kk'q} V_q u_{k+q}u_{k'-q}u_{-k}v_k\alpha^\dagger_{k+q}\delta^\dagger_{k'-q} \end{aligned} \tag{A.65}$$

Now let us take $q = k' - k$, then

$$Term1 = -\sum_{kk'q} V_q u_{k'}u_{-k'}u_{-k}v_k\alpha^\dagger_{k'}\delta^\dagger_{-k'} \tag{A.66}$$

Now we take $k \to k'$ and $k' \to k$

$$Term1 = -\sum_{kk'q} V_q u_k u_{-k} u_{-k'} v_{k'} \alpha_k^\dagger \delta_{-k}^\dagger \tag{A.67}$$

The $Term2$ is given as

$$\begin{aligned} Term2 = & \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_k v_{k'} \delta_{-k-q} \delta^\dagger_{-k} \alpha_{-k'+q} \alpha^\dagger_{-k'} \\ = & \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_k v_{k'} (\delta_{-k-q,-k} - \delta^\dagger_k \delta_{-k-q})(\delta_{-k'+q,-k'} \alpha^\dagger_{-k'} \alpha_{-k'+q}) \\ = & \sum_{kk'q} V_q v_{k+q} v_{k'-q} v_k v_{k'} (\delta_{-k-q,-k} \delta_{-k'+q,-k'} - \alpha^\dagger_{-k'} \alpha_{-k'+q} \delta_{-k-q,-k} \\ & - \delta^\dagger_k \delta_{-k-q} \delta_{-k'+q,-k'}) \\ = & \sum_{kk'q} V_0 (v_k v_{k'} v_k v_{k'} - v_k v_{k'} v_k v_{k'} \alpha^\dagger_{-k'} \alpha_{-k'} - \delta^\dagger_{-k} \delta_{-k}) \end{aligned} \tag{A.68}$$

The $Term3$ is given as

$$\begin{aligned} Term3 = & \sum_{kk'q} V_q v_{k+q} v_{k'-q} u_{k'} v_k \delta_{-k-q} \alpha_{-k'+q} (\delta_{k',-k} - \delta^\dagger_{-k} \delta_{k'}) \\ & = \sum_{kk'q} V_q v_{k+q} v_{-k-q} u_{-k} v_k \delta_{-k-q} \alpha_{k+q} \\ & - \sum_{kk'q} V_q v_{k+q} v_{k'-q} u_{k'} v_k \delta_{-k-q} \delta^\dagger_{-k} \delta_{k'} \alpha_{-k'+q} \\ & = \sum_{kk'} V_{k-k'} v_k v_{-k'} u_{k'} v_{k'} \delta_{-k} \alpha_k \\ & - \sum_{kk'q} V_q v_{k+q} v_{k'-q} u_{k'} v_k (\delta_{-k-q,-k} - \delta^\dagger_{-k} \delta_{-k-q}) \delta_{k'} \alpha_{-k'+q} \\ & = \sum_{kk'q} V_{k-k'} v_k v_{-k} u_{-k'} v_{k'} \delta_{-k} \alpha_k \\ & + V_0 \; term \end{aligned} \tag{A.69}$$

Let us now evaluate the $Term4$.

$$\begin{aligned} Term4 = & -\sum_{kk'q} V_q u_{k'-q} v_{k+q} u_k u_{k'} (\delta_{-k,k'} - \delta^\dagger_{k'-q} \delta_{-k-q}) \delta_{k'} \alpha_k \\ = & -\sum_{kk'q} V_q u_{-k-q} v_{k+q} u_k u_{-k} \delta_{-k} \alpha_k \\ = & -\sum_{kk'q} V_q u_{-k'} v_{k'} u_k u_{-k} \delta_{-k} \alpha_k \end{aligned} \tag{A.70}$$

Let us evaluate the $Term5$.

$$\begin{aligned} Term5 = & \sum_{kk'q} V_q u_{k'-q} v_{k+q} v_k v_{k'} (\delta_{-k,k'} - \delta^\dagger_{k'-q}\delta_{-k-q})(-\delta^\dagger_{-k}\alpha^\dagger_{-k'}) \\ = & -\sum_{kk'q} V_q u_{-k-q} v_{k+q} v_k v_{-k} \delta^\dagger_{-k}\alpha^\dagger_k \\ & + \sum_{kk'q} V_q u_{k'-q} v_{k+q} v_k v_{k'} \delta^\dagger_{k'-q}(\delta_{-k,k'} - \delta^\dagger_{-k}\delta_{-k-q})\alpha^\dagger_{-k'} \\ = & -\sum_{kk'} V_{k-k'} u_{-k'} v_{k'} v_k v_{-k} \delta^\dagger_{-k}\alpha^\dagger_k \\ & + V_0 \; term \end{aligned} \tag{A.71}$$

Let us now evaluate the $Term6$.

$$\begin{aligned} Term6 = & -\sum_{kk'q} V_q u_{k'-q} v_{k+q} u_k v_{k'} (\delta_{-k,k'} - \delta^\dagger_{k'-q}\delta_{-k-q})\alpha^\dagger_{-k'}\alpha_k \\ = & -\sum_{kk'q} V_q u_{-k-q} v_{k+q} u_k v_{-k} \alpha^\dagger_k \alpha_k \\ = & -\sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_k v_{-k} \alpha^\dagger_k \alpha_k \end{aligned} \tag{A.72}$$

Let us now evaluate the $Term7$.

$$\begin{aligned} Term7 = & \sum_{kk'q} V_q u_{k'-q} v_{k+q} u_{k'} v_k (\delta_{-k,k'} - \delta^\dagger_{k'-q}\delta_{-k-q})\delta_{k'}\delta^\dagger_{-k} \\ = & \sum_{kk'q} V_q u_{-k-q} v_{k+q} u_{-k} v_k \delta_{-k}\delta^\dagger_{-k} \\ & - \sum_{kk'q} V_q u_{k'-q} v_{k+q} u_{k'} v_k \delta^\dagger_{k'-q}\delta_{-k-q}\delta_{k'}\delta^\dagger_{-k} \\ = & \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \delta_{-k}\delta^\dagger_{-k} \\ & - \sum_{kk'q} V_q u_{k'-q} v_{k+q} u_{k'} v_k \delta^\dagger_{k'-q}\delta_{-k-q}(\delta_{-k,k'} - \delta^\dagger_{-k}\delta_{k'}) \\ = & \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \delta_{-k}\delta^\dagger_{-k} \\ & - \sum_{kk'q} V_q u_{-k-q} v_{k+q} u_{-k} v_k \delta^\dagger_{-k-q}\delta_{-k-q} \\ & + \sum_{kk'q} V_q u_{k'-q} v_{k+q} u_{k'} v_k \delta^\dagger_{k'-q}\delta_{-k-q}\delta^\dagger_{-k}\delta_{k'}) \end{aligned}$$

$$
\begin{aligned}
= \quad & \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \delta_{-k} \delta^\dagger_{-k} \\
& - \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \delta^\dagger_{-k'} \delta_{-k'} \\
& - \sum_{kk'q} V_q u_{k'-q} v_{k+q} u_{k'} v_k \delta^\dagger_{k'-q} (\delta_{-k-q,-k} - \delta^\dagger_{-k} \delta_{-k-q}) \delta_{k'} \\
= \quad & \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k (1 - \delta^\dagger_{-k} \delta_{-k}) \\
& - \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \delta^\dagger_{-k} \delta_{-k} \\
& - V_0 \; term \\
= \quad & \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \\
& -2 \sum_{kk'} V_{k'-k} u_{-k'} v_{k'} u_{-k} v_k \delta^\dagger_{-k} \delta_{-k} \qquad \text{(A.73)}
\end{aligned}
$$

Let us now evaluate the $Term8$.

$$
\begin{aligned}
Term8 = \quad & - \sum_{kk'q} V_q u_{k+q} v_{k'-q} u_{k'} v_k \alpha^\dagger_{k+q} \alpha_{-k'+q} (\delta_{-k,k'} - \delta^\dagger_{k'} \delta_{-k}) \\
= \quad & - \sum_{kk'q} V_q u_{k+q} v_{-k-q} u_{-k} v_k \alpha^\dagger_{k+q} \alpha_{k+q} \qquad \text{(A.74)}
\end{aligned}
$$

Now if we have $q = k' - k$, then

$$
Term8 = \quad - \sum_{kk'} V_{k'-k} u_{k'} v_{-k'} u_{-k'} v_{k'} \alpha^\dagger_{k'} \alpha_{k'} \qquad \text{(A.75)}
$$

Now if we have $k \to k' \; and \; k' \to k$

$$
\begin{aligned}
Term8 = \quad & - \sum_{kk'} V_{k'-k} u_k v_{-k} u_{-k'} v_{k'} \alpha^\dagger_k \alpha_k \\
= \quad & - \sum_{kk'} V_{k'-k} u_k v_k u_{k'} v_{k'} \alpha^\dagger_k \alpha_k \qquad \text{(A.76)}
\end{aligned}
$$

We have used the fact that $v_{-k} = v_k$. Now we add all the eight terms evaluated term by term above.

$$
1^{st} = \quad \sum_{kk'q} V_{k'-k} [-u_k u_{-k} u_{-k'} v_{k'} \alpha^\dagger_k \delta^\dagger_{-k}
$$

$$
\begin{aligned}
+ \quad & v_k v_{-k} u_{-k'} v_{k'} \delta_{-k} \alpha_k \\
- \quad & u_{-k'} v_{k'} u_k u_{-k} \delta_{-k} \alpha_k \\
- \quad & u_{-k'} v_{k'} v_k v_{-k} \delta^{\dagger}_{-k} \alpha^{\dagger}_k \\
- \quad & u_{-k'} v_{k'} u_k v_{-k} \alpha^{\dagger}_k \alpha_k \\
+ \quad & u_{-k'} v_{k'} u_{-k} v_k \\
- \quad & 2u_{-k'} v_{k'} u_{-k} v_k \delta^{\dagger}_{-k} \delta_{-k} \\
- \quad & u_k v_k u_{k'} v_{k'} \alpha^{\dagger}_k \alpha_k]
\end{aligned} \tag{A.77}
$$

$$
\begin{aligned}
1^{st} \quad & = \sum_{kk'q} V_{k'-k}[-u_k^2 u_{-k'} v_{k'} \alpha^{\dagger}_k \delta^{\dagger}_{-k} \\
& + v_k^2 u_{k'} v_{k'} \delta_{-k} \alpha_k \\
& - u_k^2 u_{'k} v_{k'} \delta_{-k} \alpha_k \\
& - v_k^2 u_{k'} v_{k'} \delta^{\dagger}_{-k} \alpha^{\dagger}_k \\
& + u_k v_k u_{k'} v_{k'} \\
& - 2u_{-k'} v_{k'} u_{-k} v_k \delta^{\dagger}_{-k} \delta_{-k} \\
& - 2u_k v_k u_{k'} v_{k'} \alpha^{\dagger}_k \alpha_k] \\
& = \sum_{kk'q} V_{k'-k}[u_k v_k u_{k'} v_{k'} - 2u_k v_k u_{k'} v_{k'} (\alpha^{\dagger}_k \alpha_k + \delta^{\dagger}_{-k} \delta_{-k}) \\
& - u_{-k'} v_{k'} (u_k^2 \alpha^{\dagger}_k \delta^{\dagger}_{-k} + v_k^2 \delta^{\dagger}_{-k} \alpha^{\dagger}_k) - u_{'k} v_{k'} (u_k^2 \delta_{-k} \alpha_k - v_k^2 \delta_{-k} \alpha_k)] \\
& = \sum_{kk'q} V_{k'-k}[u_k v_k u_{k'} v_{k'} - 2u_k v_k u_{k'} v_{k'} (\alpha^{\dagger}_k \alpha_k + \delta^{\dagger}_{-k} \delta_{-k}) \\
& - u_{-k'} v_{k'} (u_k^2 - v_k^2) \alpha^{\dagger}_k \delta^{\dagger}_{-k} - u_{'k} v_{k'} (u_k^2 - v_k^2) \delta_{-k} \alpha_k]
\end{aligned} \tag{A.78}
$$

The 2^{nd} term in the electron-hole part of the Hamiltonian is given as

$$
2^{nd} \quad = \sum_{kk'q} V_q c^{\dagger}_{k+q,\downarrow} d^{\dagger}_{k'-q,\uparrow} d_{k'\uparrow} c_{k\downarrow} \tag{A.79}
$$

We know that

$$
c^{\dagger}_{k+q,\downarrow} = \bar{u}_{k+q} \gamma^{\dagger}_{k+q} - \bar{v}_{k+q} \beta_{-k-q} \tag{A.80}
$$

$$d^{\dagger}_{k'-q,\uparrow} = \bar{u}_{k'-q}\beta^{\dagger}_{k'-q} + \bar{v}_{k'-q}\gamma_{-k'+q} \tag{A.81}$$

$$d_{k',\uparrow} = \bar{u}_{k'}\beta_{k'} + \bar{v}_{k'}\gamma^{\dagger}_{-k'} \tag{A.82}$$

$$c_{k,\downarrow} = \bar{u}_{k}\gamma_{k} - \bar{v}_{k}\beta^{\dagger}_{-k} \tag{A.83}$$

Let us transform the 2^{nd} term of the electron-hole part of interaction. The 2^{nd} term of the electron-hole part of interaction is structurally similar to the 1^{st} part if we identify $\alpha \rightarrow \gamma,\ \delta \rightarrow \beta,\ u \rightarrow \bar{u}\ and\ v \rightarrow \bar{v}$. Then we can easily write down the 2^{nd} part as

$$\begin{aligned} 2^{nd} = \sum_{kk'q} V_{k'-k}[&\bar{u}_k\bar{v}_k\bar{u}_{k'}\bar{v}_{k'} - 2\bar{u}_k\bar{v}_k\bar{u}_{k'}\bar{v}_{k'}(\gamma^{\dagger}_k\gamma_k + \beta^{\dagger}_{-k}\beta_{-k}) \\ &-\bar{u}_{k'}\bar{v}_{k'}(\bar{u}^2_k - \bar{v}^2_k)\gamma^{\dagger}_k\beta^{\dagger}_{-k} - \bar{u}_{'k}\bar{v}_{k'}(\bar{u}^2_k - \bar{v}^2_k)\beta_{-k}\gamma_k] \end{aligned} \tag{A.84}$$

Therefore the total transformed electron-hole part of the transformed Hamiltonian is given as

$$\begin{aligned} H^T_{eh} = -\sum_{kk'} V_{k-k'}[&(u_kv_ku_{k'}v_{k'} - 2u_kv_ku_{k'}v_{k'}(\alpha^{\dagger}_k\alpha_k + \delta^{\dagger}_{-k}\delta_{-k}) \\ &-u_{-k'}v_{k'}(u^2_k - v^2_k)\alpha^{\dagger}_k\delta^{\dagger}_{-k} - u_{'k}v_{k'}(u^2_k - v^2_k)\delta_{-k}\alpha_k) \\ &+(\bar{u}_k\bar{v}_k\bar{u}_{k'}\bar{v}_{k'} - 2\bar{u}_k\bar{v}_k\bar{u}_{k'}\bar{v}_{k'}(\gamma^{\dagger}_k\gamma_k + \beta^{\dagger}_{-k}\beta_{-k}) \\ &-\bar{u}_{k'}\bar{v}_{k'}(\bar{u}^2_k - \bar{v}^2_k)\gamma^{\dagger}_k\beta^{\dagger}_{-k} - \bar{u}_{'k}\bar{v}_{k'}(\bar{u}^2_k - \bar{v}^2_k)\beta_{-k}\gamma_k)] \end{aligned} \tag{A.85}$$

Now adding the $H^T_{ee},\ H^T_{hh},\ and\ H^T_{eh}$ terms together, we get,

$$
\begin{aligned}
H^T_{ee} + H^T_{hh} + H^T_{eh} \quad &= \sum_{kk'} V_{k-k'}[-(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2) \\
&-\{(u_k^2 v_{k'}^2 - v_k^2 v_{k'}^2)(\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) \\
&+(\bar{u}_k^2 \bar{v}_{k'}^2 - \bar{v}_k^2 \bar{v}_{k'}^2)(\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&+v_{k'}^2 u_k v_k (\alpha_{-k}\delta_k - \delta_{-k}\alpha_k) + \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k (\gamma_{-k}\beta_k - \beta_{-k}\gamma_k) \\
&+v_{k'}^2 u_k v_k (\delta_k^\dagger \alpha_{-k}^\dagger - \alpha_k^\dagger \delta^\dagger - k) + \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k (\beta_k^\dagger \gamma_{-k}^\dagger - \gamma_k^\dagger \beta_{-k}^\dagger)\} \\
&-\{(u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&-2u_k v_k u_{k'} v_{k'} (\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) - 2\bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'} (\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&-u_{k'} v_{k'} (u_k^2 - v_k^2)(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) - \bar{u}_{k'} \bar{v}_{k'} (\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)\}]
\end{aligned}
\tag{A.86}
$$

$$
\begin{aligned}
&= \sum_{kk'} V_{k-k'}[-(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2) \\
&-\{(u_k^2 v_{k'}^2 - v_k^2 v_{k'}^2)(\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) \\
&+(\bar{u}_k^2 \bar{v}_{k'}^2 - \bar{v}_k^2 \bar{v}_{k'}^2)(\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&-v_{k'}^2 u_k v_k 2\delta_{-k}\alpha_k - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k 2\beta_{-k}\gamma_k \\
&-v_{k'}^2 u_k v_k 2\alpha_k^\dagger \delta_{-k}^\dagger - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k 2\gamma_k^\dagger \beta_{-k}^\dagger\} \\
&-\{(u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&-2u_k v_k u_{k'} v_{k'} (\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) - 2\bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'} (\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&-u_{k'} v_{k'} (u_k^2 - v_k^2)(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) - \bar{u}_{k'} \bar{v}_{k'} (\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)\}]
\end{aligned}
\tag{A.87}
$$

The light part of the Hamiltonian is given as

$$
\tilde{H}_L = \lambda \sum_k \rho_k (c_{k\uparrow}^\dagger d_{-k\downarrow}^\dagger + c_{k\downarrow}^\dagger d_{-k\uparrow}^\dagger + d_{-k\downarrow} c_{k\uparrow} + d_{-k\uparrow} c_{k\downarrow}) \tag{A.88}
$$

Substituting B-V transformations, we have

$$\begin{aligned}\tilde{H}_L = \lambda\sum_k \rho_k[(u_k\alpha_k^\dagger - v_k\delta_{-k})(u_k\delta_{-k}^\dagger + v_k\alpha_k) + (\bar{u}_k\gamma_k^\dagger - \bar{v}\beta_{-k})(\bar{u}_k\beta_{-k}^\dagger + \bar{v}_k\gamma_k) \\ +(u_k\delta_{-k} + v_k\alpha_k^\dagger)(u_k\alpha_k - v_k\delta_{-k}^\dagger) + (\bar{u}_k\beta_{-k} + \bar{v}_k\gamma_k^\dagger)(\bar{u}_k\gamma_k - \bar{v}_k\beta_k^\dagger)]\end{aligned} \tag{A.89}$$

$$\begin{aligned}= \lambda\sum_k \rho_k[-2u_kv_k - 2\bar{u}_k\bar{v}_k + 2u_kv_k(\alpha_k^\dagger\alpha_k + \delta_k^\dagger\delta_k) + 2\bar{u}_k\bar{v}_k(\gamma_k^\dagger\gamma_k + \beta_k^\dagger\beta_k) \\ +(u_k^2 - v_k^2)(\alpha_k^\dagger\delta_{-k}^\dagger + \delta_{-k}\alpha_k) + (\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\gamma_k)]\end{aligned} \tag{A.90}$$

Now adding the $H_{ee}^T,\ H_{hh}^T,\ H_{eh}^T,\ \tilde{H}_L$, we get the total transformed Hamiltonian without the kinetic energy part as:

$$\begin{aligned}H_{ee,hh,eh,L}^T \quad &= \sum_{kk'} V_{k-k'}[-(v_k^2v_{k'}^2 + \bar{v}_k^2\bar{v}_{k'}^2) \\ &-\{(u_k^2v_{k'}^2 - v_k^2v_{k'}^2)(\alpha_k^\dagger\alpha + \delta_{-k}^\dagger\delta_{-k}) \\ &+(\bar{u}_k^2\bar{v}_{k'}^2 - \bar{v}_k^2\bar{v}_{k'}^2)(\beta_k^\dagger\beta_k + \gamma_{-k}^\dagger\gamma_k) \\ &-v_{k'}^2u_kv_k2\delta_{-k}\alpha_k - \bar{v}_{k'}^2\bar{u}_k\bar{v}_k2\beta_{-k}\gamma_k \\ &-v_{k'}^2u_kv_k2\alpha_k^\dagger\delta_{-k}^\dagger - \bar{v}_{k'}^2\bar{u}_k\bar{v}_k2\gamma_k^\dagger\beta_{-k}^\dagger\} \\ &-\{(u_kv_ku_{k'}v_{k'} + \bar{u}_k\bar{v}_k\bar{u}_{k'}\bar{v}_{k'}) \\ &-2u_kv_ku_{k'}v_{k'}(\alpha_k^\dagger\alpha + \delta_{-k}^\dagger\delta_{-k}) - 2\bar{u}_k\bar{v}_k\bar{u}_{k'}\bar{v}_{k'}(\beta_k^\dagger\beta_k + \gamma_{-k}^\dagger\gamma_k) \\ &-u_{k'}v_{k'}(u_k^2 - v_k^2)(\alpha_k^\dagger\delta_{-k}^\dagger + \delta_{-k}\alpha_k) - \bar{u}_{k'}\bar{v}_{k'}(\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\gamma_k)\}] \\ &+\lambda\sum_k \rho_k[-2u_kv_k - 2\bar{u}_k\bar{v}_k + 2u_kv_k(\alpha_k^\dagger\alpha_k + \delta_k^\dagger\delta_k) + 2\bar{u}_k\bar{v}_k(\gamma_k^\dagger\gamma_k + \beta_k^\dagger\beta_k) \\ &+(u_k^2 - v_k^2)(\alpha_k^\dagger\delta_{-k}^\dagger + \delta_{-k}\alpha_k) + (\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\gamma_k)]\end{aligned} \tag{A.91}$$

The kinetic energy part of the Hamiltonian with the photon energy is given as

$$
\begin{aligned}
H_{ke} &= \sum_{k\sigma}((\epsilon_{ck\sigma} - \frac{\hbar\omega}{2})c^\dagger_{k\sigma}c_{k\sigma} + (\epsilon_{vk\sigma} - \frac{\hbar\omega}{2})d^\dagger_{k\sigma}d_{k\sigma}) \\
&= \sum_{k\uparrow\downarrow}((\epsilon_{ck\uparrow} - \frac{\hbar\omega}{2})c^\dagger_{k\uparrow}c_{k\uparrow} + (\epsilon_{ck\downarrow} - \frac{\hbar\omega}{2}))c^\dagger_{k\downarrow}c_{k\downarrow} \\
&\quad +(\epsilon_{vk\uparrow} - \frac{\hbar\omega}{2})d^\dagger_{k\uparrow}d_{k\uparrow} + +(\epsilon_{vk\downarrow} - \frac{\hbar\omega}{2})d^\dagger_{k\downarrow}d_{k\downarrow})
\end{aligned} \tag{A.92}
$$

Using the B-V transformations, we get

$$
\begin{aligned}
H_{ke} &= \sum_{k\uparrow}(\epsilon_{ck\uparrow} - \frac{\hbar\omega}{2})(u_k^2\alpha^\dagger_k\alpha_k + v_k^2\delta_{-k}\delta^\dagger_{-k} - u_k v_{-k}\alpha^\dagger_k\delta^\dagger_{-k} - u_k v_k\delta_{-k}\alpha_k) \\
&+ \sum_{k\downarrow}(\epsilon_{ck\downarrow} - \frac{\hbar\omega}{2})(\bar{u}_k^2\gamma^\dagger_k\gamma_k + \bar{v}_k^2\beta_{-k}\beta^\dagger_{-k} - \bar{u}_k\bar{v}_{-k}\gamma^\dagger_k\beta^\dagger_{-k} - \bar{u}_k\bar{v}_k\beta_{-k}\gamma_k) \\
&+ \sum_{k\uparrow}(\epsilon_{vk\uparrow} - \frac{\hbar\omega}{2})(\bar{u}_k^2\beta^\dagger_k\beta_k + \bar{v}_k^2\gamma_k\gamma^\dagger_k + \bar{u}_k\bar{v}_k\beta^\dagger_k\gamma^\dagger_{-k} + \bar{u}_k\bar{v}_k\gamma_{-k}\beta_k) \\
&+ \sum_{k\downarrow}(\epsilon_{vk\downarrow} - \frac{\hbar\omega}{2})(u_k^2\delta^\dagger_k\delta_k + v_k^2\alpha_k\alpha^\dagger_{-k} + u_k v_k\delta^\dagger_k\alpha^\dagger_{-k} + u_k v_k\alpha_{-k}\delta_k)
\end{aligned} \tag{A.93}
$$

Now using the fact that $u_k^2 = 1 - v_k^2$ and $\eta\eta^\dagger = 1 - \eta^\dagger\eta$ and rearranging the terms, we get,

$$
\begin{aligned}
H_{ke} &= \sum_k[(\epsilon_{ckw\uparrow}v_k^2 + \epsilon_{ckw\downarrow}\bar{v}_k^2 + \epsilon_{vkw\uparrow}\bar{v}_k^2 + \epsilon_{vkw\downarrow}v_k^2) \\
&+(\epsilon_{ckw\uparrow}(1 - v_k^2) - \epsilon_{vkw\downarrow}v_k^2)\alpha^\dagger_k\alpha_k + (\epsilon_{ckw\downarrow}(1 - \bar{v}_k^2) - \epsilon_{vkw\uparrow}\bar{v}_k^2)\gamma^\dagger_k\gamma_k \\
&(\epsilon_{vkw\uparrow}(1 - \bar{v}_k^2) - \epsilon_{ckw\downarrow}\bar{v}^2)\beta^\dagger_k\beta_k + (\epsilon_{vkw\downarrow}(1 - v_k^2) - \epsilon_{ckw\uparrow}v^2)\delta^\dagger_k\delta_k \\
&+u_k v_k(\epsilon_{ckw\uparrow} + \epsilon_{vkw\downarrow})(\alpha^\dagger_k\delta^\dagger_{-k} + \delta_{-k}\alpha_k) \\
&+\bar{u}_k\bar{v}_k(\epsilon_{ckw\downarrow} + \epsilon_{vkw\uparrow})(\gamma^\dagger_k\beta^\dagger_{-k} + \beta_{-k}\gamma_k)]
\end{aligned} \tag{A.94}
$$

$$
\begin{aligned}
H_{ke} &= \sum_k[(\epsilon_{ck\omega\uparrow} + \epsilon_{vk\omega\downarrow})v_k^2 + (\epsilon_{ck\omega\downarrow} + \epsilon_{vk\omega\uparrow})\bar{v}_k^2 \\
&\{(\epsilon_{ck\omega} + J_e < M > -v_k^2(\xi^0_{k\omega} + (J_e - J_h) < M >))\alpha^\dagger_k\alpha_k
\end{aligned}
$$

$$
\begin{aligned}
&+(\epsilon_{ck\omega} - J_e < M > -\bar{v}_k^2(\xi_{k\omega}^0 - (J_e - J_h) < M >))\gamma_k^\dagger\gamma_k \\
&+(\epsilon_{vk\omega} + J_h < M > -\bar{v}_k^2(\xi_{k\omega}^0 - (J_e - J_h) < M >))\beta_k^\dagger\beta_k \\
&+(\epsilon_{vk\omega} - J_h < M > -v_k^2(\xi_{k\omega}^0 + (J_e - J_h) < M >))\delta_k^\dagger\delta\} \\
&-u_k v_k(\xi_{k\omega}^0 + (J_e - J_h) < M >)(\alpha_k^\dagger\delta_{-k}^\dagger + \delta_{-k}\alpha_k) \\
&+\bar{u}_k\bar{v}_k(\xi_{k\omega}^0 - (J_e - J_h) < M >)\gamma_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\gamma_k)]
\end{aligned} \quad \text{(A.95)}
$$

$$
\begin{aligned}
H_{ke} = &\sum_k[\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2 \\
&+(\epsilon_{ck\omega} + J_e < M > -\xi_k^+ v_k^2)\alpha_k^\dagger\alpha_k \\
&+(\epsilon_{ck\omega} - J_e < M > -\xi_k^- \bar{v}_k^2)\gamma_k^\dagger\gamma_k \\
&+(\epsilon_{vk\omega} + J_h < M > -\xi_k^- \bar{v}_k^2)\beta_k^\dagger\beta_k \\
&+(\epsilon_{vk\omega} - J_h < M > -\xi_k^+ v_k^2)\delta_k^\dagger\delta_k \\
&-u_k v_k \xi_k^+(\alpha_k^\dagger\delta_{-k}^\dagger + \delta_{-k}\alpha_k) \\
&+\bar{u}_k\bar{v}_k\xi_k^-\gamma_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\gamma_k)]
\end{aligned} \quad \text{(A.96)}
$$

where

$$\epsilon_{ck\omega} = E_g + \frac{\hbar^2 k^2}{2m_e} - \frac{\hbar\omega}{2} \quad \text{(A.97)}$$

$$\epsilon_{ck\omega} = \frac{\hbar^2 k^2}{2m_h} - \frac{\hbar\omega}{2} \quad \text{(A.98)}$$

$$\xi_{k\omega}^0 = E_g + \frac{\hbar^2 k^2}{2m_e} + \frac{\hbar^2 k^2}{2m_h} - \hbar\omega \quad \text{(A.99)}$$

$$\xi_k^\pm = \xi_{k\omega}^0 \pm (J_e - J_h) < M > \quad \text{(A.100)}$$

$$\epsilon_{ck\omega\uparrow(\downarrow)} = \epsilon_{ck\omega} + (-)J_e < M > \quad \text{(A.101)}$$

$$\epsilon_{vk\omega\uparrow(\downarrow)} = \epsilon_{vk\omega} + (-)J_h < M > \quad \text{(A.102)}$$

Adding the kinetic part (with the photon energy) of the Hamiltonian to the $H^T_{ee,hh,eh,L}$, we get the Free energy as,

$$
\begin{aligned}
F_T \quad &= \sum_k [\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2 \\
&+(\epsilon_{ck\omega} + J_e < M > -\xi_k^+ v_k^2)\alpha_k^\dagger \alpha_k \\
&+(\epsilon_{ck\omega} - J_e < M > -\xi_k^- \bar{v}_k^2)\gamma_k^\dagger \gamma_k \\
&+(\epsilon_{vk\omega} + J_h < M > -\xi_k^- \bar{v}_k^2)\beta_k^\dagger \beta_k \\
&+(\epsilon_{vk\omega} - J_h < M > -\xi_k^+ v_k^2)\delta_k^\dagger \delta_k \\
&-u_k v_k \xi_k^+ (\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) \\
&+\bar{u}_k \bar{v}_k \xi_{k\omega}^- \gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)] \\
&+ \sum_{kk'} V_{k-k'}[-(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2) \\
&-\{(u_k^2 v_{k'}^2 - v_k^2 v_{k'}^2)(\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) \\
&+(\bar{u}_k^2 \bar{v}_{k'}^2 - \bar{v}_k^2 \bar{v}_{k'}^2)(\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&-v_{k'}^2 u_k v_k 2\delta_{-k}\alpha_k - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k 2\beta_{-k}\gamma_k \\
&-v_{k'}^2 u_k v_k 2\alpha_k^\dagger \delta_{-k}^\dagger - \bar{v}_{k'}^2 \bar{u}_k \bar{v}_k 2\gamma_k^\dagger \beta_{-k}^\dagger\} \\
&-\{(u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&-2u_k v_k u_{k'} v_{k'}(\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) - 2\bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}(\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&-u_{k'} v_{k'}(u_k^2 - v_k^2)(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) - \bar{u}_{k'} \bar{v}_{k'}(\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)\}] \\
&+\lambda \sum_k \rho_k[-2u_k v_k - 2\bar{u}_k \bar{v}_k + 2u_k v_k(\alpha_k^\dagger \alpha_k + \delta_k^\dagger \delta_k) + 2\bar{u}_k \bar{v}_k(\gamma_k^\dagger \gamma_k + \beta_k^\dagger \beta_k) \\
&+(u_k^2 - v_k^2)(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) + (\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)]
\end{aligned}
\tag{A.103}
$$

We define:

$$\Omega_k = -2 \sum_{k'} V_{k-k'} v_{k'}^2 \tag{A.104}$$

$$\bar{\Omega}_k = -2 \sum_{k'} V_{k-k'} \bar{v}_{k'}^2 \tag{A.105}$$

$$\Delta_k^0 = 2\sum_{k'} V_{k-k'} u_{k'} v_{k'} \tag{A.106}$$

$$\Delta_k = 2\lambda_k \rho_k + \Delta_k^0 \tag{A.107}$$

$$\bar{\Delta}_k^0 = 2\sum_{k'} V_{k-k'} \bar{u}_{k'} \bar{v}_{k'} \tag{A.108}$$

$$\bar{\Delta}_k = 2\lambda_k \rho_k + \bar{\Delta}_k^0 \tag{A.109}$$

We can write the total Free energy as

$$\begin{aligned}
F_T \quad &= \sum_k [\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2 \\
&+(\epsilon_{ck\omega} + J_e < M > - \xi_{k\omega}^+ v_k^2)\alpha_k^\dagger \alpha_k \\
&+(\epsilon_{ck\omega} - J_e < M > - \xi_k^- \bar{v}_k^2)\gamma_k^\dagger \gamma_k \\
&+(\epsilon_{vk\omega} + J_h < M > - \xi_k^- \bar{v}_k^2)\beta_k^\dagger \beta_k \\
&+(\epsilon_{vk\omega} - J_h < M > - \xi_k^+ v^2)\delta_k^\dagger \delta_k \\
&- u_k v_k \xi_k^+ (\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) \\
&+ \bar{u}_k \bar{v}_k \xi_{k\omega}^- \gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)] \\
&+ \sum_{kk'} V_{k-k'}(-(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2)) \\
&+\{\sum_k \frac{\Omega_k}{2}(1 - 2v_k^2)(\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) \\
&+ \sum_k \frac{\Omega_k}{2}(1 - 2\bar{v}_k^2)(\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&- \sum_k \Omega_k u_k v_k (\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) - \sum_k \Omega_k \bar{u}_k \bar{v}_k (\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)\} \\
&- \sum_k V_{k-k'}(u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&+\{\sum_k \Delta_k^0 u_k v_k (\alpha_k^\dagger \alpha + \delta_{-k}^\dagger \delta_{-k}) + \sum_k \bar{\Delta}_k^0 \bar{u}_k \bar{v}_k (\beta_k^\dagger \beta_k + \gamma_{-k}^\dagger \gamma_k) \\
&+ \sum_k \frac{\Delta_k^0}{2}(u_k^2 - v_k^2)(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) + \sum_k \frac{\bar{\Delta}_k^0}{2}(\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)\} \\
&+ \lambda \sum_k \rho_k [-2u_k v_k - 2\bar{u}_k \bar{v}_k + 2u_k v_k (\alpha_k^\dagger \alpha_k + \delta_k^\dagger \delta_k) + 2\bar{u}_k \bar{v}_k (\gamma_k^\dagger \gamma_k + \beta_k^\dagger \beta_k)
\end{aligned}$$

$$+(u_k^2 - v_k^2)(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) + (\bar{u}_k^2 - \bar{v}_k^2)(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)] \tag{A.110}$$

Now rearranging the terms we finally have,

$$\begin{aligned}
F_T \quad &= \sum_k [\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2] \\
&- \sum_{kk'} V_{k-k'}(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2 + u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&-2 \sum_k \lambda \rho_k (u_k v_k + \bar{u}_k \bar{v}_k) \\
&+ \sum_k [\{\epsilon_{ck\omega} + J_e < M > + \frac{\Omega_k}{2} - (\xi_k^+ + \Omega_k) v_k^2 + (\Delta_k^0 + 2\lambda_k \rho_k) u_k v_k\} \alpha_k^\dagger \alpha_k \\
&+ \{\epsilon_{vk\omega} - J_h < M > + \frac{\Omega_k}{2} - (\xi_k^+ + \Omega_k) v_k^2 + (\Delta_k^0 + 2\lambda_k \rho_k) u_k v_k\} \delta_k^\dagger \delta_k \\
&+ \{\epsilon_{ck\omega} - J_e < M > + \frac{\bar{\Omega}_k}{2} - (\xi_k^- + \bar{\Omega}_k) \bar{v}_k^2 + (\bar{\Delta}_k^0 + 2\lambda_k \rho_k) \bar{u}_k \bar{v}_k\} \gamma_k^\dagger \gamma_k \\
&+ \{\epsilon_{vk\omega} + J_h < M > + \frac{\bar{\Omega}_k}{2} - (\xi_k^+ + \bar{\Omega}_k) \bar{v}_k^2 + (\bar{\Delta}_k^0 + 2\lambda_k \rho_k) \bar{u}_k \bar{v}_k\} \beta_k^\dagger \beta_k \\
&+ \{(\frac{\Delta_k^0}{2} + \lambda_k \rho_k)(u_k^2 - v_k^2) - (\xi_k^+ + \Omega_k) u_k v_k\} (\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k} \alpha_k) \\
&+ \{(\frac{\bar{\Delta}_k^0}{2} + \lambda_k \rho_k)(\bar{u}_k^2 - \bar{v}_k^2) - (\xi_k^- + \bar{\Omega}_k) \bar{u}_k \bar{v}_k\} (\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k} \gamma_k)]
\end{aligned} \tag{A.111}$$

$$\begin{aligned}
F_T \quad &= \sum_k [\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2] \\
&- \sum_{kk'} V_{k-k'}(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2 + u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&-2 \sum_k \lambda \rho_k (u_k v_k + \bar{u}_k \bar{v}_k) \\
&+ \sum_k [\{\epsilon_{ck\omega} + J_e < M > + \frac{\Omega_k}{2} - (\xi_k^+ + \Omega_k) v_k^2 + \Delta_k u_k v_k\} \alpha_k^\dagger \alpha_k \\
&+ \{\epsilon_{vk\omega} - J_h < M > + \frac{\Omega_k}{2} - (\xi_k^+ + \Omega_k) v_k^2 + \Delta_k u_k v_k\} \delta_k^\dagger \delta_k \\
&+ \{\epsilon_{ck\omega} - J_e < M > + \frac{\bar{\Omega}_k}{2} - (\xi_k^- + \bar{\Omega}_k) \bar{v}_k^2 + \bar{\Delta}_k \bar{u}_k \bar{v}_k\} \gamma_k^\dagger \gamma_k
\end{aligned}$$

$$+\{\epsilon_{vk\omega} + J_h < M > + \frac{\bar{\Omega}_k}{2} - (\xi_k^+ + \bar{\Omega}_k)\bar{v}_k^2 + \bar{\Delta}_k \bar{u}_k \bar{v}_k\}\beta_k^\dagger \beta_k$$
$$+\{\frac{\Delta_k}{2}(u_k^2 - v_k^2) - (\xi_k^+ + \Omega_k)u_k v_k\}(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k)$$
$$+\{\frac{\bar{\Delta}_k}{2}(\bar{u}_k^2 - \bar{v}_k^2) - (\xi_k^- + \bar{\Omega}_k)\bar{u}_k \bar{v}_k\}(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)] \qquad \text{(A.112)}$$

We rewrite the above expression for F_T as

$$
\begin{aligned}
F_T \quad &= \sum_k [\xi_k^+ v_k^2 + \xi_k^- \bar{v}_k^2] \\
&- \sum_{kk'} V_{k-k'}(v_k^2 v_{k'}^2 + \bar{v}_k^2 \bar{v}_{k'}^2 + u_k v_k u_{k'} v_{k'} + \bar{u}_k \bar{v}_k \bar{u}_{k'} \bar{v}_{k'}) \\
&-2 \sum_k \lambda \rho_k (u_k v_k + \bar{u}_k \bar{v}_k) \\
&+ \sum_k [\{\epsilon_{ck\omega} + J_e < M > + A_k\}\alpha_k^\dagger \alpha_k \\
&+\{\epsilon_{vk\omega} - J_h < M > + A_k\}\delta_k^\dagger \delta_k \\
&+\{\epsilon_{ck\omega} - J_e < M > \bar{A}_k\}\gamma_k^\dagger \gamma_k \\
&+\{\epsilon_{vk\omega} + J_h < M > + \bar{A}_k\}\beta_k^\dagger \beta_k \\
&+B_k(\alpha_k^\dagger \delta_{-k}^\dagger + \delta_{-k}\alpha_k) \\
&+\bar{B}_k(\gamma_k^\dagger \beta_{-k}^\dagger + \beta_{-k}\gamma_k)] \\
&+O(\alpha_k^\dagger \beta_k^\dagger \gamma_k^\dagger \delta_k^\dagger + ...) \\
&= E_0 + H_2 + H_4 \qquad \text{(A.113)}
\end{aligned}
$$

where

$$A_k = \frac{\Omega_k}{2} - (\xi_k^+ + \Omega_k)v_k^2 + \Delta_k u_k v_k \qquad \text{(A.114)}$$
$$B_k = \frac{\Delta_k}{2}(u_k^2 - v_k^2) - (\xi_k^+ + \Omega_k)u_k v_k \qquad \text{(A.115)}$$

This expression (A.113) is finally the transformed free energy we get by performing B-V transformation.

Appendix B

Some Expectation Values

Let us evaluate expectation values of some opeartors over the state $|\Psi>$. We use the fact that η annihilates the BCS-ground state $|\Psi>$, i.e., $\eta|\Psi>=0$, where $\eta=\alpha,\ \beta,\ \gamma,\ \delta$ are Bogoliubov operators.

$$c_{\vec{k}\uparrow}=u_{\vec{k}}\alpha_{\vec{k}}-v_{\vec{k}}\delta^{\dagger}_{-\vec{k}} \tag{B.1}$$

$$c_{\vec{k}\downarrow}=\bar{u}_{\vec{k}}\gamma_{\vec{k}}-\bar{v}_{\vec{k}}\beta^{\dagger}_{-\vec{k}} \tag{B.2}$$

$$d_{\vec{k}\uparrow}=\bar{u}_{\vec{k}}\beta_{\vec{k}}+\bar{v}_{\vec{k}}\gamma^{\dagger}_{-\vec{k}} \tag{B.3}$$

$$d_{\vec{k}\downarrow}=u_{\vec{k}}\delta_{\vec{k}}+v_{\vec{k}}\alpha^{\dagger}_{-\vec{k}} \tag{B.4}$$

We now evaluate some matrix elements which we will use in Section (5.1).

$$\begin{aligned}<\Psi|c^{\dagger}_{k1\uparrow}c_{k2\uparrow}|\Psi> \quad &=<|\Psi|u_{k1}\alpha^{\dagger}_{k1}-v_{k1}\delta_{-k1})(u_{k2}\alpha_{k2}-v_{k2}\delta^{\dagger}_{-k2})|\Psi> \\ &=<\Psi|v_{k1}v_{k2}\delta_{-k1}\delta^{\dagger}_{-k2}|\Psi> \\ &=v_{k1}v_{k2}\delta_{k1,k2}\end{aligned} \tag{B.5}$$

$$\begin{aligned}<\Psi|c^{\dagger}_{k1\uparrow}d^{\dagger}_{k2\downarrow}|\Psi> \quad &=<\Psi|u_{k1}\alpha^{\dagger}_{k1}-v_{k1}\delta_{-k1})(u_{k2}\delta^{\dagger}_{k2}+v_{k2}\alpha_{-k2}|\Psi> \\ &=<\Psi|-v_{k1}u_{k2}\delta_{-k1}\delta^{\dagger}_{k2}|\Psi> \\ &=-v_{k1}u_{k2}\delta_{-k1,k2}\end{aligned} \tag{B.6}$$

$$
\begin{aligned}
< \Psi|c^{\dagger}_{k1\uparrow}d_{k2\downarrow}|\Psi > \quad &=< \Psi|u_{k1}\alpha^{\dagger}_{k1} - v_{k1}\delta_{-k1})(u_{k2}\delta_{k2} + v_{k2}\alpha^{\dagger}_{-k2})|\Psi > \\
&= 0
\end{aligned} \tag{B.7}
$$

$$
\begin{aligned}
< \Psi|d_{k2\downarrow}c_{k1\uparrow}|\Psi > \quad &=< \Psi|(u_{k2}\delta_{k2} + v_{k2}\alpha^{\dagger}_{-k2})(u_{k1}\alpha_{k1} - v_{k1}\delta^{\dagger}_{-k1})|\Psi > \\
&=< \Psi| - u_{k2}v_{k1}\delta_{k2}\delta^{\dagger}_{-k1}|\Psi > \\
&= -u_{k2}v_{k1}\delta_{k2,-k1}
\end{aligned} \tag{B.8}
$$

$$
\begin{aligned}
< \Psi|c^{\dagger}_{k1\uparrow}c^{\dagger}_{k2\downarrow}|\Psi > \quad &=< \Psi|u_{k1}\alpha^{\dagger}_{k1} - v_{k1}\delta_{-k1})(\bar{u}_{k2}\gamma^{\dagger}_{k2} - \bar{v}_{k2}\beta_{-k2})|\Psi > \\
&= 0
\end{aligned} \tag{B.9}
$$

$$
\begin{aligned}
< \Psi|c_{k1\downarrow}c_{k2\uparrow}|\Psi > \quad &=< \Psi|(\bar{u}_{k1}\gamma_{k1} - \bar{v}_{k1}\beta^{\dagger}_{-k1})(u_{k2}\alpha_{k2} - v_{k2}\delta^{\dagger}_{-k2})|\Psi > \\
&= 0
\end{aligned} \tag{B.10}
$$

$$
\begin{aligned}
< \Psi|c^{\dagger}_{k1\uparrow}c_{k2\downarrow}|\Psi > \quad &=< |\Psi|u_{k1}\alpha^{\dagger}_{k1} - v_{k1}\delta_{-k1})(\bar{u}_{k2}\gamma_{k2} - \bar{v}_{k2}\beta^{\dagger}_{-k2})|\Psi > \\
&= 0
\end{aligned} \tag{B.11}
$$

$$
\begin{aligned}
< \Psi|c^{\dagger}_{k1\uparrow}c^{\dagger}_{k2\uparrow}|\Psi > \quad &=< |\Psi|u_{k1}\alpha^{\dagger}_{k1} - v_{k1}\delta_{-k1})(u_{k2}\alpha^{\dagger}_{k2} - v_{k2}\delta_{-k2})|\Psi > \\
&= 0
\end{aligned} \tag{B.12}
$$

$$
< \Psi|c_{k1\uparrow}c_{k2\uparrow}|\Psi >= (< \Psi|c^{\dagger}_{k2\uparrow}c^{\dagger}_{k1\uparrow}|\Psi >)^{\dagger} = 0 \tag{B.13}
$$

VITA

Subodha Mishra was born on May 28, 1965, in Puri, India. He obtained a Masters in Physics from Ravenshaw College, Cuttack in 1989; a Diploma in Advanced Physics in 1991 and a Ph.D in Physics in 1998 both from the Institute of Physics, Bhubaneswar, India. He was a Post-Doctoral Institute Research Associate in the Department of Physics, IIT, Kharagpur, India in 1999. In January 2000, Subodha came to the University of Missouri-Columbia to work on a second Ph.D. in Physics. He graduated with a Ph.D in June 2006 and joined as a Post-Doctoral Research Associate in the Department of Physics and Astronomy, University of Missouri-Columbia.