

SPIN COUPLING BY CONDUCTION ELECTRONS
EXPLORED BY DOUBLE TIME
GREEN'S FUNCTIONS

by

WILLIAM DECKER

Presented to the Faculty of the Graduate School of
The University of Texas at Arlington in Partial Fulfillment
of the Requirements
for the Degree of

MASTER OF SCIENCE IN PHYSICS

THE UNIVERSITY OF TEXAS AT ARLINGTON

April 2012

ACKNOWLEDGEMENTS

I am grateful to my advisor, Nail Fazleev, whose patience, encouragement and guidance throughout my graduate career allowed me to develop an understanding of physics beyond anything I thought was possible.

Finally, I offer my regards and blessings to all those who supported me in any respect during the completion of my thesis.

April 20th, 2012

ABSTRACT

SPIN COUPLING BY CONDUCTION ELECTRONS

EXPLORED BY DOUBLE TIME

GREEN'S FUNCTIONS

William Decker, M.S.

The University of Texas at Arlington, 2012

Supervising Professor: Nail Fazleev

The impurities containing unfilled d or f shells may have localized magnetic moments in nonmagnetic metals, semiconductors, and superconductors under certain conditions. These localized moments interact with each other through the spin polarization field of conduction electrons. The indirect coupling between magnetic impurities is referred to as the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction which is important in describing the magnetic and thermodynamic properties of magnetic nanostructures. The interaction may be expressed as a long range oscillatory function. I explored the properties of the indirect exchange interaction between localized moments in different dimensions using the s-d model and the Green's functions method. An effective Hamiltonian for the indirect interaction is obtained in terms of a Green's function using a canonical transformation applied to the s-d exchange model. The equation of motion for the Green's function has been solved by using a Hartree-Fock approximation to truncate higher order Green's functions. The asymptotic form of the indirect spin-spin interaction for large distances R for both polarized and unpolarized conduction electrons has been explored using the theory of generalized functions. The Green's function

technique is justified as the three dimensional Hamiltonian is modified by a screened Coulomb potential that is Yukawa-like in nature.

TABLE OF CONTENTS

ACKNOWLEDGEMENTS	ii
ABSTRACT	iii
LIST OF ILLUSTRATIONS.....	vii

Chapter	Page
1. INDIRECT INTERACTION BETWEEN LOCALIZED MOMENTS	1
1.1 Introduction.....	1
1.2 Derivation of the s-d model Exchange Interaction	2
1.2.1 Canonical Transformation of the Anderson Model	7
1.3 Spin Polarization	9
1.3.1 Introduction to Spin Polarization Formalism	10
1.3.2 Spin Polarization due to s-d Interaction	16
1.3.3 RKKY Interaction	22
1.3.4 RKKY Interaction In 2D and 1D	23
2. GREEN'S FUNCTION.....	35
2.1 Introduction.....	35
2.2 A Beginner's Guide to Green's Functions	36
2.2.1 Spectral Representations of Correlation Functions	39
2.2.2 Spectral Representations of Retarded and Advanced Green's Functions	40
2.2.3 Finding the Green's function of a Perfect Quantum Gas.....	43
2.2.4 Using Green's Function Method to find Spin Polarization of the s-d Model	47

3. ASYMPTOTIC ESTIMATION OF FOURIER TRANSFORMS	60
3.1 Introduction.....	60
3.2 Introduction to the Theory of Generalized Functions	60
3.2.1 Theory of the Asymptotic Expansion of Fourier Transforms.....	64
4. EFFECT OF ELECTRON-ELECTRON INTERACTION ON S-D MODEL	70
4.1 Introduction.....	70
4.2 Calculation of a New Effective Hamiltonian via Canonical Transformation	70
4.2.1 Calculation of the Green's Function.....	73
4.3 The Fourier Transform of Green's Function.....	86
5. CONCLUSION	96
REFERENCES.....	98
BIOGRAPHICAL INFORMATION	100

LIST OF ILLUSTRATIONS

Figure	Page
1.1 Plot of $F(x)$ Range Function	21
1.2 Three Dimensional Susceptibility	29
1.3 One Dimensional Susceptibility	32
1.4 Two Dimensional Susceptibility	33

CHAPTER 1

INDIRECT INTERACTION BETWEEN LOCALIZED MOMENTS

The introduction of an impurity to a periodic lattice creates many interesting and practical problems that can be explored. In principle, the impurity destroys the periodicity of the lattice and the wave vector is no longer a constant of motion, but this does not mean that all periodic properties of the lattice have been destroyed.

1.1 Introduction

The periodic properties of a pure substance used to model the properties of an impure substance in a variety of ways. A simple way is to modify the independent electron's wave function with a term to represent the scattering between an electron and a nonmagnetic impurity [1].

$$\varphi_{\mathbf{k}}(\mathbf{x}) = e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} + g_{\mathbf{k}}(\vec{\mathbf{x}})$$

The variation of the electron density is calculated as

$$\Delta\rho_{\mathbf{k}}(\vec{\mathbf{x}}) = \varphi_{\mathbf{k}}^*\varphi_{\mathbf{k}} - 1 = g_{\mathbf{k}}(\vec{\mathbf{x}})e^{-i\vec{\mathbf{k}}\cdot\vec{\mathbf{x}}} + cc + |g_{\mathbf{k}}(\vec{\mathbf{x}})|^2$$

with

$$g_{\mathbf{k}}(\vec{\mathbf{x}}) \cong f_{\mathbf{k}}(\theta) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r}$$

outside of the central charge.

The asymptotic behavior of the electronic density variation is proportional to

$$\Delta\rho(\vec{x}) \propto \frac{\cos(2k_F r + \varphi_F)}{r^3}.$$

The independent electron interacting with an impurity leads to long-range oscillatory charge density variations that fall off as r^{-3} . This effect shows up experimentally in the nuclear magnetic resonances of a material with dilute impurities. For example, the nuclear magnetic resonance of a Cu-base alloy experiences attenuation of its resonance line. The broadening occurs due to the interaction of the quadrupole moment of the Cu nuclei with the gradients in the electric field. The gradients in the electric field are caused by the screening charge surrounding the impurity [2].

The effect of a magnetic impurity on the spin polarization density of conduction electrons is similar to the effect of a charged impurity on charge density described above. The exchange interaction between a conduction electron and a magnetic impurity causes spin polarization in the conduction electrons. As above, the polarization exhibits a long range oscillatory behavior and couples the original impurity with another magnetic impurity. This indirect interaction between localized magnetic moments via the conduction electrons is known as Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction.

1.2 Derivation of the s-d model Exchange Interaction

The s-d model assumes that there are two types of electrons: s electrons that are non-localized over the entire crystal and d electrons that are localized at impurity sites. The model uses the exchange interaction between these types of electrons as a basis for exploring magnetism. Namely,

$$\mathcal{H}_{\text{ex}} = J_{ll'} S_l \cdot S_{l'}$$

where S_l and $S_{l'}$ are spin vectors associated with the intrinsic magnetic moment of each particle and $J_{ll'}$ is the matrix element representing the strength of the exchange interaction between particles l and l' . Keeping in mind the properties of the dot product, it can be seen that $J_{ll'} > 0$ favors antiparallel spins and $J_{ll'} < 0$ favors parallel spins.

It should be noted that the exchange interaction is a direct consequence of electron-electron interaction and arises because of the overlap of electronic wave functions along with the anti-symmetric nature of their wave functions [3]. The conduction electron Hamiltonian in a metal of volume Ω and with N atoms takes the form

$$H_0 = \sum_{ks} \xi_k a_{ks}^\dagger a_{ks}$$

where a_{ks}^\dagger and a_{ks} are the usual second quantized creation and annihilation operators of the electron with wave vector k and spin s . The coefficient ξ_k is the energy of a single electron moving in a general potential such as that caused by a crystal field or an external magnetic field. The Bloch function associated with a particular electron momentum state is labeled as $\phi_k(\mathbf{r})$ and its spin state is labeled as $\chi_s(\zeta)$, where ζ is the generalized spin coordinate. For an impurity atom located at \mathbf{R}_n , the localized orbital is $\phi_L(\mathbf{r} - \mathbf{R}_n)$ and a_{ns} operator is the annihilation operator of the localized electron at site \mathbf{R}_n and spin s .

Therefore, the field operator is expanded in terms of one-electron wave functions for both the conduction electron and the localized electron as

$$\Psi(\mathbf{r}, \zeta) = \sum_{ks} \phi_k(\mathbf{r}) \chi_s(\zeta) a_{ks} + \sum_{ns} \phi_L(\mathbf{r} - \mathbf{R}_n) \chi_s(\zeta) a_{ns} \quad 1.1$$

$$\Psi^\dagger(\mathbf{r}, \zeta) = \sum_{ks} \phi_k^*(\mathbf{r}) \chi_s^\dagger(\zeta) a_{ks}^\dagger + \sum_{ns} \phi_L^*(\mathbf{r} - \mathbf{R}_n) \chi_s^\dagger(\zeta) a_{ns}^\dagger \quad 1.2$$

Using 1.1 and 1.2, the two body interaction term is written as

$$\int \dots \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 d\zeta_1 d\zeta_2 \Psi^\dagger(\mathbf{r}_1, \zeta_1) \Psi^\dagger(\mathbf{r}_2, \zeta_2) V(r_{12}) \Psi(\mathbf{r}_2, \zeta_2) \Psi(\mathbf{r}_1, \zeta_1) \quad 1.3$$

with $V(r_{12})$ representing the interaction potential between two electrons and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$.

Only terms that represent the scattering between a conduction electron and a localized electron will be considered. In other words, only terms that are proportional to $\delta_{nn'}$, will be kept.

Inserting the definitions of 1.1 and 1.2 into 1.3 along with some rearranging of terms yields

$$\begin{aligned} &= \sum_{kk'n} (a_{k'\uparrow}^\dagger a_{k'\uparrow} + a_{k'\downarrow}^\dagger a_{k'\downarrow}) (a_{n\uparrow}^\dagger a_{n\uparrow} + a_{n\downarrow}^\dagger a_{n\downarrow}) \left[\langle \mathbf{k}\mathbf{n} | \mathbf{k}'\mathbf{n} \rangle - \frac{1}{2} \langle \mathbf{k}\mathbf{n} | \mathbf{n}\mathbf{k}' \rangle \right] \\ &\quad - \sum_{kk'n} [(a_{k'\uparrow}^\dagger a_{k'\uparrow} - a_{k'\downarrow}^\dagger a_{k'\downarrow}) (a_{n\uparrow}^\dagger a_{n\uparrow} - a_{n\downarrow}^\dagger a_{n\downarrow}) \\ &\quad + a_{k'\uparrow}^\dagger a_{k'\downarrow} a_{n\downarrow}^\dagger a_{n\uparrow} + a_{k'\downarrow}^\dagger a_{k'\uparrow} a_{n\uparrow}^\dagger a_{n\downarrow}] \langle \mathbf{k}\mathbf{n} | \mathbf{n}\mathbf{k}' \rangle \end{aligned} \quad 1.4$$

The electron-electron interaction Hamiltonian produces two types of integrals, $\langle \mathbf{k}\mathbf{n}|\mathbf{k}'\mathbf{n} \rangle$ and $\langle \mathbf{k}\mathbf{n}|\mathbf{n}\mathbf{k}' \rangle$. The first integral is known as the Coulomb integral and is defined as

$$\langle \mathbf{k}\mathbf{n}|\mathbf{k}'\mathbf{n} \rangle = \int \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \phi_{\mathbf{k}}^*(\mathbf{r}_1) \phi_{\mathbf{k}'}(\mathbf{r}_2 - \mathbf{R}_N) V(r_{12}) \phi_{\mathbf{k}}(\mathbf{r}_2 - \mathbf{R}_N) \phi_{\mathbf{k}'}(\mathbf{r}_1),$$

which has the classical interpretation as the electrostatic interaction between two electrons.

The Exchange integral does not have a direct classical interpretation and can be thought of as a correction to the Coulomb integral due to the anti-symmetric nature of the electron wave functions,

$$\langle \mathbf{k}\mathbf{n}|\mathbf{n}\mathbf{k}' \rangle = \int \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \phi_{\mathbf{k}}^*(\mathbf{r}_1) \phi_{\mathbf{k}'}(\mathbf{r}_2 - \mathbf{R}_N) V(r_{12}) \phi_{\mathbf{k}}(\mathbf{r}_1 - \mathbf{R}_N) \phi_{\mathbf{k}'}(\mathbf{r}_2).$$

Next, the Bloch functions are expanded in terms of Wannier functions

$$\phi_{\mathbf{k}}(\mathbf{r}) = N^{-1/2} \sum_{\mathbf{R}_n} e^{i\mathbf{k}\cdot\mathbf{R}_n} w(\mathbf{r} - \mathbf{R}_n)$$

and the exchange integral is rewritten as

$$\langle \mathbf{k}\mathbf{n}|\mathbf{n}\mathbf{k}' \rangle = \frac{1}{N} e^{i(\mathbf{k}' - \mathbf{k})\cdot\mathbf{R}_n} J(\mathbf{k}, \mathbf{k}'). \quad 1.5$$

The coupling constant in 1.5 is defined as

$$J(\mathbf{k}, \mathbf{k}') = \sum_{ij} e^{[i(\mathbf{k}' \cdot \mathbf{R}_j - \mathbf{k} \cdot \mathbf{R}_i)]} \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 w^*(\mathbf{r}_1 - \mathbf{R}_i) \phi_L^*(\mathbf{r}_2) V(r_{12}) \phi_L(\mathbf{r}_1) w^*(\mathbf{r}_2 - \mathbf{R}_j) \quad 1.6$$

and is taken to be dependent on the absolute difference between \mathbf{k} and \mathbf{k}' . Equation 1.6 can be reduced to an atomic exchange integral by assuming that the lead term, $i = j = 0$, is dominant enough to be able to discard the rest of the terms in the series. It is also convenient to assume that $J(\mathbf{k}, \mathbf{k}')$ is a constant, but for the rest of this section it will be taken in its most general form.

Assuming that there is only a single unpaired orbital electron located on a particular impurity leads to the following second quantized operator definitions

$$\frac{1}{2}(a_{n\uparrow}^\dagger a_{n\uparrow} - a_{n\downarrow}^\dagger a_{n\downarrow}) = S_{nz}; \quad a_{n\uparrow}^\dagger a_{n\downarrow} = S_{n+}; \quad a_{n\downarrow}^\dagger a_{n\uparrow} = S_{n-} \quad 1.7$$

with S_n being the spin operator of the localized electron located at n and having spin $1/2$.

Inserting the 1.7 definitions into the exchange part of the Hamiltonian yields

$$= \frac{1}{N} e^{[i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_N]} J(|\mathbf{k} - \mathbf{k}'|) [(a_{k\uparrow}^\dagger a_{k'\uparrow} - a_{k\downarrow}^\dagger a_{k'\downarrow}) S_{nz} + a_{k\uparrow}^\dagger a_{k'\downarrow} S_{n-} + a_{k\downarrow}^\dagger a_{k'\uparrow} S_{n+}].$$

By using similar definitions to 1-7 for the conduction electron spin operators and definition of the dot product between spins,

$$S \cdot \sigma = S^+ \sigma^- + S^- \sigma^+ + S_z \sigma_z.$$

the final form of the exchange interaction between conduction electrons and localized d electrons becomes

$$= \frac{1}{N} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{R}_N} J(|\mathbf{k} - \mathbf{k}'|) \sum_{\alpha\beta} (\mathbf{S}_n \cdot \boldsymbol{\sigma})_{\alpha\beta} a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}'\sigma}. \quad 1.8$$

It should be noted that the analysis of the contact hyperfine interaction between an electron and a nucleus will also lead to a similar exchange interaction term.

1.2.1 Canonical Transformation of the Anderson Model

Another model that describes the interaction of a conduction electron with a localized electron is the Anderson model,

$$H = \sum_{ks} \xi_k a_{ks}^\dagger a_{ks} + \xi_L \sum_s a_{Ls}^\dagger a_{Ls} + U a_{L\uparrow}^\dagger a_{L\uparrow} a_{L\downarrow}^\dagger a_{L\downarrow} + \sum_{ks} M_k (a_{ks}^\dagger a_{Ls} + a_{Ls}^\dagger a_{ks})$$

$$= H_0 + H_M.$$

The H_0 term represents the single particle operators and H_M , the term proportional to M_k , represents a mixing or hopping term. There is a canonical transformation that can transform the Anderson model into a Hamiltonian with exchange terms like equation 1.8 [4]. A byproduct of this derivation is that the transformed Hamiltonian has a much richer display of all the different types of interactions that can occur in a system of interacting localized moments and conduction electrons.

The overall plan is to find a canonical transformation to the Anderson Model that will eliminate terms which are linear in M_k .

$$\tilde{H} = e^S H e^{-S}$$

1.9

$$= H_0 + H_M + [S, H_0] + [S, H_M] + \frac{1}{2}[S, [S, H_0]] + \frac{1}{2}[S, [S, H_M]] + \dots$$

Equation 1.9 is arrived at by expanding the exponential terms and rearranging the terms into a series of commutation relations. The required condition so that the terms linear in M_k vanish is

$$H_M = [H_0, S]. \quad 1.10$$

After some minor manipulation of the terms, equation 1.9 becomes

$$\tilde{H} = H_0 + \frac{1}{2}[S, H_M] + 0(M_k^3).$$

All terms $0(M_k^3)$ are taken to vanish and only with terms that are $0(M_k^2)$ are left. The transformation factor S is calculated by using 1.10 and the Heisenberg equation of motion,

$$[H_0, S(t)] = i \frac{dS(t)}{dt}.$$

Solving the resulting differential equation gives [4]

$$S = \sum_{ks} M_k \left(\frac{1 - n_{-s}}{\xi_L - \xi_k} + \frac{n_{-s}}{\xi_L + U - \xi_k} \right) (a_{Ls}^\dagger a_{ks} - a_{ks}^\dagger a_{Ls})$$

Although S has some rather unwieldy commutation relations, it does satisfy the condition stated in equation 1.10. To simplify the final form of the Hamiltonian, an effective exchange constant is defined as:

$$\bar{L}_{kk'} = M_k M_{k'} \left(\frac{1}{\bar{\xi}_L - \xi_k} + \frac{1}{\bar{\xi}_L - \xi_{k'}} - \frac{1}{\bar{\xi}_L + U - \xi_k} - \frac{1}{\bar{\xi}_L + U - \xi_{k'}} \right).$$

From here, the second term of \tilde{H} in terms of $\bar{L}_{kk'}$ is calculated to be

$$\begin{aligned} \frac{1}{2} [S, H_M] = & \sum_{kk's} \bar{L}_{kk'} \left[n_{-s} a_{ks}^\dagger a_{k's} + a_{ks}^\dagger a_{k'-s} a_{L-s}^\dagger a_{Ls} - \delta_{kk} n_s n_{-s} \right. \\ & \left. + \frac{1}{4} (a_{k-s}^\dagger a_{k's}^\dagger a_{L-s} a_{Ls} + h.c.) \right] + 2 \sum_k \frac{M_k^2}{\bar{\xi}_L - \xi_k} n_s \\ & - \sum_{kk's} a_{ks}^\dagger a_{k's} M_k M_{k'} \left(\frac{1}{\bar{\xi}_L - \xi_k} + \frac{1}{\bar{\xi}_L - \xi_{k'}} \right) \end{aligned} \quad 1.11$$

The first two terms in 1.11 represent a scattering only event and a scattering with spin-flip event, the same exchange interaction term that we found in the s-d interaction Hamiltonian. The s-d model represents a subset of the interactions contained within the Anderson Model. Also of note, is that taking even higher order commutator terms from 1.9 will result in even more types of interactions.

1.3 Spin Polarization

In analogy with polarized light, an ensemble of electrons is considered to be polarized if the up and down states are not equally populated in a sample. This build up of spin density will lead to a change in the magnetic field felt within the sample. Spin-polarized electrons play

an important role in the development of spintronics and uncovering the magnetic properties of a material [6].

1.3.1 Introduction to Spin Polarization Formalism

The observable spin obeys similar commutation relations to the angular momentum of an electron in atomic orbit. Namely,

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k \quad 1.12$$

where ϵ_{ijk} is the Levi-Civita symbol and i,j,k represent Cartesian coordinates and $\epsilon_{xyz} = 1$. By defining $S = \frac{\hbar}{2}\sigma$ and requiring that σ_z be diagonal, the Pauli matrices are defined as

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad 1.13$$

An arbitrary state $\chi = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ as a linear superposition in terms of the eigenfunctions of σ_z .

$$\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + a_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Here, $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ have eigenvalues of 1 and -1 respectively. Assuming $\langle \chi | \chi \rangle = 1$ allows the interpretation of $|a_1|^2$ and $|a_2|^2$ as the probabilities of finding χ in either $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ state.

Since operators that can be measured simultaneously must commute, 1.12 reveals that all the components of electronic spin cannot be measured simultaneously. However, the S^2 operator does commute with each individual spin direction and a precise measurement on that quantity and one of the particular components of spin can be made. For a $s = 1/2$ particle, the eigenvalue of S^2 is $s(s + 1)\hbar^2 = 3\hbar^2/4$.

Now, there is a definite way to interpret the statement “the spin of the electron is in the z direction”. It means that the z-component of the spin is $\hbar/2$, but s_x and s_y are undefined with the constraint that

$$s_x^2 + s_y^2 = 3\hbar^2/4 - s_z^2 = \hbar^2/2$$

This concept can be pictured as a conical shell with a height of $\hbar/2$ and a hypotenuse of $\sqrt{3/4} \hbar$.

Moving on from the basic review of spin, the polarization of an electron shall be defined along a particular axis and in an arbitrary state, $\chi = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$. First, let $\hat{e} = (e_x, e_y, e_z)$ be a unit vector in the θ, ϕ direction of a unit sphere with the following component definitions

$$e_x = \sin \theta \cos \phi \quad e_y = \sin \theta \sin \phi \quad e_z = \cos \theta.$$

Now, the eigenvalue equation that relates to the projection of the Pauli Spin Matrices in the direction of \hat{e} must be solved,

$$(\boldsymbol{\sigma} \cdot \hat{e} - \lambda)\chi = 0.$$

After performing the dot product calculations and applying some simple trigonometric identities, the following is arrived at

$$a_1(\cos \theta - \lambda) + a_2 \sin \theta e^{-i\phi} = 0$$

$$a_1 \sin \theta e^{i\phi} - a_2(\cos \theta + \lambda) = 0.$$

The condition for a nontrivial solution to this system of equations requires that the determinant vanishes.

$$-\cos^2 \theta + \lambda^2 - \sin^2 \theta = 0$$

$$\xrightarrow{\text{yields}} \lambda = \pm 1$$

Using these eigenvalues, the a_i coefficients are solved for

$$a_1 = \cos \frac{\theta}{2} \quad a_2 = \sin \frac{\theta}{2} e^{i\phi} \quad \text{for } \lambda = 1$$

1.14

$$a_1 = \sin \frac{\theta}{2} \quad a_2 = \cos \frac{\theta}{2} e^{i\phi} \quad \text{for } \lambda = -1.$$

The above spin functions represent the states where the spin in the direction θ, ϕ has eigenvalues $\pm \hbar/2$. It is easily seen that the $\lambda = -1$ solution is the same as the $\lambda = 1$ in the $-\hat{e}$ direction, which can be found by just shifting the angles $\theta, \phi \rightarrow \pi - \theta, \phi + \pi$. Therefore, only one set of solutions is considered since the other set can be found just by shifting them by π .

These equations give the mathematical framework to consider the polarization of electrons. Defining the polarization as the expectation value of the Pauli spin operators,

$$\mathbf{P} = \langle \chi | \boldsymbol{\sigma} | \chi \rangle = (a_1^*, a_2^*) \boldsymbol{\sigma} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

and using the 1.13 definitions for $\boldsymbol{\sigma}$ and 1.14 for the coefficients. The expressions for the polarization in different directions are found to be

$$P_x = (a_1^*, a_2^*) \sigma_x \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = a_1^* a_2 + a_2^* a_1 = \sin \theta \cos \phi$$

$$P_y = i(a_2^* a_1 - a_1^* a_2) = \sin \theta \sin \phi$$

$$P_z = |a_1|^2 - |a_2|^2 = \cos \theta.$$

If the polarization is normalized by dividing through by $\langle \chi | \chi \rangle$, the magnitude of the polarization for different directions becomes

$$P_x = \frac{a_1^* a_2 + a_2^* a_1}{|a_1|^2 + |a_2|^2}$$

$$P_y = \frac{i(a_2^* a_1 - a_1^* a_2)}{|a_1|^2 + |a_2|^2}$$

$$P_z = \frac{|a_1|^2 - |a_2|^2}{|a_1|^2 + |a_2|^2}.$$

Finally, the methods of Statistical Mechanics must be used to consider an ensemble of electrons with more than one spin state. In this case, the polarization of the system is considered to be the average of the polarization vectors for each individual spin state. Assuming the states χ^n are normalized, the polarization averaged over the different ensembles of spin states becomes

$$\mathbf{P} = \sum_n w^n \mathbf{P}^n = \sum_n \langle \chi^n | \boldsymbol{\sigma} | \chi^n \rangle. \quad 1.15$$

$$w^n = \frac{N^n}{\sum_n N^n}$$

Where the weighting factor, w^n , takes into account the proportion of each spin state compared to the overall mixture with N^n being the number of electrons in state χ^n .

The density matrix, ρ , shall be defined in the usual manner.

$$\rho = \sum_n w^n |\chi^n\rangle \langle \chi^n| = \sum_n w^n \begin{pmatrix} a_1^n \\ a_2^n \end{pmatrix} (a_1^{(n)*}, a_2^{(n)*}) \quad 1.16$$

$$= \sum_n w^n \begin{pmatrix} |a_1^n|^2 & a_2^{(n)*} a_1^n \\ a_1^{(n)*} a_2^n & |a_2^n|^2 \end{pmatrix}$$

Now, the polarization rewritten in terms of the density operator is

$$\mathbf{P} = \text{Tr}\{\rho \boldsymbol{\sigma}\}.$$

The density matrix can also be expressed in terms of the components of polarization.

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + P_z & P_x - iP_y \\ P_x + iP_y & 1 - P_z \end{pmatrix} = \frac{1}{2} (\mathbf{1} + \mathbf{P} \cdot \boldsymbol{\sigma})$$

If the polarization of the ensemble is taken to be only in the z-direction, then the density matrix is diagonalized as

$$\rho = \frac{1}{2} \begin{pmatrix} 1+P & 0 \\ 0 & 1-P \end{pmatrix}.$$

Given that the probability of obtaining the eigenvalue of $\hbar/2$ from a measurement in the z direction for a particular nth subsystem is $|a_1^n|^2$. Then the total probability of all the subsystems is $\sum_n w^n |a_1^n|^2$. This probability can also be rewritten as the ratio of N_\uparrow to the total number of particles in the system. From these definitions, it is possible to make a connection between fraction of particles in the spin-up state and the polarization of the system.

$$\sum_n w^n |a_1^n|^2 = \frac{N_\uparrow}{N_\uparrow + N_\downarrow} = \frac{1}{2}(1+P)$$

The same process can be done for eigenvalue $-\hbar/2$ to get

$$\frac{N_\downarrow}{N_\uparrow + N_\downarrow} = \sum_n w^n |a_2^n|^2 = \frac{1}{2}(1-P).$$

From these two equations, the unidirectional polarization is simply

$$P = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}.$$

1.3.2 Spin Polarization due To s-d Interaction

In this section, how the polarization of the conduction electrons arises out of the s-d interaction is demonstrated using perturbation theory. Beginning with the exchange interaction derived as equation 1.8, the dot product is expanded to give

$$\mathcal{H}_{s-d} = -\frac{1}{N} \sum_{k,k',n} \exp[i(k' - k) \cdot R_N] J(|k - k'|) [(a_{k'\uparrow}^\dagger a_{k\uparrow} - a_{k'\downarrow}^\dagger a_{k\downarrow}) S_{nz} + a_{k'\uparrow}^\dagger a_{k\downarrow} S_{n-} + a_{k'\downarrow}^\dagger a_{k\uparrow} S_{n+}].$$

The first order perturbation to the energy can be found by identifying the diagonal elements of the interaction (*i. e.* $k = k'$):

$$-\frac{J}{N} (n_\uparrow - n_\downarrow) \sum_n S_{nz}$$

where n_\uparrow and n_\downarrow are the total number of electrons for spin \uparrow and \downarrow .

The first thing to notice about the first order perturbation to the energy is that the interaction energy of the system is lowered as the polarization, $(n_\uparrow - n_\downarrow)$, increases. Therefore, the system of conduction electrons tends to be spin-polarized. However, the diagonal terms are independent of the distance from the impurity and the polarization is uniform due to the first order effect.

The first order correction to the Fermi energy is

$$E_f^\pm = \frac{\hbar^2}{2m} (k_\pm)^2 \mp \frac{J}{N} \sum_n S_{nz}. \quad 1.17$$

with k_{\pm} being the maximum wave vector of an electron with spins \uparrow and \downarrow . E_f^+ and E_f^- are the corrections to the Fermi energy associated with spin \uparrow and \downarrow , respectively.

Next, the maximum wave vector for the unpolarized electron is defined as k and putting it in terms of the polarized wave vectors

$$k_{\pm} = k \pm \Delta k. \quad 1.18$$

Placing 1.18 into the first order correction of the Fermi energy, 1.17, yields

$$E_f^{\pm} = E_f \pm 2E_f \frac{\hbar}{2m} \frac{\Delta k}{k} \mp \frac{J}{N} \sum_n S_{nz}$$

with E_f being the unperturbed Fermi energy.

Now, the total number of electrons is related to the unpolarized wave vector, k , by

$$n = \left(\frac{V}{6\pi^2} \right) k^3$$

and related to the polarized n_{\pm} by

$$n_{\pm} = n \pm 3n \left(\frac{\Delta k}{k} \right).$$

By requiring that E_f^+ and E_f^- are equal to each other, $(\Delta k/k)$ can be solved for

$$\frac{\Delta k}{k} = \frac{J}{2NE_f} \sum_n S_{nz} \quad 1.19$$

Placing this into our equation for n_{\pm} , an expression is obtained that describes the polarization of the electrons,

$$n_{\pm} = n \pm \frac{3nJ}{2NE_f} \sum_n S_{nz}. \quad 1.20$$

At first glance, the uniform polarization in 1.20 is a surprising result because the Friedel theorem states that the perturbing potential due to impurities is screened out except in the immediate neighborhood of the impurity [1,7]. This suggests that off-diagonal terms might have a first order contribution to the polarization.

Starting with the first-order correction to the perturbed wave function of the conduction electron,

$$\phi_k = \phi_k^0 + \sum_{k'} \frac{\langle k' | \mathcal{H}_{s-d} | k \rangle}{E_k - E_{k'}} \phi_{k'}^0,$$

yields

$$\phi_{k\pm} = \phi_{k\pm}^0 - \frac{2m}{\hbar^2} N^{-1} \sum_{k'} \frac{J(|k-k'|)}{k^2 - k'^2} \sum_n e^{i(k-k') \cdot R_n} \left\{ \pm S_n^z \phi_{k\pm}^0 + S_n^{\pm} \phi_{k\mp}^0 \right\}.$$

In this case, +/− refers to spin-up/spin-down particles, the prime on the summation indicates that the $k = k'$ is excluded, and the wave functions are represented by plane waves in the above equation.

$$\phi_k^0 = \left(\frac{1}{V}\right)^{\frac{1}{2}} e^{ik \cdot r}$$

The spin density at $T = 0$ can be found by calculating the wave function density over the Fermi sea.

$$\rho_{\pm}(r) = \sum_s \sum_k^{k_F} \phi_{k\pm}^* \phi_{k\pm}$$

Using the expression for the perturbed wave function and the 1st order uniform polarization term,

$$\rho_{\pm}(r) = \frac{1}{V} \left\{ n \pm \frac{3n}{2E_f} N^{-1} J(0) \sum_n S_n^z \right\} \mp \frac{2m}{V\hbar^2} N^{-1} \sum_k^{k_F} \sum_{k'}' \frac{J(|k-k'|)}{k^2 - k'^2} \sum_n \left\{ e^{i(k-k') \cdot R_n} + e^{-i(k-k') \cdot R_n} \right\} S_n^z$$

Making the replacement of $k - k' = q$ and then integrating over k yields (see 1.24 for details and also note [8] as a different integral that yields the same results)

$$\rho_{\pm}(r) = \frac{1}{V} \left\{ n \pm \frac{3n}{2E_f} N^{-1} J(0) \sum_n S_n^z \right\} \\ \pm \frac{2m}{V \hbar^2} \frac{V}{16\pi^2} N^{-1} \sum_q' J(q) \left\{ k_F + \frac{4k_F^2 - q^2}{4q} \ln \left| \frac{2k_F + q}{2k_F - q} \right| \right\} \sum_n \{ e^{iq \cdot (r-R_n)} + e^{-iq \cdot (r-R_n)} \} S_n^z.$$

The expression is rewritten as

$$\rho_{\pm}(r) = \frac{n}{V} \pm \frac{3n}{2E_f V} N^{-1} J(0) \sum_n S_n^z \pm \frac{3n}{8E_f} \frac{N^{-1}}{V} \sum_q' J(q) f(q) \sum_n \{ e^{iq \cdot (r-R_n)} + e^{-iq \cdot (r-R_n)} \} S_n^z$$

with

$$f(q) = 1 + \frac{4k_F^2 - q^2}{4qk_F} \ln \left| \frac{2k_F + q}{2k_F - q} \right|. \quad 1.21$$

The term $J(0)$ is omitted from the summation but is equal to the second term of $\rho_{\pm}(r)$ because $f(0) = 2$. After absorbing the second term into the summation over q , the expression takes the form,

$$\rho_{\pm}(r) = \frac{n}{V} \pm \frac{3n}{8E_f} \frac{N^{-1}}{V} \sum_q J(q) f(q) \sum_n \{ e^{iq \cdot (r-R_n)} + e^{-iq \cdot (r-R_n)} \} S_n^z,$$

with the sum now going over all values of q . It should also be emphasized that the equation for $\rho_{\pm}(r)$ includes the diagonal terms calculated in 1.20 which were absorbed into the summation over q . Therefore, the calculation of $\rho_{\pm}(r)$ represent the complete modification of the first order

energy perturbation. By assuming that $J(q) = J$, the integration over q can be performed which yields

$$\rho_{\pm}(r) = \frac{n}{V} \pm \frac{(3n)^2 N^{-1}}{E_f} \frac{2\pi J(0)}{V} \sum_n F(2k_F|r - R_n|) S_n^z$$

and

$$F(x) = (1/x^4)(x \cos x - \sin x).$$

The polarization is defined to be the difference the up and down spin densities as noted in section 1.3.1. This simple calculation at long distances gives

$$\rho_{\downarrow} - \rho_{\uparrow} \sim \frac{9\pi n^2}{4\varepsilon_F} J I_n^z \frac{\cos(2k_F r)}{(k_F r)^3}.$$

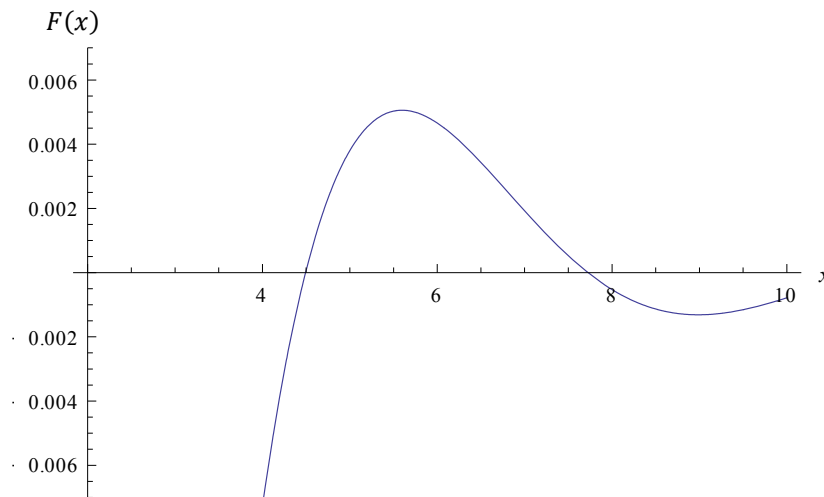


Figure 1.1-Plot of $F(x)$ Range Function

The final expression for the spin density reveals that the uniform polarization term is modified by a long range oscillatory term that depends upon the distance from the impurity as R^{-3} . It is also noted how elongated the oscillations are by comparing the order of magnitude of the y-axis to the x-axis and how rapidly the polarization vanishes as $r \rightarrow \infty$. Therefore, the polarization of the conduction electrons is confined to the neighborhood of the impurity much in line with the expectations from Friedel's theorem.

1.3.3 RKKY Interaction

So far, the system being dealt with has consisted of a sea of conduction electrons and a magnetic impurity. If there were a second impurity in the system, it will be perturbed by the spin the polarization of the conduction electrons produced by the first impurity and first will be perturbed in the same way by second. The system has become two magnetic moments that are indirectly coupled by the conduction electrons. The second order interaction between two spins can be written as

$$H''(\mathbf{r}) = \sum_{\substack{\mathbf{k}\mathbf{k}' \\ s s'}}' \frac{\langle \mathbf{k}s | \mathcal{H}_{sd} | \mathbf{k}'s' \rangle \langle \mathbf{k}'s' | \mathcal{H}_{sd} | \mathbf{k}s \rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'}}$$

with $\varepsilon_{\mathbf{k}} = k^2/2m$, the prime on the summation again means that the $\mathbf{k} = \mathbf{k}'$ is excluded from the sum, and assuming that $J(|\mathbf{k} - \mathbf{k}'|) = J$.

Beginning with the summation over the spins and using a standard relation, allows the second order spin summation to be rewritten as

$$\sum_s (\boldsymbol{\sigma} \cdot \mathbf{S}_n)(\boldsymbol{\sigma} \cdot \mathbf{S}_m) = \mathbf{S}_n \cdot \mathbf{S}_m + i\boldsymbol{\sigma} \cdot \mathbf{S}_n \times \mathbf{S}_m = \mathbf{S}_n \cdot \mathbf{S}_m.$$

The last part of equality uses the fact that the trace of any component of $\boldsymbol{\sigma}$ must vanish.

From here, the integrations are very similar to ones already calculated which yield

$$H''(\mathbf{r}) = S_n \cdot S_m \frac{4J^2 m k_F^4}{(2\pi)^3} F(2k_F r). \quad 1.22$$

Once again,

$$F(x) = (1/x^4)(x \cos x - \sin x).$$

The oscillatory nature of the indirect exchange interaction causes a variety of polarized spin structures in magnetic crystals, even including spirals!

1.3.4 RKKY Interaction In 2D and 1D

So far, only crystals in three dimensions have been considered. However, an understanding of the RKKY polarization effects in lower dimensions is essential to understanding polarization effects of nanostructures. First, the susceptibility associated with the exchange energy of a crystal is calculated.

Beginning with definition of the local magnetic field at the site \mathbf{R}_i which is labeled as \mathbf{H}_i . This magnetic field induces a localized magnetic moment at \mathbf{R}_j in the form of

$$\mathbf{m}_j = \sum_i \chi_{ij} \mathbf{H}_i.$$

Here, \mathbf{m}_j is the localized magnetic at \mathbf{R}_j induced by \mathbf{H}_i with a magnetic susceptibility of χ_{ij} .

Assuming isotropic conditions and translational invariance imposes the conditions that χ_{ij} is a scalar and $\chi_{ij}(\mathbf{R}_{ij}) = \chi_{ij}(R_{ij})$.

The energy of the system is calculated by

$$E = -\frac{1}{2} \sum_i \mathbf{m}_j \cdot \mathbf{H}_i = -\frac{1}{2} \sum_{ij} \chi_{ij}(R_{ij}) \mathbf{H}_j \cdot \mathbf{H}_i.$$

Here, $\mathbf{H}_i = \frac{A\mathbf{S}_i}{2\mu_B}$ and focusing only on the exchange term between two magnetic moments, the exchange energy becomes

$$E_{EX} = -\frac{A^2}{4\mu_B^2} \chi_{ij}(R_{ij}) \mathbf{S}_j \cdot \mathbf{S}_i.$$

Now, E will be written in terms of $\chi(q)$ through the use of Fourier transforms. Starting with this definition of the transform,

$$\mathbf{H}_i = \frac{1}{\sqrt{N}} \sum_q e^{-iq \cdot \mathbf{R}_i} \mathbf{H}_q$$

E can be rewritten as

$$E = -\frac{1}{2} \sum_{ij} \chi_{ij}(R_{ij}) \mathbf{H}_j \cdot \mathbf{H}_i$$

$$\begin{aligned}
&= -\frac{1}{2N} \sum_{qq'} \sum_{ij} \chi_{ij}(R_{ij}) e^{-i(q \cdot R_i + q' \cdot R_j)} \mathbf{H}_q \cdot \mathbf{H}_{q'} \\
&= -\frac{1}{2N} \sum_{qq'} \sum_i \sum_{i-j} \chi_{ij}(R_{ij}) e^{-i(q+q') \cdot R_i} e^{-iq' \cdot R_{ij}} \mathbf{H}_q \cdot \mathbf{H}_{q'}.
\end{aligned}$$

Taking the sum over the i index yields and applying the $\delta_{q,-q'}$ to the summation gives

$$= -\frac{1}{2} \sum_q \sum_{i-j} \chi_{ij}(R_{ij}) e^{iq \cdot R_{ij}} \mathbf{H}_q \cdot \mathbf{H}_{-q}.$$

Finally, defining $\chi(q) = \sum_{i-j} \chi_{ij}(R_{ij}) e^{iq \cdot R_{ij}}$ allows for

$$E = -\frac{1}{2} \sum_q \chi(q) \mathbf{H}_q \cdot \mathbf{H}_{-q}.$$

Next, $\chi(q')$ is calculated by assuming a magnetic field of the form

$$\mathbf{H}_i = \frac{1}{\sqrt{N}} \mathbf{H}_q (e^{iq \cdot R_i} + e^{-iq' \cdot R_j}) \hat{x}.$$

The energy due to the magnetic moment of an electron interacting with a magnetic field is given by

$$E_{EX} = -\frac{1}{2} \sum_i g_s \mu_B \mathbf{S}_i \cdot \mathbf{H}_i.$$

Using the fact that $g_s = 2$ for an electron and $s_i^x = \frac{1}{2}(a_{i\uparrow}^\dagger a_{i\downarrow} + a_{i\downarrow}^\dagger a_{i\uparrow})$, the exchange energy is found to be

$$E_{EX} = -\frac{1}{\sqrt{N}} \sum_i \mu_B \mathbf{H}_q (a_{i\uparrow}^\dagger a_{i\downarrow} + a_{i\downarrow}^\dagger a_{i\uparrow}) (e^{iq \cdot \mathbf{R}_i} + e^{-iq' \cdot \mathbf{R}_j}).$$

Now a Fourier transform must be applied to the creation and annihilation operators. Defining the transforms for a_i^\dagger and a_i as

$$a_i = \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot \mathbf{R}_i} a_k$$

$$a_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ik \cdot \mathbf{R}_i} a_k^\dagger.$$

Next, the exchange energy can be rewritten as

$$\begin{aligned} E_{EX} &= -\frac{1}{N\sqrt{N}} \sum_i \sum_{kk'} \mu_B \mathbf{H}_q (a_{k'\uparrow}^\dagger a_{k\downarrow} e^{i(k-k') \cdot \mathbf{R}_i} + a_{k'\downarrow}^\dagger a_{k\uparrow} e^{i(k-k') \cdot \mathbf{R}_i}) (e^{iq \cdot \mathbf{R}_i} + e^{-iq' \cdot \mathbf{R}_j}) \\ &= -\frac{1}{N\sqrt{N}} \sum_i \sum_{kk'} \mu_B \mathbf{H}_q (a_{k'\uparrow}^\dagger a_{k\downarrow} e^{i(k-k'+q) \cdot \mathbf{R}_i} + a_{k'\uparrow}^\dagger a_{k\downarrow} e^{i(k-k'-q') \cdot \mathbf{R}_i} + a_{k'\downarrow}^\dagger a_{k\uparrow} e^{i(k-k'+q) \cdot \mathbf{R}_i} \\ &\quad + a_{k'\downarrow}^\dagger a_{k\uparrow} e^{i(k-k'-q') \cdot \mathbf{R}_i}) \\ &= -\frac{1}{N\sqrt{N}} \sum_{kk'} \mu_B \mathbf{H}_q (a_{k'\uparrow}^\dagger a_{k\downarrow} N \delta_{k+q, k'} + a_{k'\uparrow}^\dagger a_{k\downarrow} N \delta_{k-q, k'} + a_{k'\downarrow}^\dagger a_{k\uparrow} N \delta_{k+q, k'} + a_{k'\downarrow}^\dagger a_{k\uparrow} N \delta_{k-q, k'}) \end{aligned}$$

$$= -\frac{1}{\sqrt{N}} \sum_{kk'} \mu_B \mathbf{H}_q (a_{k+q\uparrow}^\dagger a_{k\downarrow} + a_{k-q\uparrow}^\dagger a_{k\downarrow} + a_{k+q\downarrow}^\dagger a_{k\uparrow} + a_{k-q\downarrow}^\dagger a_{k\uparrow})$$

Now, second order perturbation theory is applied to E_{EX} . First, it must be kept in mind that

$$\begin{aligned} \sum_n |\langle n | a_{k+q}^\dagger a_k | m \rangle|^2 &= \sum_n \langle m | a_k^\dagger a_{k+q} | n \rangle \langle n | a_{k+q}^\dagger a_k | m \rangle = \langle m | a_k^\dagger a_{k+q} a_{k+q}^\dagger a_k | m \rangle \\ &= \langle m | a_{k+q} a_{k+q}^\dagger a_k^\dagger a_k | m \rangle = \sum_n \langle m | a_{k+q} a_{k+q}^\dagger | n \rangle \langle n | a_k^\dagger a_k | m \rangle. \end{aligned}$$

Then, the second order perturbed term is written as

$$H'' = \frac{-2\mu_B^2 H_q^2}{N} \sum_k \left[\frac{f(k)[1-f(k+q)]}{\epsilon_{k+q} - \epsilon_k} + \frac{f(k)[1-f(k-q)]}{\epsilon_{k-q} - \epsilon_k} \right].$$

Next, replacing $k \rightarrow k - q$ in the first term yields

$$H'' = \frac{-2\mu_B^2 H_q^2}{N} \sum_k \frac{f(k) - f(k-q)}{\epsilon_{k-q} - \epsilon_k}.$$

From this equation, the susceptibility can be identified as

$$\chi(q) = \frac{2\mu_B^2}{N} \sum_k \frac{f(k) - f(k-q)}{\epsilon_{k-q} - \epsilon_k}. \quad 1.23$$

The new magnetic susceptibility will first be explored in three dimensions by taking the Fourier transform of $\chi(q)$ to be compared with the original calculation of the RKKY interaction, equation 1.20. The integral in 1.23 is a very well studied function called the Lindhard function and finds many applications with respect to response functions [9].

The general conversion formula of a summation into an integral in d dimensions is

$$\frac{1}{N} \sum_k \rightarrow \frac{1}{N} \frac{V_d}{(2\pi)^d} \int d^d k,$$

where d is the dimension under consideration. The assumptions for the calculation are that $V_d = 1$, $T = 0$ and the standard energy term

$$\varepsilon_k = \frac{k^2}{2m}.$$

After converting the summation to an integral, the susceptibility becomes

$$\chi(q) = \frac{2\mu_B^2}{N} \frac{2m}{(2\pi)^3} \int_0^{k_F} k^2 dk \int_0^{2\pi} d\phi \int_{-1}^1 d\mu \left[\frac{1}{q^2 - 2kq\mu} + \frac{1}{q^2 + 2kq\mu} \right].$$

Taking the angular integrals yields

$$\chi(q) = \frac{\mu_B^2}{N} \frac{m}{\pi^2} \int_0^{k_F} \frac{k}{q} \ln \left| \frac{q+2k}{q-2k} \right| dk.$$

After integrating up to k_F , the expression for the three dimensional susceptibility is

$$\chi(q) = \frac{\mu_B^2 m}{N \pi^2} \left[\frac{k_F}{2} + \frac{1}{8} \frac{(4k_F^2 - q^2)}{q} \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \right]. \quad 1.24$$

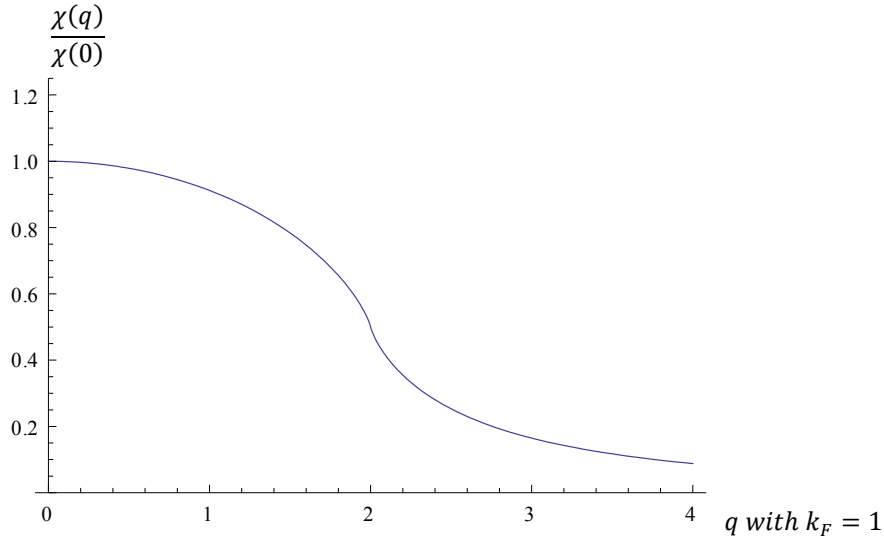


Figure 1.2-Three Dimensional Susceptibility

The logarithmic singularity is a first derivative singularity at $q = 2k_F$ that is called a Kohn anomaly in both dielectric and magnetic response functions. Generally, Kohn anomalies are related to the Fermi surface and can result in important physical effects such as subtle kinks in a dispersion curve. The similarity of 1.24 to 1.21 should also be noted as it shows how the Lindhard function can arise naturally in a physical problem.

Next, the Fourier transform of $\chi(q)$ is taken and then compared to the results in 1.20.

$$\chi(r) = \frac{2\mu_B^2}{N^2} \frac{1}{(2\pi)^6} \int d^3k d^3k' \frac{f(k) - f(k - q)}{\epsilon_{k-q} - \epsilon_k} e^{i(k'-k) \cdot R}$$

$$\chi(r) = 2\mu_B^2 \frac{2m}{N^2} \frac{8}{(2\pi)^4 r^2} \int_0^{k_F} k dk \int_{k_F}^{\infty} k' dk' \frac{\sin(kr) \sin(k'r)}{k'^2 - k^2}$$

The integral on k' can be extended down to 0 because it will not affect the final result. This allows us to perform a contour integration which leaves the integral (with coefficients set to unity)

$$\int_0^{k_F} dk \sin(kr) \cos(kr).$$

Using the trigonometric identity,

$$2 \sin x \cos x = \sin 2x,$$

leaves a simple integral to calculate which gives

$$\chi(r) = 2\mu_B^2 \frac{m}{N^2} \frac{1}{\pi^4} \left[\frac{\sin(2k_F r) - 2k_F r \cos(2k_F r)}{8r^4} \right].$$

We see from the above equation that we recovered the RKKY effect for the three dimensional case, namely

$$\chi(r) \sim \frac{\cos x}{x^3}.$$

Similar calculations for the two and one dimensional Fourier transform yield

$$\chi(r) \sim \frac{\sin x}{x^2} \quad D = 2$$

$$\chi(r) \sim \frac{\cos x}{x} \quad D = 1.$$

What is immediately noticeable about reducing the dimensionality of the system is that the strength of the RKKY effect goes up noticeably. The reason for this difference lies in the singularity of $\chi(q)$ for each dimension. The stronger the singularity at $k = 2k_F$ in $\chi(q)$, the slower the RKKY effect falls off with distance [10]. The effect stems entirely from the nature of the Fourier transform. A function with stronger singularities will tend to have a broader spectrum in the transformed variable's space. To examine this more carefully, the magnetic susceptibilities are calculated for the one dimensional and two dimensional cases and then their singularities are explored.

Beginning with the one-dimensional case, the summation in 1.21 is converted into the one-dimensional integral,

$$\chi(q) = \frac{2\mu_B}{N} \frac{2m}{2\pi} \int_{-k_F}^{k_F} dk \left[\frac{1}{(k-q)^2 - k^2} + \frac{1}{(k+q)^2 - k^2} \right].$$

This integral is calculated to be

$$\chi(q) = \frac{2\mu_B}{N} \frac{m}{2\pi q} \ln \left| \frac{q + 2k_F}{q - 2k_F} \right|$$

$$\chi(0) = \frac{2\mu_B m}{N 2\pi}$$

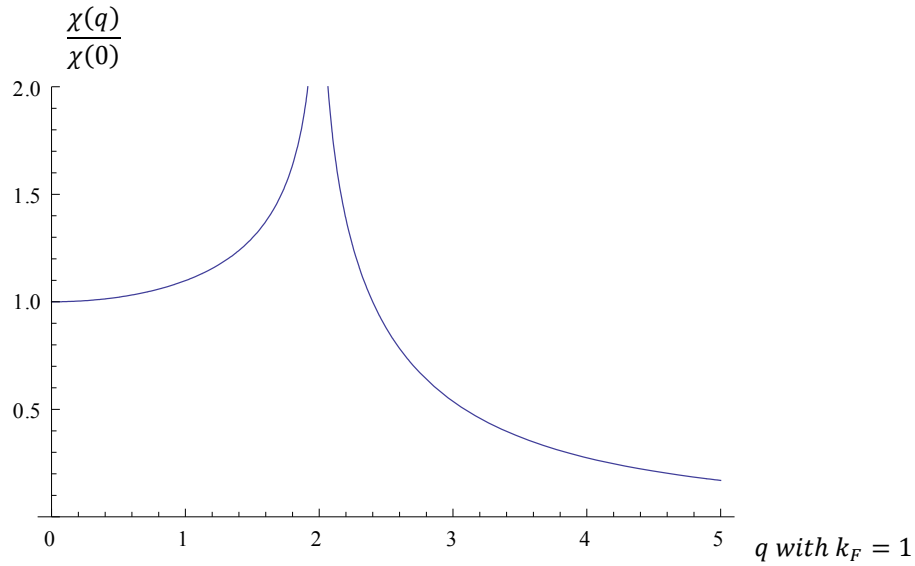


Figure 1.3-One Dimensional Susceptibility

The magnetic susceptibility in one dimension has a singularity at $q = 0$ in the actual function. Therefore, the one dimensional singularity is expected to be stronger than the three-dimensional case where the singularity was in the first derivative.

Moving to the calculation of the two-dimensional case of the susceptibility, summation in 1.21 becomes

$$\chi(q) = \frac{2\mu_B^2 m}{N (2\pi)^2} \int k dk \int_0^{2\pi} d\varphi \left[\frac{1}{q(q - 2k \cos \varphi)} + \frac{1}{q(q + 2k \cos \varphi)} \right].$$

Using the standard integral

$$\int_0^{\frac{\pi}{2}} \frac{1}{1 - a^2 \cos^2 \varphi} = \begin{cases} \frac{\pi}{2\sqrt{1-a^2}} & a < 1 \\ 0 & a > 1 \end{cases} ,$$

the integrals for both cases are calculated to be

$$\chi(q) = 4 \frac{\mu_B^2 m}{N \pi} \quad q < 2k_F$$

$$\chi(q) = 4 \frac{\mu_B^2 m}{N \pi} \left(1 - \sqrt{1 - \frac{4k_F^2}{q^2}} \right) \quad q \geq 2k_F$$

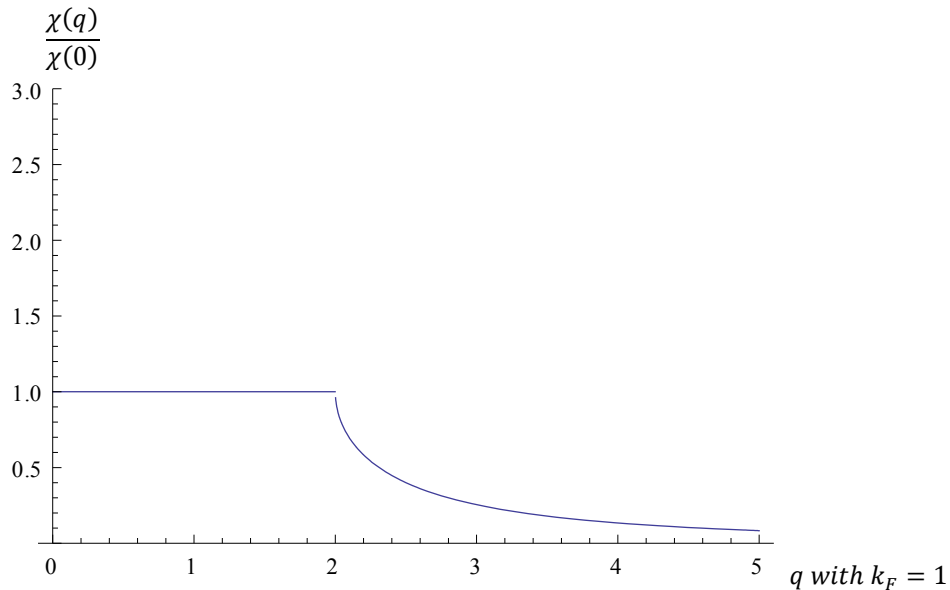


Figure 1.4-Two Dimensional Susceptibility

The singularity in the two dimensional case comes from the kink where the square root part of the piecemeal function meets the constant function. Once again the singularity is in the function and not the derivative of the function as it was in the three dimensional case.

Therefore, we expect once again for the two-dimensional case to have a longer range than the three-dimensional case which is born out in the comparison between the magnetic susceptibilities in real space. However, the singularity in the two-dimensional case is due to a discontinuity in the function. For this reason, it is expected that the RKKY effect in two dimensions will have weaker range than in one-dimension as is borne out by direct calculation of the transform of the susceptibility from momentum space to real space.

CHAPTER 2

GREEN'S FUNCTIONS

2.1 Introduction

The methods of quantum field theory have found uses in statistical physics due to the fact that both fields deal with basic problems that are essentially the same. Both methods investigate systems that infinite in volume and therefore have an infinite number of degrees of freedom. These methods also both describe themselves in terms of a second-quantized Hamiltonian, which gives the interaction of a particle with a quantized field and a large system of interacting particles common mathematical ground.

The application of perturbation theory to a system with a large number of interacting particles is fraught with many difficulties. Typical calculations in statistical mechanics analyze the asymptotic properties of the system in the thermodynamic limit, the number of particles $N \rightarrow \infty$ while V/N remains constant (V is the volume of the system). However, the application of perturbation theory directly to a large system of interacting particles can lead to terms proportional in V , which become divergent in the thermodynamic limit. Also, a statistical mechanical system can have a very dense energy spectrum where the distance between the energy levels tends to zero as $V \rightarrow \infty$. The application of perturbation theory to the system of particles leads to a situation where the perturbation energy is much larger than the distance between the energy levels. Therefore, these perturbations can lead to large changes in the wave function and the energy of the system [11].

A convenient way to eliminate these difficulties is through the use of Green's Function techniques. For example, the use of Green's functions can find expansions for the energy that

are not proportional to arbitrary powers of volume. In this way, the technique allows for the application of perturbation theory to systems of a large number of particles indirectly. Therefore, many of the complications mentioned above are avoided using the Green's function method.

2.2 A Beginner's Guide to Green's Functions

Green's functions are a generalization of the correlation function and are intimately connected with the calculation of observed quantities. This section will focus on what is called double time Green's functions. The three types of double time Green's functions are defined as

$$G_c(t, t') = \langle\langle A(t)|B(t') \rangle\rangle_c = -i\langle TA(t)B(t') \rangle \quad 2.1$$

$$G_r(t, t') = \langle\langle A(t)|B(t') \rangle\rangle_r = -i\theta(t - t')\langle[A(t), B(t')]_\eta \rangle \quad 2.2$$

$$G_a(t, t') = \langle\langle A(t)|B(t') \rangle\rangle_a = i\theta(t' - t)\langle[A(t), B(t')]_\eta \rangle. \quad 2.3$$

In 2.1, 2.2, and 2.3 the $\langle \dots \rangle$ operator is taken to be the statistical average over the grand canonical ensemble and Q is taken to be the partition function for the grand ensemble as shown below.

$$\langle \dots \rangle = Q^{-1} \text{Tr}(e^{-\beta\mathcal{H}} \dots)$$

$$Q = \text{Tr}(e^{-\beta\mathcal{H}})$$

\mathcal{H} is the Hamiltonian defined in the grand canonical ensemble in the usual manner as

$$\mathcal{H} = H - \mu N.$$

This relation has H as the time independent Hamiltonian operator, N as the operator of the total number of particles, and μ as the chemical potential of the system. The use of the grand canonical ensemble lifts the restriction that number of particles or quantized fields must be constant in the system.

The terms $A(t)$ and $B(t')$ are the Heisenberg representations of the operators A and B , expressed in the language of second quantization,

$$A(t) = e^{i\mathcal{H}t} A e^{-i\mathcal{H}t}.$$

The Heisenberg equation of motion for $A(t)$ is

$$i \frac{dA(t)}{dt} = [A(t), H]$$

with $\hbar = 1$.

The time-ordered operator, T , is defined as

$$TA(t)B(t') = \theta(t - t')A(t)B(t') + \eta\theta(t' - t)B(t')A(t)$$

and the step function as

$$\theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases}$$

Finally, $[A, B]_\eta$ indicates either commutator ($\eta = 1$) or the anticommutator ($\eta = -1$)

$$[A, B]_\eta = AB - \eta BA.$$

For double time Green's Functions, the choice of the sign of η is taken as a matter of convenience for a particular problem. Generally, η is taken in relation to the commutation relations for the Boson and Fermion operators as will be discussed later on.

The cyclic properties of the trace can be used along with the definition of the Heisenberg representation to show that

$$G_c(t, t') = G_c(t - t')$$

$$G_r(t, t') = G_r(t - t')$$

$$G_a(t, t') = G_a(t - t').$$

The Green's functions do not rely upon a separate time variable for each operator, but rather on the difference between the two times. This is an advantageous characteristic of double time Green's functions that allows the use of spectral expansions to help with the solution of the Green's function equations [12].

The equation of motion that must be solved can be built by first taking the derivative of a general double time Green's function, G , which yields

$$i \frac{dG}{dt} = i \frac{d}{dt} \langle\langle A|B \rangle\rangle = \frac{d\theta(t-t')}{dt} \langle[A(t), B(t')]_\eta\rangle + \langle\langle i \frac{dA(t)}{dt} | B(t') \rangle\rangle.$$

Using the equation of motion for A in the Heisenberg representation gives

$$i \frac{dG}{dt} = \frac{d\theta(t-t')}{dt} \langle [A(t), B(t')]_{\eta} \rangle + \langle \langle [A(t), H] | B(t') \rangle \rangle$$

$$i \frac{dG}{dt} = \delta(t-t') \langle [A(t), B(t')]_{\eta} \rangle + \langle \langle [A(t), H] | B(t') \rangle \rangle.$$

Where the final line uses the relation

$$\theta(t) = \int_{-\infty}^t \delta(t') dt'. \quad 2.4$$

It should be noted that the Green's function that appears on the right hand side, $\langle \langle [A(t), H] | B(t') \rangle \rangle$, is generally of higher order than the original one. Constructing another equation of motion for the new higher order Green's function will generally lead to terms of even higher order. Continued construction of the equations of motion will lead to an infinite chain of coupled equations in most cases of interacting particles and the solution of these equations is an extremely complicated endeavor. The general approach is to use some sort of approximation scheme to decouple the equations and reduce the chain to a finite number of equations that can be solved. However, there is no general prescription for this uncoupling process.

2.2.1 Spectral Representations of Correlation Functions

The Green's function equations of motion must be supplemented with boundary conditions by means of spectral theorems. These spectral relations will reveal a relationship between the Green's functions and statistical mechanical correlation functions.

After defining correlation functions as

$$F_{AB} = \langle A(t)B(t') \rangle; F_{BA} = \langle B(t')A(t) \rangle,$$

the spectral representations can be found to be [13]

$$F_{BA}(t - t') = \int e^{-i\omega(t-t')} J(\omega) d\omega$$

$$F_{AB}(t - t') = \int e^{-i\omega(t-t')} e^{\frac{\omega}{\theta}} J(\omega) d\omega$$

$$J(\omega) = Q^{-1} \sum_{\alpha\beta} e^{\frac{E_\beta}{\theta}} A_{\alpha\beta} B_{\beta\alpha} \delta(\omega - E_\beta + E_\alpha).$$

The method is to expand the statistical averaging brackets in terms of eigenfunctions of the Hamiltonian and then use the cyclical properties of the trace to rearrange terms. The above equations use the eigenfunction relationship

$$\mathcal{H}|\alpha\rangle = E_\alpha|\alpha\rangle.$$

Also, $J(\omega)$ is known as the spectral intensity of the correlation function.

2.2.2 Spectral Representations of Retarded and Advanced Green's functions

The spectral representation of the retarded and advanced Green's functions can be found by starting with the Fourier transform of G_r defined as

$$G_r(t - t') = \int e^{iE(t-t')} G_r(E) dE$$

$$G_r(E) = \frac{1}{2\pi} \int e^{iE(t)} G_r(t) dt.$$

Using the spectral representation of the correlation functions and the definition of the retarded Green's function, a new form for the retarded Green's function is found as

$$G_r(E) = \frac{-i}{2\pi} \int d\omega J(\omega) [e^{\frac{\omega}{\theta}} - \eta] \int dt \theta(t) e^{i(E-\omega)t}.$$

A relationship between the E and ω is found by using the integral form of the step function, 2.4, and performing a contour integration over the t variable,

$$G_r(E) = \frac{1}{2\pi} \int d\omega J(\omega) [e^{\frac{\omega}{\theta}} - \eta] \frac{1}{(E - \omega + i\varepsilon)}.$$

A similar calculation of the Fourier component of G_a can be done and then combined with G_r to get

$$G_a(E) = \frac{1}{2\pi} \int d\omega J(\omega) [e^{\frac{\omega}{\theta}} - \eta] \frac{1}{E - \omega \pm i\varepsilon} \quad 2.5$$

All the calculations up to this point have assumed that E is a real number, by considering E to be a complex quantity the function can be extended analytically into the complex plane.

$$G_a(E) = \begin{cases} G_r(E) & \text{Im } E > 0 \\ G_a(E) & \text{Im } E < 0 \end{cases}$$

If a cut is made along the real axis, the new complex function consists of two branches with G_r in the upper half-plane and G_a in the lower half-plane.

Now, $J(\omega)$ can be solved for by taking the difference between these two Green's functions.

$$G_r(E) - G_a(E) = \frac{1}{2\pi} \int d\omega J(\omega) [e^{\frac{\omega}{\theta}} - \eta] \left(\frac{1}{E - \omega + i\varepsilon} - \frac{1}{E - \omega - i\varepsilon} \right)$$

Applying the δ -function representation

$$\delta(x) = \frac{1}{2\pi i} \left(\frac{1}{x - i\varepsilon} - \frac{1}{x + i\varepsilon} \right),$$

to the above gives a relationship between the spectral intensity $J(\omega)$ and $G_a(E)$.

$$G_r(E) - G_a(E) = iJ(\omega) [e^{\frac{\omega}{\theta}} - \eta] \tag{2.6}$$

The steps to finding an expression for the double time correlation functions are

1. Solve for the Green's function by finding a way to truncate the infinite chain of equations
2. Construct the spectral intensity from our retarded and advanced Green's functions
3. Solve for the correlation function

$$\begin{aligned}
F_{BA}(t - t') &= \int e^{-i\omega(t-t')} J(\omega) d\omega \\
&= \int e^{-i\omega(t-t')} i \frac{G_a(E) - G_r(E)}{e^{\frac{\omega}{\theta}} - \eta} d\omega
\end{aligned}$$

Also, the symbolical identity for the delta function,

$$\frac{1}{x \pm i\varepsilon} = PV \frac{1}{x} \mp i\pi\delta(x),$$

shows a connection between the imaginary and real parts of the Green's functions that have the form of dispersion relations. In this equation, PV stands for the principal value of the integral.

Using the identity in 2.6 yields

$$\text{Re } G_r(E) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\text{Im } G_r(E)}{\omega - E} d\omega$$

$$\text{Re } G_a(E) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\text{Im } G_a(E)}{\omega - E} d\omega.$$

2.2.3 Finding the Green's function of a Perfect Quantum Gas

As an example of using Green's Function techniques, consider a perfect quantum gas where interactions between particles are negligible compared the kinetic energies. The Hamiltonian for a non-interacting gas composed entirely of identical fermions or bosons is

$$\mathcal{H} = \sum_k T_k a_k^\dagger a_k.$$

Here k is the momentum, $T_k = k^2/2m - \mu$, and with μ as the chemical potential. The operators a_k^\dagger and a_k represent creation and annihilation operators obeying the Fermi-Dirac or Bose-Einstein commutation relations

$$[a_f, a_{f'}^\dagger]_\epsilon = a_f a_{f'}^\dagger - \epsilon a_{f'}^\dagger a_f = \delta_{ff'}, \text{ and } a_f a_{f'} - \epsilon a_{f'} a_f = a_f^\dagger a_{f'}^\dagger - \epsilon a_{f'}^\dagger a_f^\dagger = 0.$$

Bose-Einstein particles have $\epsilon = 1$ and Fermi-Dirac particles use $\epsilon = -1$.

The Green's function related to the double time correlation function $\langle a_f^\dagger(t) a_f(t') \rangle$ will be calculated. Using the definitions of the Green's functions as expressed in 2.1, 2.2, and 2.3, we introduce the following function

$$G_f(t - t') = \langle \langle a_f(t) | a_f^\dagger(t') \rangle \rangle.$$

The equation of motion for $G_f(t - t')$ is calculated as

$$i \frac{dG_f}{dt} = \delta(t - t') \langle [a_f(t), a_f^\dagger(t')]_\epsilon \rangle + \langle \langle i \frac{da_f^\dagger}{dt} | a_f^\dagger(t') \rangle \rangle.$$

The inhomogeneous term is only non-zero when $t = t'$, therefore both operators in the commutator have the same time argument and the commutation relations can be applied.

$$i \frac{dG_f}{dt} = \delta(t - t') + T_f G_f$$

To solve the equation of motion, the Fourier transform of the Green's function is defined as

$$G_f(t - t') = \int dE e^{-(t-t')E} G_f(E).$$

In order to complete the transform, we use the following identity for the transform of the delta function.

$$\delta(t - t') = \frac{1}{2\pi} \int dE e^{-(t-t')E}$$

The equation of motion in Fourier space then becomes the simple algebraic equation

$$E G_f(E) - T_f G_f(E) = \frac{1}{2\pi}.$$

This can easily be solved for G_f as

$$G_f(E) = \frac{1}{2\pi} \frac{1}{E - T_f}$$

From this equation, it can be seen that the poles of the Green's function are directly related to the energy of a particle in state f . In the case of non-interacting particles of the

current system, the poles are on the real axis and represent the elementary excitation energies of the system. Taking into consideration interaction of particles will generally lead to singularities of a more complicated nature than just poles on the real axis or a shifting of the poles off the real axis and into the complex plane.

Using the solved form of the Green's Function and 2.6, we can solve for the Spectral Density Function

$$G_f(\omega + i\varepsilon) - G_f(\omega - i\varepsilon) = -i \left(e^{\frac{\omega}{\theta}} - \eta \right) J_f(\omega).$$

This in turn allows us to find an expression for the correlation function

$$\mathcal{F}_f(t - t') = \langle a_f^\dagger(t) a_f(t') \rangle = \int d\omega J_f(\omega) e^{-i\omega(t-t')}$$

$$\mathcal{F}_f(t - t') = \langle a_f^\dagger(t) a_f(t') \rangle = \frac{e^{-iT_f(t-t')}}{e^{\frac{T_f}{\theta}} - \eta}$$

If $t = t'$, then the correlation function reverts to the familiar occupation number for a boson or a fermion of a perfect quantum gas.

$$\langle a_f^\dagger a_f \rangle = \frac{1}{e^{\frac{T_f}{\theta}} - \eta}$$

2.2.4 Using the Green's Function Method to find Spin Polarization of the s-d Model

The system under consideration shall consist of conduction electrons interacting with localized magnetic moments through the exchange interaction as derived in section 1.2 and is placed in an external magnetic field. The Hamiltonian has the form

$$H = \sum_{k\sigma} \xi_{k\sigma} a_{k\sigma}^\dagger a_{k\sigma} - \omega_0 S_z - \frac{J}{2N} \sum_{k,k';\alpha\beta} (\mathbf{S} \cdot \boldsymbol{\sigma}_{\alpha\beta}) a_{k\sigma}^\dagger a_{k'\sigma}.$$

The first term represents the non-interacting terms for the electrons in a magnetic field \mathbf{H} . The operator $a_{k\sigma}^\dagger$ creates a particle of momentum \mathbf{k} and spin equal to $\frac{1}{2}\sigma$ (where $\sigma = \pm 1$). The coefficient on the single particle operator term is defined to be

$$\xi_{k\sigma} = (k^2/2m) - \epsilon_F - \mu_B |H|$$

with $k^2/2m$ being the usual kinetic energy, ϵ_F being the Fermi energy, and $\mu_B |H|$ representing the interaction of the electron with a magnetic field of strength $|H|$. The second term represents the interaction of the magnetic impurity with the magnetic field and $\omega_0 = g\mu_B |H|$ and g being the Lande factor ($g = 2$ for electrons). The final term represents interaction between the electron and the impurity in the form of a simple exchange interaction. In this case, J represents the strength of the interaction, N is the number of electrons, and $\boldsymbol{\sigma}$ are the Pauli spin matrices.

The retarded Green's function used in these calculations is

$$G_{kk'}^\sigma(t) = -i\theta(t) \langle [a_{k'\sigma}(t), a_{k\sigma}^\dagger(0)] \rangle = \langle \langle a_{k'\sigma}(t) | a_{k\sigma}^\dagger(0) \rangle \rangle.$$

The Fourier Transform is defined as

$$G_{kk'}^\sigma(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G_{kk'}^\sigma(\omega).$$

The density of electrons with spin σ can be calculated by

$$n^\sigma(\mathbf{r}) = \lim_{\mathbf{r} \rightarrow \mathbf{r}'} \Omega \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot \mathbf{r}} \int \frac{d^3k'}{(2\pi)^3} e^{ik' \cdot \mathbf{r}'} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) [-2\text{Im} G_{kk'}^\sigma(\omega)]$$

where Ω is the volume of the system.

The equations of motion in ω -space of the system are found to be

$$(\omega - \xi_{k'\sigma}) G_{kk'}^\sigma(\omega) + \frac{J}{2N} \sum_l (\langle \langle a_{l,-\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle + \sigma \langle \langle a_{l,\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle) = \delta_{kk'} \quad 2.7$$

$$\begin{aligned} & (\omega - \xi_{k'\sigma}) \langle \langle a_{k'\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle + \frac{J}{2N} \sum_l [\langle \langle a_{l,-\sigma} S_{-\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle + \sigma \langle \langle a_{l,\sigma} S_z^2 | a_{k\sigma}^\dagger \rangle \rangle] \\ & + \frac{J}{2N} \sum_{l,l'} \sigma [\langle \langle a_{l,\sigma} a_{l,-\sigma}^\dagger a_{l',\sigma}^\dagger S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle - \langle \langle a_{k',\sigma} a_{l,\sigma}^\dagger a_{l',-\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle] \\ & = \langle S_z \rangle \delta_{kk'} \end{aligned} \quad 2.8$$

$$\begin{aligned}
& (\omega - \xi_{k' - \sigma} + \sigma \omega_0) \langle \langle a_{k' - \sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle \\
& + \frac{J}{2N} \sum_l [S(S+1) G_{kl}^\sigma(\omega) - \langle \langle a_{l\sigma} S_z^2 | a_{k\sigma}^\dagger \rangle \rangle - \sigma \langle \langle a_{l, -\sigma} S_z S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle \\
& + \sigma \langle \langle a_{l\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle] \\
& + \frac{J}{2N} \sum_{l, l'} [\langle \langle a_{k', -\sigma} a_{l, \sigma}^\dagger a_{l', \sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle - \langle \langle a_{k', -\sigma} a_{l, -\sigma}^\dagger a_{l', -\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle \\
& - 2\sigma \langle \langle a_{k', -\sigma} a_{l, -\sigma}^\dagger a_{l', \sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle] = 0
\end{aligned} \tag{2.9}$$

As an example, 2.7 is worked out explicitly to give a feeling on how these kinds of calculations are performed.

$$\omega G_{kk'}^\sigma(\omega) = \langle \langle [a_{k'\sigma}, a_{k\sigma}^\dagger]_\pm \rangle \rangle + \langle \langle [a_{k'\sigma}, H]_- | a_{k\sigma}^\dagger \rangle \rangle$$

It should be noted in the first line that it has not been decided whether to have a commutator or anti-commutator in the inhomogeneous term of the differential equation. Below the choice becomes the anti-commutator to take advantage of the Fermi operator's anti-commutation relations.

After inserting the definition of the Hamiltonian, the linearity property of Green's functions is used to rewrite the equation of motion.

$$\omega G_{kk'}^\sigma(\omega) = \langle [a_{k'\sigma}, a_{k\sigma}^\dagger]_+ \rangle + \left\langle \left[a_{k'\sigma}, \sum_{l\sigma} \xi_{l\sigma} a_{l\sigma}^\dagger a_{l\sigma} - \omega_0 S_z - \frac{J}{2N} \sum_{l,l';\alpha\beta} (\mathbf{s} \cdot \boldsymbol{\sigma}_{\alpha\beta}) a_{l\sigma}^\dagger a_{l'\sigma} \right]_- \right| a_{k\sigma}^\dagger \rangle$$

$$\begin{aligned} \omega G_{kk'}^\sigma(\omega) &= \langle [a_{k'\sigma}, a_{k\sigma}^\dagger]_+ \rangle + \sum_{l\sigma} \xi_{l\sigma} \langle [a_{k'\sigma}, a_{l\sigma}^\dagger a_{l\sigma}]_- | a_{k\sigma}^\dagger \rangle - \omega_0 \langle [a_{k'\sigma}, S_z]_- | a_{k\sigma}^\dagger \rangle \\ &\quad - \frac{J}{2N} \sum_{l,l'\sigma} \langle [a_{k'\sigma}, (S_\sigma a_{l-\sigma}^\dagger a_{l\sigma} + \sigma' S_z a_{l\sigma}^\dagger a_{l'\sigma}')]_- | a_{k\sigma}^\dagger \rangle \end{aligned}$$

$$\begin{aligned} \omega G_{kk'}^\sigma(\omega) &= \langle [a_{k'\sigma}, a_{k\sigma}^\dagger]_+ \rangle + \sum_{l\sigma} \xi_{l\sigma} \langle [a_{k'\sigma}, a_{l\sigma}^\dagger a_{l\sigma}]_- | a_{k\sigma}^\dagger \rangle - \omega_0 \langle [a_{k'\sigma}, S_z]_- | a_{k\sigma}^\dagger \rangle \\ &\quad - \frac{J}{2N} \sum_{l,l'\sigma} \{ \langle [S_\sigma [a_{k'\sigma}, a_{l-\sigma}^\dagger a_{l'\sigma}']]_- | a_{k\sigma}^\dagger \rangle + \sigma' \langle [S_z [a_{k'\sigma}, a_{l\sigma}^\dagger a_{l'\sigma}']]_- | a_{k\sigma}^\dagger \rangle \} \end{aligned}$$

Now, solving the equation of motion is simply calculating commutation relation for raising and lowering operators. By definition, the inhomogeneous term becomes

$$[a_{k'\sigma}, a_{k\sigma}^\dagger]_+ = \delta_{k'k}$$

The kinetic term is

$$\begin{aligned} [a_{k'\sigma}, a_{l\sigma}^\dagger a_{l\sigma}]_- &= a_{k'\sigma} a_{l\sigma}^\dagger a_{l\sigma} - a_{l\sigma}^\dagger a_{l\sigma} a_{k'\sigma} \\ &= a_{k'\sigma} a_{l\sigma}^\dagger a_{l\sigma} + (\delta_{kl} - a_{k'\sigma} a_{l\sigma}^\dagger) a_{l\sigma} \end{aligned}$$

$$= a_{l\sigma} \delta_{kl}$$

Since any creation or annihilation electron operator will commute with a localized moment operator, that term becomes

$$[a_{k',\sigma}, S_z]_- = 0.$$

The raising and lowering term in the exchange interaction yields

$$\begin{aligned} [a_{k',\sigma}, a_{l-\sigma'}^\dagger a_{l'\sigma'}]_- &= a_{k',\sigma} a_{l-\sigma'}^\dagger a_{l'\sigma'} - a_{l-\sigma'}^\dagger a_{l'\sigma'} a_{k',\sigma} \\ &= a_{k',\sigma} a_{l-\sigma'}^\dagger a_{l'\sigma} - (\delta_{k'l} \delta_{\sigma,-\sigma'} - a_{k',\sigma} a_{l-\sigma'}^\dagger) a_{l'\sigma'} \\ &= \delta_{k'l} \delta_{\sigma,-\sigma'} a_{l'\sigma'}. \end{aligned}$$

Finally, the z component term of the exchange interaction is

$$\begin{aligned} [a_{k',\sigma}, a_{l\sigma'}^\dagger a_{l'\sigma'}]_- &= a_{k',\sigma} a_{l\sigma'}^\dagger a_{l'\sigma'} - a_{l\sigma'}^\dagger a_{l'\sigma'} a_{k',\sigma} \\ &= a_{k',\sigma} a_{l\sigma'}^\dagger a_{l'\sigma'} + (\delta_{k'l} \delta_{\sigma\sigma'} - a_{k',\sigma} a_{l\sigma'}^\dagger) a_{l'\sigma'} \\ &= \delta_{k'l} \delta_{\sigma\sigma'} a_{l'\sigma'} \end{aligned}$$

Now putting the results back in the equation of motion, the equation of motion are found to be

$$\omega G_{kk'}^\sigma(\omega) = \langle \delta_{klk} \rangle + \sum_{l\sigma} \xi_{l\sigma} \langle \langle a_{l\sigma} \delta_{kl} | a_{k\sigma}^\dagger \rangle \rangle - \frac{J}{2N} \sum_{l,l'\sigma'} \{ \langle \langle \delta_{k'l} \delta_{\sigma,-\sigma'} S_\sigma a_{l'\sigma'} | a_{k\sigma}^\dagger \rangle \rangle + \sigma' \langle \langle \delta_{k'l} \delta_{\sigma\sigma'} S_z a_{l'\sigma} | a_{k\sigma}^\dagger \rangle \rangle \}.$$

After applying our Kronecker symbols to the summations, replacing $l' \rightarrow l$, and isolating the inhomogeneous term on the right hand side, the equation of motion becomes

$$(\omega - \xi_{k\sigma}) G_{kk'}^\sigma(\omega) + \frac{J}{2N} \sum_l \{ \langle \langle S_{-\sigma} a_{l-\sigma} | a_{k\sigma}^\dagger \rangle \rangle + \sigma \langle \langle S_z a_{l\sigma} | a_{k\sigma}^\dagger \rangle \rangle \} = \delta_{klk}.$$

As mentioned above, construction of the equation of motion for 2.7 led to Green's functions of higher order when the commutation of $a_{k',\sigma}$ with interaction part of the Hamiltonian is calculated. Further calculations of the equations of motion of those higher order Green's functions (2.8 and 2.9) created even higher order Green's functions. In this manner, the infinite chain of coupled equations of motion that results can be seen.

The chain of equations will be truncated by attempting a reasonable approximation that eliminates all higher order Green's functions and allows us to solve our original equation of motion. For this particular problem, only keep terms that are of $O(J)$ in 2.8 and 2.9 were kept. This approximation will lead to terms $O(J^2)$ in our original equation of motion 2.7.

The first order of business is to examine the equations of motion for the Green's functions in 2.8 and 2.9 for any terms that are of zero order in J since any other terms will be of $O(J^2)$ when we insert them back into 2.8 and 2.9.

Applying this approximation, yields the following equations to $O(J)$.

$$(\omega - \xi_{k'\sigma}) \langle\langle a_{k'\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle + \frac{J}{2N} \sum_l \langle S_z^2 \rangle \frac{\delta_{kl}}{(\omega - \xi_{l\sigma})} = \langle S_z \rangle \delta_{kk'} \quad 2.10$$

$$\begin{aligned} (\omega - \xi_{k'-\sigma} + \sigma\omega_0) \langle\langle a_{k'-\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle\rangle + \frac{J}{2N} \sum_l \langle S_\sigma S_{-\sigma} \rangle \frac{\delta_{kl}}{(\omega - \xi_{l\sigma})} \\ - 2\sigma \frac{J}{2N} \sum_{l,l'} \langle\langle a_{k',-\sigma} a_{l,-\sigma}^\dagger a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle = 0 \end{aligned} \quad 2.11$$

The terms in 2.10 can be rearranged to give

$$\langle\langle a_{k'\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle = \frac{1}{(\omega - \xi_{k'\sigma})} \left\{ \langle S_z \rangle \delta_{kk'} - \frac{J}{2N} \sum_l \langle S_z^2 \rangle \frac{\delta_{kl}}{(\omega - \xi_{l\sigma})} \right\}.$$

The application the Kronecker symbol to the summation in 2.10 finally yields

$$\langle\langle a_{k'\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle = \frac{\langle S_z \rangle \delta_{kk'}}{(\omega - \xi_{k'\sigma})} - \frac{J}{2N} \frac{\langle S_z^2 \rangle}{(\omega - \xi_{k'\sigma})(\omega - \xi_{k\sigma})}. \quad 2.12$$

In 2.11, a commutation relation will be used on the last Green's function before applying any approximations

$$\langle\langle a_{k',-\sigma} a_{l,-\sigma}^\dagger a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle = \langle\langle (\delta_{lk'} - a_{l,-\sigma}^\dagger a_{k',-\sigma}) a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle$$

$$\begin{aligned}
&= \delta_{lk'} \langle \langle a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle + \langle \langle a_{l,-\sigma}^\dagger a_{k',-\sigma} a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle \\
&= \delta_{lk'} \langle \langle a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle + \frac{\delta_{l'k} \langle a_{l,-\sigma}^\dagger a_{k',-\sigma} S_z \rangle}{\omega - \xi_{l'\sigma} - \xi_{k',-\sigma} + \xi_{l,-\sigma}} + O(J).
\end{aligned}$$

Also, the expectation value on the inhomogeneous term will be approximated to zeroth order,

$$\langle a_{l,-\sigma}^\dagger a_{k',-\sigma} S_z \rangle = \delta_{lk'} \langle S_z \rangle f(\xi_{l,-\sigma}).$$

Where $f(\xi_{l,-\sigma})$ is the Fermi-Dirac distribution function for the system.

The application of these approximations gives

$$\langle \langle a_{k',-\sigma} a_{l,-\sigma}^\dagger a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle = \delta_{lk'} \langle \langle a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle + \frac{\delta_{l'k} \delta_{lk'} \langle S_z \rangle f(\xi_{l,-\sigma})}{\omega - \xi_{l'\sigma} - \xi_{k',-\sigma} + \xi_{l,-\sigma}} + O(J)$$

for the higher order Green's function in 2.11. By dropping the terms that are $O(J)$ since they will be $O(J^2)$ when reinserted into 2.11, the order of the Green's function is reduced and an inhomogeneous term has been introduced through the approximation.

Inserting this result back into 2.11 gives

$$\begin{aligned}
&(\omega - \xi_{k',-\sigma} + \sigma\omega_0) \langle \langle a_{k',-\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle \rangle + \frac{J}{2N} \sum_l \langle S_\sigma S_{-\sigma} \rangle \frac{\delta_{kl}}{(\omega - \xi_{l\sigma})} \\
&- 2\sigma \frac{J}{2N} \sum_{l,l'} \left\{ \delta_{lk'} \langle \langle a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle \rangle + \frac{\delta_{l'k} \delta_{lk'} \langle S_z \rangle f(\xi_{l,-\sigma})}{\omega - \xi_{l'\sigma} - \xi_{k',-\sigma} + \xi_{l,-\sigma}} \right\} = 0.
\end{aligned}$$

Taking the $\langle\langle a_{l',\sigma} S_z | a_{k\sigma}^\dagger \rangle\rangle$ term to $O(J)$ gives

$$(\omega - \xi_{k'-\sigma} + \sigma\omega_0) \langle\langle a_{k'-\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle\rangle + \frac{J}{2N} \sum_l \langle S_\sigma S_{-\sigma} \rangle \frac{\delta_{kl}}{(\omega - \xi_{l\sigma})} - 2\sigma \frac{J}{2N} \sum_{l,l'} \left\{ \delta_{lk'} \frac{\delta_{kl'} \langle S_z \rangle}{(\omega - \xi_{l'\sigma})} + \frac{\delta_{l'k} \delta_{lk'} \langle S_z \rangle f(\xi_{k',-\sigma})}{\omega - \xi_{l'\sigma} - \xi_{k',-\sigma} + \xi_{l,-\sigma}} \right\} = 0.$$

Some algebraic rearranging of terms and keeping in mind that $[S_\sigma, S_{-\sigma}] = 2\sigma S_z$ gives the final expression for 2.11 as

$$\langle\langle a_{k'-\sigma} S_{-\sigma} | a_{k\sigma}^\dagger \rangle\rangle = \frac{-J/2N}{(\omega - \xi_{k'-\sigma} + \sigma\omega_0)(\omega - \xi_{k\sigma})} \{ \langle S_{-\sigma} S_\sigma \rangle - 2\sigma \langle S_z \rangle f(\xi_{k',-\sigma}) \}. \quad 2.13$$

Next, both of the equations of motion that have been approximated to $O(J)$ (now 2.12 and 2.13) are placed in the original Green's function for $G_{kk'}^\sigma(\omega)$ to develop an equation of motion that is $O(J^2)$.

$$(\omega - \xi_{k\sigma}) G_{kk'}^\sigma(\omega) = \delta_{kk'} - \frac{J}{2N} \sum_l \frac{-J/2N}{(\omega - \xi_{l-\sigma} + \sigma\omega_0)(\omega - \xi_{k\sigma})} \{ \langle S_{-\sigma} S_\sigma \rangle - 2\sigma \langle S_z \rangle f(\xi_{l,-\sigma}) \} + \sigma \frac{J}{2N} \sum_l \frac{\langle S_z \rangle \delta_{kl}}{(\omega - \xi_{l\sigma})} - \frac{J}{2N} \frac{\sigma \langle S_z^2 \rangle}{(\omega - \xi_{l\sigma})(\omega - \xi_{k\sigma})}$$

The expression can be simplified by assuming a constant density of states with this definition,

$$\sum_k \frac{1}{\omega - \xi_k} = -i\pi\rho.$$

After doing some algebraic rearranging, we arrive at the following expression

$$G_{kk'}^\sigma(\omega) = \delta_{kk'} - \frac{J/2N \left(\frac{-J}{2N} \left\{ -i\pi\rho \langle S_{-\sigma} S_\sigma \rangle - \sum_l \frac{2\sigma \langle S_z \rangle f(\xi_{l-\sigma})}{(\omega - \xi_{l-\sigma} + \sigma\omega_0)} \right\} + \sigma \langle S_z \rangle + \frac{i\pi J\rho}{2N} \langle S_z^2 \rangle \right)}{(\omega - \xi_{k'\sigma})(\omega - \xi_{k\sigma})}$$

Next, applying the identity

$$\frac{1}{x \pm i\varepsilon} = PV \frac{1}{x} \mp i\pi\delta(x)$$

to the remaining summation and convert the remaining summation into an integral. The application of the identity to the term with the summation yields

$$-2\sigma \langle S_z \rangle \rho \int d\xi \left(PV \frac{1}{(\omega + \sigma\omega_0 - \xi)} - i\pi\delta(\omega + \sigma\omega_0 - \xi) \right) f(\xi)$$

$$\rightarrow -2\sigma \langle S_z \rangle \rho (g(\omega + \sigma\omega_0) - i\pi f(\omega + \sigma\omega_0)).$$

Where

$$g(\omega) \simeq \text{Re} \rho \int_{-D}^D d\xi \frac{f(\xi)}{\omega - \xi}$$

and D is the cutoff on the integral that is assumed to be of the order of ϵ_F , the Fermi energy.

Putting this result back into the equation for $G_{kk'}^\sigma(\omega)$ gives the result

$$G_{kk'}^{\sigma}(\omega) = \frac{\delta_{kk'}}{(\omega - \xi_{k'\sigma})} - \frac{J/2N \left(\sigma \langle S_z \rangle + \frac{Ji\pi\rho \{ \langle S_{-\sigma} S_{\sigma} \rangle + \frac{\langle S_z^2 \rangle}{2N} + f(\omega + \sigma\omega_0) \}}{2N} + \sigma \langle S_z \rangle \frac{J}{N} g(\omega + \sigma\omega_0) \right)}{(\omega - \xi_{k'\sigma})(\omega - \xi_{k\sigma})}$$

The function $g(\omega)$ can be evaluated in terms of $\beta(\equiv 1/kT)$ and the cutoff variable to give

$$g(\omega) = \rho \left[\ln \frac{2\pi}{\beta D} + \text{Re} \Psi \left(\frac{1}{2} + \frac{i\beta\omega}{2\pi} \right) \right]$$

where $\Psi(z)$ is the digamma function defined as

$$\Psi(z) = [d/dz] \ln \Gamma(z).$$

Based upon the properties of $\Psi(z)$, the limiting form of $g(\omega)$ as $\beta\omega \gg 1$ ($T \rightarrow 0$)

$$g(\omega) \rightarrow \rho \ln \frac{|\omega|}{D}$$

In the calculation of the spin polarization, the assumption will be that the polarization is due to some sort of internal crystalline field by letting $\xi_{k\sigma} \rightarrow \xi_k = (k^2/2m) - \epsilon_F$. Starting with the definition of electron density

$$n^{\sigma}(\mathbf{r}) = \Omega \int \frac{d^3k}{(2\pi)^3} e^{ik \cdot \mathbf{r}} \int \frac{d^3k'}{(2\pi)^3} e^{-ik' \cdot \mathbf{r}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) [-2\text{Im} G_{kk'}^{\sigma}(\omega)],$$

the polarization is defined to be

$$P(\mathbf{r}) = \sum_{\sigma} \sigma n^{\sigma}(\mathbf{r}) = \Omega \int \frac{d^3 k}{(2\pi)^3} e^{ik \cdot \mathbf{r}} \int \frac{d^3 k'}{(2\pi)^3} e^{-ik' \cdot \mathbf{r}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) \left[-2Im \sum_{\sigma} \sigma G_{kk'}^{\sigma}(\omega) \right].$$

Calculating the summation over the spins of the Green's functions and recombining terms yields

$$\begin{aligned} \sum_{\sigma} \sigma G_{kk'}^{\sigma}(\omega) &= \frac{J/2N}{(\omega - \xi_{k'\sigma})(\omega - \xi_{k\sigma})} \left(-2\langle S_z \rangle - \langle S_z \rangle \frac{J}{N} (g(\omega + \omega_0) + g(\omega - \omega_0)) \right) \\ &\quad + \frac{Ji\pi\rho}{2N} \{f(\omega - \omega_0) - f(\omega + \omega_0)\} \end{aligned}$$

Next, the integrations over k, k' are calculated and give

$$\begin{aligned} P(\mathbf{r}) &= \frac{-\pi m^2}{r^2} \frac{\Omega}{(2\pi^2)^2} \left[\int_{-\epsilon_F}^{\infty} d\omega f(\omega) \frac{J}{2N} \left(2\langle S_z \rangle + \langle S_z \rangle \frac{J}{N} (g(\omega + \omega_0) + g(\omega - \omega_0)) \right) \sin 2kr \right. \\ &\quad + \int_{-\epsilon_F}^{\infty} d\omega f(\omega) \frac{\pi\rho}{2} \left(\frac{J}{N} \right)^2 \langle S_z \rangle \{1 - f(\omega - \omega_0) - f(\omega + \omega_0)\} \cos 2kr \\ &\quad \left. + \int_{-\infty}^{-\epsilon_F} d\omega f(\omega) \frac{\pi\rho}{2} \left(\frac{J}{N} \right)^2 \langle S_z \rangle \{1 - f(\omega - \omega_0) - f(\omega + \omega_0)\} e^{-2k'r} \right]. \end{aligned}$$

Now, calculating the integral at $T = 0$ for the term that is linear in J gives for the polarization

$$P_{\text{RKKY}}(\mathbf{r}) = 3\pi n \left(\frac{J\rho}{N} \right) \langle S_z \rangle \frac{j_1(2k_F r)}{(k_F r)^2}.$$

In the above, $j_1(z)$ is the spherical Bessel function of the first kind and $n = k_F^3/6\pi^2$. This matches the standard RKKY polarization result using a different method of calculation, but note that there will be a modification the RKKY polarization due to the terms that are of higher order in J . For more details on the terms that modify the RKKY polarization, the reader is referred to [14].

CHAPTER 3
ASYMPTOTIC ESTIMATION OF FOURIER TRANSFORMS

3.1 Introduction

An asymptotic expansion of a given function is a series of functions that when truncated provides an approximation to the given function as the argument of the function tends to a particular point. Repeated applications of the integration by parts technique to an integral will often produce an asymptotic expansion. Although a Taylor series fits the above definition, the term asymptotic series generally implies a non-convergent series.

It is not always possible to calculate an exact expression for the Fourier transform of a particular function. In these cases it is necessary to construct an asymptotic expression to be able to calculate an approximate expression of the Fourier transform. The asymptotic expression of a Fourier transform is defined as an expression that is the sum of a simpler Fourier transform and a remainder which tends to zero as the argument of the function tends to a particular point. However, the building of asymptotic expressions requires generalized function theory.

3.2 Introduction to the Theory of Generalized Functions

Before the concept of generalized functions can be introduced, *good functions* and *fairly good functions* must be defined [15].

A *good function* is an ordinary function that is differentiable any number of times and the function and all its derivative are $O(|x|^{-N})$ as $|x| \rightarrow \infty$ for all N . In other words, A *good function* is a function that obeys

$$\lim_{x \rightarrow \pm\infty} x^m f^{(n)}(x) = 0$$

for any positive integers m, n . Some examples of *good functions* include

$$e^{-x^2}, xe^{-x^2}, \frac{e^{-x^2}}{1+x^2}.$$

In contrast, $e^{-|x|}$ is not a good function since it is not differentiable at zero and $\frac{1}{1+x^2}$ is not a good function because

$$\lim_{x \rightarrow \infty} \frac{x^3}{1+x^2} \rightarrow \infty.$$

Therefore it fails the basic limit test set forth above.

A *fairly good* function is one which differentiable everywhere any number of times and such that the function and all its derivatives are $O(|x|^N)$ as $|x| \rightarrow \infty$ for all N . Any polynomial function is a fairly good function as the n th order term is $O(|x|^N)$ and it can be differentiated any number of times. Note that the definitions of *fairly good* functions differs from *good functions* by $O(|x|^N)$ instead of $O(|x|^{-N})$.

The derivative of a *good function* is a *good function*. The sum of two *good functions* is a *good function*. The product of a *fairly good function* with a *good function* is a *good function*.

These statements are offered without proof and the interested reader is referred to [16] for details.

If $f(x)$ is a *good function*, then

$$g(y) = \int_{-\infty}^{\infty} f(x)e^{-2\pi ixy} dx,$$

is a *good function*.

The theorem can be proven by differentiating the transform p times with respect to y and then using integration by parts N times. Next, the application of the definition of a *good function* eliminates the boundary terms left by multiple applications of integration by parts which gives

$$\begin{aligned} |g^p(y)| &= \left| \frac{1}{(2\pi i)^N} \int_{-\infty}^{\infty} \frac{d^N}{dx^N} \{(-2\pi i x)^p f(x)\} e^{-2\pi ixy} dx \right| \\ &\leq \frac{(2\pi)^{p-N}}{|y|^N} \int_{-\infty}^{\infty} \left| \frac{d^N}{dx^N} x^p f(x) \right| dx \\ &= O(|y|^{-N}). \end{aligned}$$

A sequence, $f_n(x)$, of *good functions* is called *regular* if

$$\lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} f_n(x) F(x) dx$$

exists for any *good function* $F(x)$.

The function e^{-x^2/n^2} is *regular* as can be shown.

$$\lim_{n \rightarrow \infty} \int_{-\infty}^{\infty} e^{-x^2/n^2} F(x) dx = \int_{-\infty}^{\infty} \lim_{n \rightarrow \infty} e^{-x^2/n^2} F(x) dx$$

$$= \int_{-\infty}^{\infty} F(x) dx.$$

A generalized function is defined as a *regular* sequence of *good functions*. Furthermore, any two *regular* sequences of *good functions* that each has the same effect on another *good function* $F(x)$ are considered to be the same generalized function.

An example of a generalized function that familiar to every physicist is the delta function, $\delta(x)$. The delta function can be represented as several different *regular* function sequences that all have the same effect on the $F(x)$ they are acting on. An example of a generalized function representing $\delta(x)$ is

$$\lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} e^{-|2x|/\epsilon}.$$

Applying test for a *regular* sequence gives

$$\lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{1}{\epsilon} e^{-|2x|/\epsilon} F(x) dx$$

$$\int_{-\infty}^{\infty} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} e^{-|2x|/\epsilon} F(x) dx.$$

As the limit $\epsilon \rightarrow 0$ is taken, the *regular* sequence define above takes a value of 1 at $x = 0$ and zero for $x \neq 0$. Therefore, the result of the integral is $F(0)$.

A second example of a sequence representing $\delta(x)$ is

$$\lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[1 - \frac{|x|}{\epsilon} \right]$$

$$\int_{-\infty}^{\infty} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[1 - \frac{|x|}{\epsilon} \right] F(x) dx$$

$$= F(0).$$

There are many other *regular* sequences of *good functions* that all have the same effect, namely

$$\int_{-\infty}^{\infty} \delta(x) F(x) dx = F(0).$$

The entire class of *regular* sequences of *good functions* is known as the Dirac delta function and represented with the symbol $\delta(x)$.

3.2.1 Theory of the Asymptotic Expansion of Fourier Transforms

After deriving the Green's function in Fourier space, the Fourier transform must be taken again to have a function in real space in order to develop physical meaning of the solution. Unfortunately, it is not possible to know the transform of certain functions. Fortunately, the theory of generalized functions makes it possible to state the generalized function $f(x)$ as a sum of a simpler function whose transform we can calculate and a remainder that tends to zero at a certain point. The method for doing constructing the asymptotic expression of the Fourier transform will rely upon $f(x)$ having a finite number of singularities.

A generalized function has a finite number of singularities $x = x_1, x_2, x_3, \dots, x_M$ if, in each one of the intervals, $-\infty < x < x_1, x_1 < x < x_2, \dots, x_{m-1} < x < x_m, x_M < x < \infty$, $f(x)$ is equal to an ordinary function that is differentiable any number of times at every point in the interval.

A generalized function is defined as being "well behaved at infinity" if for some R the function $f(x) - F(x)$ is absolutely integrable in the interval $(-\infty, -R)$ and (R, ∞) , where $F(x)$ is some linear combination of the functions

$$e^{ikx}|x|^\beta, e^{ikx}|x|^\beta \operatorname{sgn}(x), e^{ikx}|x|^\beta \ln|x|, e^{ikx}|x|^\beta \ln|x| \operatorname{sgn}(x)$$

for different values of β and k .

The generalized Riemann-Lebesgue Lemma must also be used:

If a generalized function, $f(x)$, is absolutely integrable from $-\infty$ to ∞ , and $g(y)$ is the Fourier transform of $f(x)$, then $g(y) \rightarrow 0$ as $|y| \rightarrow \infty$.

From the definition for a finite number of singularities and the Riemann-Lebesgue Lemma, the following theorem is obtained:

If a generalized function, $f(x)$, has a finite number of singularities $x = x_1, x_2, x_3, \dots, x_M$ and if (and for each m from 1 to M) $f(x) - F_m(x)$ has an absolutely integrable N th derivative in an interval including x_m , where $F_m(x)$ is a linear combination of the type

$$|x-x_n|^\beta, |x-x_n|^\beta \operatorname{sgn}(x-x_n), |x-x_n|^\beta \ln|x-x_n|,$$

3.1

$$e^{ikx}|x-x_n|^\beta \ln|x-x_n| \operatorname{sgn}(x-x_n), \delta^p(x-x_n)$$

for different values of β and p , and if $f^{(n)}(x)$ is “well behaved at infinity” then the Fourier transform of $f(x)$ satisfies

$$g(y) = \sum_{m=1}^M G_m(y) + o(|y|^{-N}) \text{ as } |y| \rightarrow \infty,$$

where $G_m(y)$ is the Fourier transform of $F_m(x)$.

In layman's terms, the function around each singularity will give a term similar to one in 3.1 whose transform can be calculated. If each of these terms are summed together, the result is an asymptotic expression which is accurate to a certain error.

As an example of using this method, the asymptotic expression is found for the Fourier transform of $f(x) = |x||x + 1|^{1/2}|x - 1|^{-1/2}$ to $o(y^{-2})$. The singularities are seen to be $x = -1, 0$, and 1 and $f(x)$ needs to be expressed around each singularity as a summation of terms like those found 3.1. However, the sum of terms must have an error whose second derivative must be absolutely integrable in an interval that includes the singularity. Given the nature of $f(x)$, it is natural to use the binomial series to expand the function around each singularity to generate the summation of 3.1 terms.

Beginning with the $x = 0$ singularity,

$$\begin{aligned} f(x) &= |x| \left| 1 + \frac{x}{2} + \dots \right| \left| 1 + \frac{x}{2} + \dots \right| \\ &= |x| + O(|x|^2). \end{aligned}$$

The expansion of $f(x)$ around $x = -1$ yields

$$\begin{aligned} f(x) &= |x + 1 - 2|^{-1/2} |(x + 1) - 1| |x + 1|^{1/2} \\ &= \frac{1}{\sqrt{2}} \left| 1 + \frac{x + 1}{2} + \dots \right| |1 - (x + 1)| |x + 1|^{1/2} \\ &= \frac{1}{\sqrt{2}} |x + 1|^{1/2} + O(|x + 1|^{3/2}). \end{aligned}$$

Finally, expanding $f(x)$ around $x = 1$ gives

$$\begin{aligned}
f(x) &= |x-1|^{-1/2} |(x-1) + 1| |(x-1) + 2|^{1/2} \\
&= \sqrt{2} |x-1|^{-1/2} |(x-1) + 1| \left| \frac{(x-1)}{2} + 1 \right|^{1/2} \\
&= \sqrt{2} |x-1|^{-1/2} |(x-1) + 1| \left| 1 + \frac{(x-1)}{4} + \dots \right| \\
&= \sqrt{2} |x-1|^{-1/2} + \frac{5}{2\sqrt{2}} |x-1|^{1/2} \operatorname{sgn}(x-1) + O(|x-1|^{3/2}).
\end{aligned}$$

The second term relation can be gotten by recalling the definition of $\operatorname{sgn}(x) = \frac{x}{|x|}$ and

$$|x|^{-1/2} |x| = |x|^{-1/2} \sqrt{x^2} = \sqrt{\frac{x^2}{|x|}} = \sqrt{x} \operatorname{sgn}(x) = |x| \operatorname{sgn}(x).$$

Defining functions representing the 3.1 terms as

$$F_1(x) = |x|$$

$$F_2(x) = \frac{1}{\sqrt{2}} |x+1|^{1/2}$$

$$F_3(x) = \sqrt{2} |x-1|^{-1/2} + \frac{5}{2\sqrt{2}} |x-1|^{1/2} \operatorname{sgn}(x-1).$$

We can now easily check the functions for the condition that the second derivative must be $f(x) - F_m(x)$ absolutely integrable over an interval including the singularity x_m . For example around $x = 0$,

$$f(x) - F_1(x) = |x| + O(|x|^2) - |x| = O(|x|^2).$$

We calculate the first derivative of $|x|^2$ to be

$$\frac{d}{dx} |x||x| = \text{sgn}(x) |x| + |x| \text{sgn}(x) = 2|x| \text{sgn}(x) = 2x.$$

The last part of the calculation used the relation $\text{sgn}(x) = \frac{x}{|x|}$. Thus, the second derivative of $f(x) - F_1(x)$ is absolutely integrable around $x = 0$.

Next, we must take the Fourier transforms of each $F_m(x)$ so that the Fourier transform of $f(x)$ can be put into the form,

$$g(y) = \sum_{m=1}^M G_m(y) + o(|y|^{-2}).$$

The following transforms are needed are needed to complete the calculation,

$$\int_{-\infty}^{\infty} |x|^\alpha e^{-2\pi ixy} dx = -2 \sin\left(\frac{\pi}{2} \alpha\right) \alpha! (2\pi|y|)^{-\alpha-1}$$

$$\int_{-\infty}^{\infty} |x|^\alpha \text{sgn}(x) e^{-2\pi ixy} dx = -2i \cos\left(\frac{\pi}{2} \alpha\right) \alpha! (2\pi|y|)^{-\alpha-1} \text{sgn}(y)$$

$$\int_{-\infty}^{\infty} f(x \pm 1)e^{-2\pi ixy} dx = g(y)e^{\pm 2\pi iy}$$

Using the transforms and applying some algebraic manipulation yields,

$$g(y) = \sqrt{2}e^{-2\pi iy}|y|^{-1/2} - \left\{ \frac{1}{4\pi\sqrt{2}}e^{2\pi iy} + \frac{5i \operatorname{sgn}(y)}{8\pi\sqrt{2}}e^{-2\pi iy} \right\} |y|^{-3/2} - \frac{1}{2\pi^2}y^{-2} + o(|y|^{-2}).$$

To reiterate, $f(x)$ was expanded around each of its singularities and applied an approximation to write $f(x)$ as a series of terms like in the 3.1 list and an error term. Next, the 2nd derivative of each term was checked to make sure that was absolutely integrable over an interval including the singularity. Finally, the known Fourier transforms of the terms from 3.1 were calculated which lead directly to an asymptotic expression for the Fourier transform of $f(x)$ with error $o(|y|^{-2})$.

It should be noted that by including more terms from the binomial expansion around each singularity, even higher order derivatives of $f(x) - F_1(x) - F_2(x) - F_3(x)$ would be absolutely integrable over an interval including the singularity. This would lead to a smaller error in the asymptotic expression for the Fourier transform.

CHAPTER 4
EFFECT OF ELECTRON-ELECTRON INTERACTION ON S-D MODEL

4.1 Introduction

While the RKKY interaction describes the indirect interaction between two localized magnetic moments through the medium of conduction electrons, the calculations only take into account the exchange interactions between the conduction and localized electrons in the three dimensional case. In this chapter, how the addition of electron-electron interaction modifies the RKKY interaction is explored.

The first step is to calculate an effective Hamiltonian for the s-d interaction by using a canonical transformation to eliminate terms that are linear in the exchange interaction.

4.2 Calculation of a New Effective Hamiltonian via Canonical Transformation

The canonical transformation method is particularly well suited for the creation of effective Hamiltonians in indirect interactions [17]. The Hamiltonian is split into two parts, the independent and interactive part,

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int}.$$

In a similar manner to section 1.2.1, I canonically transformed the Hamiltonian and looked for an operator, S , that eliminated linear terms of the exchange interaction.

From section 1.2.1, the expansion of the transformation in terms of the original Hamiltonian

$$\tilde{\mathcal{H}} = e^S \mathcal{H} e^{-S} = \mathcal{H}_0 + \mathcal{H}_{int} + [S, \mathcal{H}_0] + [S, \mathcal{H}_{int}] + \frac{1}{2} [S, [S, \mathcal{H}_0]] + \frac{1}{2} [S, [S, \mathcal{H}_{int}]] + \dots,$$

shows that the requirement to eliminate linear interaction terms is

$$\mathcal{H}_{int} + [S, \mathcal{H}_0] = 0.$$

I used this condition along with the equation of motion for operators in the Heisenberg representation to arrive at the simple differential equation,

$$i\hbar \frac{\partial S(t)}{\partial t} = \mathcal{H}_{int}.$$

Fortunately, the differential equation has a simple solution for S ,

$$S(t) = -\frac{i}{\hbar} \int_{-\infty}^t dt' \mathcal{H}_{int}(t').$$

Next, I placed the integral equation into the series equation for $\tilde{\mathcal{H}}$ and kept just terms to second order of the interaction,

$$\tilde{\mathcal{H}} = \mathcal{H}_0(t) - \frac{i}{2\hbar} \int_{-\infty}^t dt' [\mathcal{H}_{int}(t), \mathcal{H}_{int}(t')]. \quad 4.1$$

I replaced $\mathcal{H}_{int}(t)$ with the form of the s-d interaction,

$$\mathcal{H}_{int} = - \sum_{\alpha} \sum_{k',k} \sum_n \frac{J}{N} \left[S_{\alpha}^n a_{k',-\alpha}^{\dagger} a_{k,\alpha} + \alpha S_z^n a_{k',\alpha}^{\dagger} a_{k,\alpha} \right].$$

Where J is assumed to be a constant, S_{σ}^n is the spin operator for a localized moment at site n and α , which indicates the raising (\uparrow) or lowering (\downarrow) operator. The conduction electrons are represented by $a_{k,\alpha}^{\dagger}$ and $a_{k,\alpha}$, the usual creation and annihilation operators for an electron with momentum k and spin $\alpha = \uparrow, \downarrow$. After inserting the s-d interaction into 4.1, the transformed Hamiltonian becomes

$$\begin{aligned} \tilde{\mathcal{H}} = \mathcal{H}_0(t) - \frac{i}{2\hbar} \sum_{k,k',\alpha} \sum_{l,l',\alpha'} \sum_{n,n'} \left(\frac{J}{N} \right)^2 \int_{-\infty}^t dt' & \left[S_{\alpha}^n(t) a_{k',-\alpha}^{\dagger}(t) a_{k,\alpha}(t) \right. \\ & \left. + \alpha S_z^n(t) a_{k',\alpha}^{\dagger}(t) a_{k,\alpha}(t) \right], S_{\alpha'}^{n'}(t') a_{l',-\alpha'}^{\dagger}(t') a_{l,\alpha'}(t') + \alpha' S_z^{n'}(t') a_{k',\alpha'}^{\dagger}(t') a_{k,\alpha'}(t') \left. \right]. \end{aligned}$$

Next, basic commutation relations were applied to the commutator to expand it as

$$\begin{aligned} & \left[S_{\alpha}^n(t) a_{k',-\alpha}^{\dagger}(t) a_{k,\alpha}(t), S_{\alpha'}^{n'}(t') a_{l',-\alpha'}^{\dagger}(t') a_{l,\alpha'}(t') \right] + \\ & \left[S_{\alpha}^n(t) a_{k',-\alpha}^{\dagger}(t) a_{k,\alpha}(t), \alpha' S_z^{n'}(t') a_{k',\alpha'}^{\dagger}(t') a_{k,\alpha'}(t') \right] + \\ & \left[\alpha S_z^n(t) a_{k',\alpha}^{\dagger}(t) a_{k,\alpha}(t), S_{\alpha'}^{n'}(t') a_{l',-\alpha'}^{\dagger}(t') a_{l,\alpha'}(t') \right] + \\ & \left[\alpha S_z^n(t) a_{k',\alpha}^{\dagger}(t) a_{k,\alpha}(t), \alpha' S_z^{n'}(t') a_{k',\alpha'}^{\dagger}(t') a_{k,\alpha'}(t') \right]. \end{aligned}$$

Since each of the above commutators can be treated the same in the following calculation, I worked with the a general form of the above commutators

$$\left[S^n(t) a_{k',\alpha}^\dagger(t) a_{k,\alpha'}(t) , S^{n'}(t') a_{l',s}^\dagger(t') a_{l,s'}(t') \right].$$

Assuming the operators representing the impurities are not functions of time allowed me to pull the S operators out of the commutator. Next, I averaged over the conduction electrons to convert the argument of the integral into familiar looking correlation functions

$$\langle [a_{k',\sigma}^\dagger a_{k,\sigma'}(t) , a_{l',s}^\dagger a_{l,s'}(t')] \rangle.$$

$$-\frac{i}{2\hbar} \sum_{k,k'} \sum_{l,l'} \sum_{n,n'} \sum_{\alpha,\alpha';s,s'} \left(\frac{J}{N}\right)^2 S^n S^{n'} \int_{-\infty}^t dt' \langle [a_{k',\sigma}^\dagger a_{k,\sigma'}(t) , a_{l',s}^\dagger a_{l,s'}(t')] \rangle$$

Next, the step function $\theta(t - t')$ was used to extend the upper limit of the integral to infinity and rewrite the argument as a retarded Green's function,

$$-\frac{i}{2\hbar} \sum_{k,k'} \sum_{l,l'} \sum_{n,n';\sigma,\sigma'} \sum_{\alpha,\alpha';s,s'} \left(\frac{J}{N}\right)^2 S^n S^{n'} \int_{-\infty}^{\infty} dt' \langle \langle a_{k',\sigma}^\dagger a_{k,\sigma'}(t) | a_{l',s}^\dagger a_{l,s'}(t') \rangle \rangle_r \quad 4.2$$

As can be seen from the above, the next step will be to calculate the retarded Green's function that modifies the transformed Hamiltonian.

4.2.1 Calculation of the Green's Function

The form of the Green's function used for calculations is

$$K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = \langle \langle a_{\sigma}^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}') \rangle \rangle = i\theta(t - t') \langle [a_{\sigma}^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') , a_s^\dagger(\bar{y}) a_{s'}(\bar{y}')] \rangle.$$

where \bar{x} , \bar{x}' , and \bar{y} denote arguments of three dimensional space-time. The operator $a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')$ acts directly on the field at the locations \bar{x} and \bar{x}' to annihilate and then create a particle. The positions of \bar{x} and \bar{x}' can be different, but the time must be same for both space-time coordinates in order to be able to apply double-time Green's function theory.

Since the static magnetic susceptibility is a three dimensional tensor, I formulated the Green's functions as rank two tensors. An example of how to show the relationship between the Green's functions, $K_{\sigma\sigma'}^{s's}(\mathbf{r}_{ij})$, and the Green's function tensor is shown below, $\phi_{\alpha\beta}(\mathbf{r}_{ij})$. The form of the Green's function tensor is assumed to be

$$\phi_{xx}(\mathbf{r}_{ij}) = \langle\langle\sigma_x(\mathbf{r}_i)|\sigma_x(\mathbf{r}_j)\rangle\rangle$$

and has the Fourier transform

$$\phi_{xx}(\mathbf{r}_{ij}) = \int \frac{d^3p}{(2\pi)^3} \phi_{xx}(\mathbf{p}, \omega) e^{ip \cdot (\mathbf{r}_i - \mathbf{r}_j)}.$$

Here, $\sigma_x(\mathbf{r}_i)$ is the electron spin density operator associated with the x-direction and \mathbf{r}_{ij} is $|\mathbf{r}_i - \mathbf{r}_j|$.

The electron spin density operators $\sigma_{\alpha}(\mathbf{r})$ are defined by the following expressions:

$$\sigma_x(r) = a_{\uparrow}^{\dagger}(r)a_{\downarrow}(r) + a_{\downarrow}^{\dagger}(r)a_{\uparrow}(r)$$

$$\sigma_y(r) = i \left(a_{\uparrow}^{\dagger}(r)a_{\downarrow}(r) - a_{\downarrow}^{\dagger}(r)a_{\uparrow}(r) \right) \quad 4.3$$

$$\sigma_z(r) = a_{\uparrow}^{\dagger}(r)a_{\uparrow}(r) - a_{\downarrow}^{\dagger}(r)a_{\downarrow}(r).$$

Next, $\phi_{xx}(r_{ij})$ is constructed from the electron density functions as

$$\begin{aligned} &= \langle\langle a_{\uparrow}^{\dagger}(r_i)a_{\downarrow}(r_i) + a_{\downarrow}^{\dagger}(r_i)a_{\uparrow}(r_i) | a_{\uparrow}^{\dagger}(r_j)a_{\downarrow}(r_j) + a_{\downarrow}^{\dagger}(r_j)a_{\uparrow}(r_j) \rangle\rangle \\ &= \langle\langle a_{\uparrow}^{\dagger}(r_i)a_{\downarrow}(r_i) | a_{\uparrow}^{\dagger}(r_j)a_{\downarrow}(r_j) \rangle\rangle + \langle\langle a_{\uparrow}^{\dagger}(r_i)a_{\downarrow}(r_i) | a_{\downarrow}^{\dagger}(r_j)a_{\uparrow}(r_j) \rangle\rangle + \langle\langle a_{\downarrow}^{\dagger}(r_i)a_{\uparrow}(r_i) | a_{\uparrow}^{\dagger}(r_j)a_{\downarrow}(r_j) \rangle\rangle \\ &\quad + \langle\langle a_{\downarrow}^{\dagger}(r_i)a_{\uparrow}(r_i) | a_{\downarrow}^{\dagger}(r_j)a_{\uparrow}(r_j) \rangle\rangle. \end{aligned}$$

Here, the definition of the retarded Green's function is applied to the first and fourth terms.

Since the commutator for these terms vanishes, the equation simply becomes

$$\phi_{xx}(r_{ij}) = K_{\uparrow\downarrow}^{\downarrow\uparrow}(r_{ij}) + K_{\downarrow\uparrow}^{\uparrow\downarrow}(r_{ij}).$$

For the calculation, I used the following Hamiltonian with a single particle operator and a two particle operator that includes the electron-electron interaction,

$$H = \sum_{\sigma} \int d\bar{x} a_{\sigma}^{\dagger}(\bar{x}) T_{\sigma}(\bar{x}) a_{\sigma}(\bar{x}) \quad 4.4$$

$$+ \frac{1}{2} \sum_{\sigma\sigma'} \int d\bar{x} d\bar{x}' a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}^{\dagger}(\bar{x}') V(\bar{x} - \bar{x}') a_{\sigma'}(\bar{x}') a_{\sigma}(\bar{x})$$

The equation of motion for the Green's function of interest is

$$i \frac{\partial}{\partial t} K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = -\frac{d}{dt} \theta(\bar{t} - \bar{t}') \langle [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), a_{\sigma'}^{\dagger}(\bar{y}) a_{\sigma}(\bar{y})] \rangle \quad 4.5$$

$$+ \langle \langle i \frac{\partial}{\partial t} [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}')] | a_{\sigma'}^{\dagger}(\bar{y}) a_{\sigma}(\bar{y}') \rangle \rangle.$$

Applying the relations,

$$\frac{d}{dt} \theta(\bar{t} - \bar{t}') = \delta(t - t')$$

and

$$i \frac{\partial}{\partial t} [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}')] = [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), H]$$

gave the following form for the equation of motion,

$$i \frac{\partial}{\partial t} K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = -\delta(t - t') \langle [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), a_{\sigma'}^{\dagger}(\bar{y}) a_{\sigma}(\bar{y})] \rangle$$

$$+ \langle \langle [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), H] | a_{\sigma'}^{\dagger}(\bar{y}) a_{\sigma}(\bar{y}') \rangle \rangle.$$

Next, I inserted 4.4 into 4.5 which yielded three parts to calculate for the equation of motion. The right hand side has an inhomogeneous term, a term due to the single particle operators, and a term due to the two particle operators.

$$i \frac{\partial}{\partial t} K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = -\delta(t - t') \langle [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), a_{\sigma'}^{\dagger}(\bar{y}) a_{\sigma}(\bar{y})] \rangle$$

$$\begin{aligned}
& + \langle \langle \left[a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), \sum_{\sigma} \int d\bar{x} a_{\sigma}^{\dagger}(\bar{x}) T_{\sigma}(\bar{x}) a_{\sigma}(\bar{x}) \right] | a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}') \rangle \rangle \\
& + \langle \langle \left[a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), \frac{1}{2} \sum_{\sigma\sigma'} \int d\bar{x} d\bar{x}' a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}^{\dagger}(\bar{x}') V(\bar{x} - \bar{x}') a_{\sigma'}(\bar{x}') a_{\sigma}(\bar{x}) \right] | a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}') \rangle \rangle.
\end{aligned}$$

The first step involved calculating the commutators on the right hand side of the equation of motion by using fermionic commutation relations.

$$a_f a_{f'}^{\dagger} + a_{f'}^{\dagger} a_f = \delta_{ff'}; \quad a_f a_{f'} + a_{f'} a_f = a_f^{\dagger} a_{f'}^{\dagger} + a_{f'}^{\dagger} a_f^{\dagger} = 0.$$

For these relations, the f state represents both the spin σ and momentum k of the electron.

Beginning with the inhomogeneous term, I calculated

$$\begin{aligned}
& [a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}'), a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y})] \\
& = a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}') a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}) - a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}) a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}') \\
& = a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}') a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}) - a_s^{\dagger}(\bar{y}) \{ \delta_{s'\sigma} \delta(\bar{x} - \bar{y}) - a_{\sigma}^{\dagger}(\bar{x}) a_{s'}(\bar{y}) \} a_{\sigma'}(\bar{x}') \\
& = a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}') a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}) + a_s^{\dagger}(\bar{y}) a_{\sigma}^{\dagger}(\bar{x}) a_{s'}(\bar{y}) a_{\sigma'}(\bar{x}') - a_s^{\dagger}(\bar{y}) a_{\sigma'}(\bar{x}') \delta_{s'\sigma} \delta(\bar{x} - \bar{y}) \\
& = a_{\sigma}^{\dagger}(\bar{x}) a_{\sigma'}(\bar{x}') a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}) + a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{y}) a_{\sigma'}(\bar{x}') a_{s'}(\bar{y}) - a_s^{\dagger}(\bar{y}) a_{\sigma'}(\bar{x}') \delta_{s'\sigma} \delta(\bar{x} - \bar{y})
\end{aligned}$$

$$\begin{aligned}
&= a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{y})a_{s'}(\bar{y}') + a_{\sigma}^{\dagger}(\bar{x})\{\delta_{s\sigma'}\delta(\bar{x}' - \bar{y}) - a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{y})\}a_{s'}(\bar{y}) \\
&\quad - a_s^{\dagger}(\bar{y})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{y}) \\
&= a_{\sigma}^{\dagger}(\bar{x})a_{s'}(\bar{y})\delta_{s\sigma'}\delta(\bar{x}' - \bar{y}) - a_s^{\dagger}(\bar{y})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{y}) \\
&\quad \xrightarrow{\text{yields}} -\delta(t - t')\langle a_{\sigma}^{\dagger}(\bar{x})a_{s'}(\bar{y})\delta_{s\sigma'}\delta(\bar{x}' - \bar{y}) - a_s^{\dagger}(\bar{y})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{y}) \rangle.
\end{aligned}$$

Finally, I was able to re-arrange the average value brackets to yield

$$= -\delta(t - t')\{\langle a_{\sigma}^{\dagger}(\bar{x})a_{s'}(\bar{y})\delta_{s\sigma'}\delta(\bar{x}' - \bar{y}) \rangle - \langle a_s^{\dagger}(\bar{y})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{y}) \rangle\}.$$

By defining

$$\langle a_{\sigma}^{\dagger}(\bar{x})a_{s'}(\bar{y}) \rangle = n_{\sigma}(\bar{x}, \bar{y}) \delta_{s'\sigma}.$$

the inhomogenous term down was simplified down to

$$= -\delta(t - t')\delta_{\sigma's}\delta_{s'\sigma}\{n_{\sigma}(\bar{x}, \bar{y})\delta(\bar{x}' - \bar{y}) - n_{\sigma}(\bar{x}', \bar{y})\delta(\bar{x} - \bar{y})\}.$$

Next, I calculated the single particle operator term.

$$\left[a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}'), \sum_s \int d\bar{z} a_s^{\dagger}(\bar{z})T_s(\bar{z})a_s(\bar{z}) \right]$$

$$\begin{aligned}
&= \sum_s \int d\bar{z} T_s(\bar{z}) \{a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}')a_s^\dagger(\bar{z})a_s(\bar{z}) - a_s^\dagger(\bar{z})a_s(\bar{z})a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}')\} \\
&= \sum_s \int d\bar{z} T_s(\bar{z}) [a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}')a_s^\dagger(\bar{z})a_s(\bar{z}) - a_s^\dagger(\bar{z})\{\delta_{s\sigma}\delta(\bar{x} - \bar{z}) - a_\sigma^\dagger(\bar{x})a_s(\bar{z})\}a_{\sigma'}(\bar{x}')] \\
&= \sum_s \int d\bar{z} T_s(\bar{z}) [a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}')a_s^\dagger(\bar{z})a_s(\bar{z}) + a_s^\dagger(\bar{z})a_\sigma^\dagger(\bar{x})a_s(\bar{z})a_{\sigma'}(\bar{x}') - a_s^\dagger(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \sum_s \int d\bar{z} T_s(\bar{z}) [a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}')a_s^\dagger(\bar{z})a_s(\bar{z}) + a_\sigma^\dagger(\bar{x})a_s^\dagger(\bar{z})a_{\sigma'}(\bar{x}')a_s(\bar{z}) - a_s^\dagger(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \sum_s \int d\bar{z} T_s(\bar{z}) [a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}')a_s^\dagger(\bar{z})a_s(\bar{z}) + a_\sigma^\dagger(\bar{x})\{\delta_{s\sigma'}\delta(\bar{x}' - \bar{z}) - a_{\sigma'}(\bar{x}')a_s^\dagger(\bar{z})\}a_s(\bar{z}) \\
&\quad - a_s^\dagger(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \sum_s \int d\bar{z} T_s(\bar{z}) [a_\sigma^\dagger(\bar{x})a_s(\bar{z})\delta_{s\sigma'}\delta(\bar{x}' - \bar{z}) - a_s^\dagger(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= T_{\sigma'}(\bar{x}')a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}') - T_\sigma(\bar{x})a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}') \\
&= (T_{\sigma'}(\bar{x}') - T_\sigma(\bar{x}))a_\sigma^\dagger(\bar{x})a_{\sigma'}(\bar{x}') \\
&\xrightarrow{\text{yields}} -(T_{\sigma'}(\bar{x}') - T_\sigma(\bar{x}))K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}).
\end{aligned}$$

Now, I tackled the two particle operator term

$$\begin{aligned}
& \left[a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}'), \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}' V(\bar{z} - \bar{z}') a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')V(\bar{z} - \bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \right] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}' V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z})a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}' V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')\{\delta_{s\sigma}\delta(\bar{x} - \bar{z}) \\
&\quad - a_{\sigma}^{\dagger}(\bar{x})a_s(\bar{z})\}a_{\sigma'}(\bar{x}')] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}' V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma}^{\dagger}(\bar{x})a_s(\bar{z})a_{\sigma'}(\bar{x}') - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}' V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')\{\delta_{s'\sigma}\delta(\bar{x} - \bar{z}') \\
&\quad - a_{\sigma}^{\dagger}(\bar{x})a_{s'}(\bar{z}')\}a_s(\bar{z})a_{\sigma'}(\bar{x}') - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}' V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{\sigma}^{\dagger}(\bar{x})a_{s'}(\bar{z}')a_s(\bar{z})a_{\sigma'}(\bar{x}') + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_s(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s,\sigma}\delta(\bar{x} - \bar{z}') \\
&\quad - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})]
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}'V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad - a_{\sigma}^{\dagger}(\bar{x})a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{\sigma'}(\bar{x}')a_{s'}(\bar{z}')a_s(\bar{z}) + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_s(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{z}') \\
&\quad - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}'V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) - a_{\sigma}^{\dagger}(\bar{x})a_s^{\dagger}(\bar{z})\{\delta_{s'\sigma}\delta(\bar{x}' - \bar{z}') \\
&\quad - a_{\sigma'}(\bar{x}')a_{s'}^{\dagger}(\bar{z}')\}a_{s'}(\bar{z}')a_s(\bar{z}) + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_s(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{z}') \\
&\quad - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}'V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad + a_{\sigma}^{\dagger}(\bar{x})a_s^{\dagger}(\bar{z})a_{\sigma'}(\bar{x}')a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) - a_{\sigma}^{\dagger}(\bar{x})a_s^{\dagger}(\bar{z})a_{s'}(\bar{z}')a_s(\bar{z})\delta_{s'\sigma}\delta(\bar{x}' - \bar{z}') \\
&\quad + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_s(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{z}') - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})] \\
&= \frac{1}{2} \sum_{ss'} \int d\bar{z}d\bar{z}'V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x})a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad + a_{\sigma}^{\dagger}(\bar{x})\{\delta_{s'\sigma}\delta(\bar{x}' - \bar{z}) - a_{\sigma'}(\bar{x}')a_s^{\dagger}(\bar{z})\}a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_s(\bar{z}) \\
&\quad - a_{\sigma}^{\dagger}(\bar{x})a_s^{\dagger}(\bar{z})a_{s'}(\bar{z}')a_s(\bar{z})\delta_{s'\sigma}\delta(\bar{x}' - \bar{z}') + a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_s(\bar{z})a_{\sigma'}(\bar{x}')\delta_{s'\sigma}\delta(\bar{x} - \bar{z}') \\
&\quad - a_s^{\dagger}(\bar{z})a_{s'}^{\dagger}(\bar{z}')a_{s'}(\bar{z}')a_{\sigma'}(\bar{x}')\delta_{s\sigma}\delta(\bar{x} - \bar{z})]
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{2} \sum_{ss'} \int d\bar{z} d\bar{z}' V(\bar{z} - \bar{z}') [a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}') a_{s'}(\bar{z}') a_s(\bar{z}) \delta_{s\sigma'} \delta(\bar{x}' - \bar{z}) \\
&\quad - a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_{s'}(\bar{z}') a_s(\bar{z}) \delta_{s'\sigma'} \delta(\bar{x}' - \bar{z}') + a_s^{\dagger}(\bar{z}) a_{s'}^{\dagger}(\bar{z}') a_s(\bar{z}) a_{\sigma'}(\bar{x}') \delta_{s'\sigma} \delta(\bar{x} - \bar{z}') \\
&\quad - a_s^{\dagger}(\bar{z}) a_{s'}^{\dagger}(\bar{z}') a_{s'}(\bar{z}') a_{\sigma'}(\bar{x}') \delta_{s\sigma} \delta(\bar{x} - \bar{z})] \\
&= \frac{1}{2} \sum_s \int d\bar{z} [V(\bar{x}' - \bar{z}) a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_s(\bar{z}) a_{\sigma'}(\bar{x}') - V(\bar{z} - \bar{x}') a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_{\sigma'}(\bar{x}') a_s(\bar{z}) \\
&\quad + V(\bar{z} - \bar{x}) a_s^{\dagger}(\bar{z}) a_{\sigma}^{\dagger}(\bar{x}) a_s(\bar{z}) a_{\sigma'}(\bar{x}') - V(\bar{x} - \bar{z}) a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_s(\bar{z}) a_{\sigma'}(\bar{x}')] \\
&= \frac{1}{2} \sum_s \int d\bar{z} [2V(\bar{x}' - \bar{z}) a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_s(\bar{z}) a_{\sigma'}(\bar{x}') - 2V(\bar{x} - \bar{z}) a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_s(\bar{z}) a_{\sigma'}(\bar{x}')] \\
&= \sum_s \int d\bar{z} [V(\bar{x}' - \bar{z}) - V(\bar{x} - \bar{z})] a_{\sigma}^{\dagger}(\bar{x}) a_s^{\dagger}(\bar{z}) a_s(\bar{z}) a_{\sigma'}(\bar{x}') \\
&\xrightarrow{yields} - \sum_{\nu} \int d\bar{z} [V(\bar{x}' - \bar{z}) - V(\bar{x} - \bar{z})] \langle\langle a_{\sigma}^{\dagger}(\bar{x}) a_{\nu}^{\dagger}(\bar{z}) a_{\nu}(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^{\dagger}(\bar{y}) a_{s'}(\bar{y}) \rangle\rangle.
\end{aligned}$$

In the last line, the summation is changed from $s \rightarrow \nu$ when the operators are inserted back into the Green's function.

At this point, all the results back were inserted back into the equation of motion for the Green's function and the linearity of the Green's function was used to give

$$i \frac{\partial}{\partial t} K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = -\delta(t - t') \delta_{\sigma's} \delta_{s'\sigma} \{n_{\sigma}(\bar{x}, \bar{y}) \delta(\bar{x}' - \bar{y}) - n_{\sigma'}(\bar{x}', \bar{y}) \delta(\bar{x} - \bar{y})\} \quad 4.6$$

$$-(T_\sigma - T_{\sigma'})K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; y)$$

$$-\sum_v \int d\bar{z} [V(\bar{x}' - \bar{z}) - V(\bar{x} - \bar{z})] \langle\langle a_\sigma^\dagger(\bar{x}) a_v^\dagger(\bar{z}) a_v(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle\rangle$$

As expected, the calculation of the equation of motion lead to higher order Green's function terms from the commutators with the interaction terms. From the two particle Green's function equation of motion, a three particle Green's function was gained. Next, I truncated the chain of equations through approximation.

In the earlier calculation of section 2.1.3, I relied on perturbation orders to eliminate the higher order terms and calculated the consequences of dropping higher order terms. In this section, we will seek a direct approximation to the higher order Green's function that will look something like this

$$G_2 \cong \lambda G_1,$$

with G_2 as the higher order Green's function and λ is some known or easily calculated/measured constant. This sort of approximation enables me to solve the equation of motion by moving it to the left hand side and factoring out G_1 . The constant that I will be factoring out is the number of particles in a state or $\langle a_f^\dagger a_f \rangle$.

To justify the approximation to be used later, I looked at a three particle Green's function where A , B , and C each represent fermion operators of the type $a_f^\dagger a_f$.

$$\langle\langle AB|C \rangle\rangle = \pm i\theta(t)\langle[AB, C]\rangle$$

$$= \pm i\theta(t)\langle A[B, C] + [A, C]B \rangle$$

$$\approx \pm i\theta(t)\{\langle A \rangle \langle [B, C] \rangle + \langle [A, C] \rangle \langle B \rangle\}$$

$$= \langle A \rangle \langle B|C \rangle + \langle B \rangle \langle A|C \rangle$$

The approximation used in the third line uncorrelates A and B from the operators in the commutator. This approximation scheme is generally described as a Hartree-Fock approximation because it decouples the higher order interaction into a simpler interaction that has the strength by the average value of the uncorrelated operator, $\langle a_f^\dagger a_f \rangle$, the number of other particles.

I applied this approximation to the higher order Green's function and use fermion commutation relations to pair up operators of the type $a_f^\dagger a_{f'}$,

$$\begin{aligned} \langle \langle a_\sigma^\dagger(\bar{x}) a_\nu^\dagger(\bar{z}) a_\nu(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle &= \langle \langle a_\sigma^\dagger(\bar{x}) \{1 - a_\nu(\bar{z}) a_\nu^\dagger(\bar{z})\} a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\ &= \langle \langle a_\sigma^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{z}) a_{s'}(\bar{z}) \rangle \rangle - \langle \langle a_\sigma^\dagger(\bar{x}) a_\nu(\bar{z}) a_\nu^\dagger(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\ &\approx \langle \langle a_\sigma^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{z}) a_{s'}(\bar{z}) \rangle \rangle - \langle a_\sigma^\dagger(\bar{x}) a_\nu(\bar{z}) \rangle \langle \langle a_\nu^\dagger(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\ &\quad - \langle a_\nu^\dagger(\bar{z}) a_{\sigma'}(\bar{x}') \rangle \langle \langle a_\sigma^\dagger(\bar{x}) a_\nu(\bar{z}) | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle. \end{aligned}$$

The job is not done at this point as there are four possible pairs of operators that can be factored out and all four must be accounted for since they are all of the same order in strength. Using fermion commutation relations to pair up the other pairs of operators,

$$\begin{aligned}
\langle \langle a_\sigma^\dagger(\bar{x}) a_v^\dagger(\bar{z}) a_v(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle &= - \langle \langle a_v^\dagger(\bar{z}) a_\sigma^\dagger(\bar{x}) a_v(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\
&= - \langle \langle a_v^\dagger(\bar{z}) \{ \delta(\bar{z} - \bar{x}) \delta_{\sigma v} - a_v(\bar{z}) a_\sigma^\dagger(\bar{x}) \} a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\
&= - \langle \langle a_v^\dagger(\bar{z}) a_{\sigma'}(\bar{x}') \delta(\bar{z} - \bar{x}) \delta_{\sigma v} | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle + \langle \langle a_v^\dagger(\bar{z}) a_v(\bar{z}) a_\sigma^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\
&\approx - \langle \langle a_\sigma^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle + \langle a_v^\dagger(\bar{z}) a_v(\bar{z}) \rangle \langle \langle a_\sigma^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle \\
&\quad + \langle a_\sigma^\dagger(\bar{x}) a_{\sigma'}(\bar{x}') \rangle \langle \langle a_v^\dagger(\bar{z}) a_v(\bar{z}) | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle.
\end{aligned}$$

Next, I added all six terms together and used the definition

$$\langle a_\sigma^\dagger(\bar{x}) a_{s'}(\bar{y}) \rangle = n_\sigma(\bar{x}, \bar{y}) \delta_{s'\sigma}$$

to get

$$\begin{aligned}
\langle \langle a_\sigma^\dagger(\bar{x}) a_v^\dagger(\bar{z}) a_v(\bar{z}) a_{\sigma'}(\bar{x}') | a_s^\dagger(\bar{y}) a_{s'}(\bar{y}) \rangle \rangle &\approx n_\nu(\bar{z}, \bar{z}) K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) + \delta_{\sigma\sigma'} n_\sigma(\bar{x}, \bar{x}') K_{\nu\nu}^{ss'}(\bar{z}, \bar{z}; \bar{y}) \\
&\quad - \delta_{\sigma v} n_\sigma(\bar{x}, \bar{z}) K_{\nu\sigma'}^{ss'}(\bar{z}, \bar{x}'; \bar{y}) - \delta_{\sigma'v} n_{\sigma'}(\bar{z}, \bar{x}') K_{\sigma v}^{ss'}(\bar{x}, \bar{z}; \bar{y}).
\end{aligned}$$

To simplify the notation, I redefined the approximation term as

$$\begin{aligned}
P(\bar{z}, \nu) &= n_\nu(\bar{z}, \bar{z}) K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) + \delta_{\sigma\sigma'} n_\sigma(\bar{x}, \bar{x}') K_{\nu\nu}^{ss'}(\bar{z}, \bar{z}; \bar{y}) \\
&\quad - \delta_{\sigma v} n_\sigma(\bar{x}, \bar{z}) K_{\nu\sigma'}^{ss'}(\bar{z}, \bar{x}'; \bar{y}) - \delta_{\sigma'v} n_{\sigma'}(\bar{z}, \bar{x}') K_{\sigma v}^{ss'}(\bar{x}, \bar{z}; \bar{y}).
\end{aligned}$$

Now, the approximated equation of motion of $K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y})$ is rewritten as

$$i \frac{\partial}{\partial t} K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = -\delta(t - t') \delta_{\sigma's} \delta_{s'\sigma} \{n_{\sigma}(\bar{x}, \bar{y}) \delta(\bar{x}' - \bar{y}) - n_{\sigma'}(\bar{x}', \bar{y}) \delta(\bar{x} - \bar{y})\} \\ - (T_{\sigma}(\bar{x}) - T_{\sigma'}(\bar{x}')) K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) - \sum_{\nu} \int d\bar{z} [V(\bar{x}' - \bar{z}) - V(\bar{x} - \bar{z})] P(\bar{z}, \nu)$$

While the Hartree-Fock approximation made all the Green's functions of the same order, they are still functions of different variables in the problem. To solve the differential equation for the Green's function of interest, I had to transform the equation of motion to Fourier space.

4.3 The Fourier Transform of Green's Function

Next, I took the Fourier transform of the equation of motion and attempt to solve the equation in Fourier space. Two types of Green's function terms were considered, those where $\sigma = \sigma'$ and others where $\sigma \neq \sigma'$.

Beginning with the $\sigma \neq \sigma'$ case, the equation of motion becomes

$$\left(\frac{\partial}{\partial t} + T_{\sigma}(\bar{x}) - T_{\sigma'}(\bar{x}') \right) K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) \\ = -\delta(t - t') \delta_{\sigma's} \delta_{s'\sigma} \{n_{\sigma}(\bar{x}, \bar{y}) \delta(\bar{x}' - \bar{y}) - n_{\sigma'}(\bar{x}', \bar{y}) \delta(\bar{x} - \bar{y})\} \\ + \int d\bar{z} [V(\bar{x} - \bar{z}) - V(\bar{x}' - \bar{z})] \{n_{\sigma'}(\bar{z}, \bar{x}') K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{z}; \bar{y}) + n_{\sigma}(\bar{x}, \bar{z}) K_{\sigma\sigma'}^{ss'}(\bar{z}, \bar{x}'; \bar{y})\}$$

Then, I defined the Fourier transforms as

$$K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}) = \frac{1}{(2\pi)^7} \int d^3 p_1 d^3 p_2 d\omega e^{ip_1 \cdot (\bar{x} - \bar{y}) + ip_2 \cdot (\bar{x}' - \bar{y}) - iE(t - t')} K(p_1, p_2; \omega)$$

$$V(\bar{x}) = \int \frac{d^3 p}{(2\pi)^3} e^{ip \cdot \bar{x}} V(p)$$

$$n(\bar{x} - \bar{y}) = \int \frac{d^3 p}{(2\pi)^3} e^{ip \cdot (\bar{x} - \bar{y})} n(p).$$

Taking the transform with respect to t and ω yielded

$$(E + T_\sigma(\bar{x}) - T_{\sigma'}(\bar{x}')) K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{x}'; \bar{y}; E) = -\delta_{\sigma's} \delta_{s'\sigma} \{n_\sigma(\bar{x}, \bar{y}) \delta(\bar{x}' - \bar{y}) - n_{\sigma'}(\bar{x}', \bar{y}) \delta(\bar{x} - \bar{y})\} \\ + \int d\bar{z} [V(\bar{x} - \bar{z}) - V(\bar{x}' - \bar{z})] \{n_{\sigma'}(\bar{z}, \bar{x}') K_{\sigma\sigma'}^{ss'}(\bar{x}, \bar{z}; \bar{y}; E) + n_\sigma(\bar{x}, \bar{z}) K_{\sigma\sigma'}^{ss'}(\bar{z}, \bar{x}'; \bar{y}; E)\}.$$

Now, I took the transform with respect to the spatial variables to give

$$(E + T_\sigma(p_1) - T_{\sigma'}(p_2)) K_{\sigma\sigma'}^{ss'}(p_1, p_2; E) = -\delta_{\sigma's} \delta_{s'\sigma} \{n_\sigma(p_1) - n_{\sigma'}(p_2)\} \\ + \int \frac{d^3 p}{(2\pi)^3} [n_\sigma(p) V(p_2 + p) - n_{\sigma'}(p) V(p_1 + p)] K_{\sigma\sigma'}^{ss'}(p_1, p_2; E) \\ + \int \frac{d^3 p}{(2\pi)^3} [n_{\sigma'}(p_2) + n_\sigma(p_1)] V(p - p_1) K_{\sigma\sigma'}^{ss'}(p, p_1 + p_2 - p; E)$$

Combining like-terms and not explicitly writing the E in the Green function's argument gave

$$\begin{aligned}
& \left(E + T_\sigma(p_1) - T_{\sigma'}(p_2) + \int \frac{d^3 p}{(2\pi)^3} [n_{\sigma'}(p)V(p_2 + p) - n_\sigma(p)V(p_1 + p)] \right) K_{\sigma\sigma'}^{ss'}(p_1, p_2) \\
& = -\delta_{\sigma's} \delta_{s'\sigma} \{n_\sigma(p_1) - n_{\sigma'}(p_2)\} \\
& + \int \frac{d^3 p}{(2\pi)^3} [n_{\sigma'}(p_2) + n_\sigma(p_1)] V(p - p_1) K_{\sigma\sigma'}^{ss'}(p, p_1 + p_2 - p).
\end{aligned}$$

Now, I took $\rightarrow p'$, $p_1 \rightarrow q$, and redefined $p = q + p_2$ to get

$$\begin{aligned}
& \left(E + T_\sigma(q) - T_{\sigma'}(p - q) + \int \frac{d^3 p'}{(2\pi)^3} [n_{\sigma'}(p' + q - p)V(p') - n_\sigma(p' - q)V(p')] \right) K_{\sigma\sigma'}^{ss'}(q, p - q) \\
& = \delta_{\sigma's} \delta_{s'\sigma} \{n_{\sigma'}(p - q) - n_\sigma(q)\} \\
& + \int \frac{d^3 p'}{(2\pi)^3} [n_{\sigma'}(p - q) + n_\sigma(q)] V(p' - q) K_{\sigma\sigma'}^{ss'}(p', p - p').
\end{aligned}$$

To compact the notation a bit, the coefficient of $K_{\sigma\sigma'}^{ss'}(q, p - q)$ is rewritten as

$$\Sigma_{\sigma\sigma'} = E + T_\sigma(q) - T_{\sigma'}(p - q) + \int \frac{d^3 p'}{(2\pi)^3} [n_{\sigma'}(p' + q - p) - n_\sigma(p' - q)] V(p')$$

This definition finally leads to

$$K_{\sigma\sigma'}^{ss'}(q, p - q) = \frac{\delta_{\sigma's} \delta_{s'\sigma} \{n_{\sigma'}(p - q) - n_\sigma(q)\}}{\Sigma_{\sigma\sigma'}}$$

$$+ \frac{[n_{\sigma'}(p-q) + n_{\sigma}(q)]}{\Sigma_{\sigma\sigma'}} \int \frac{d^3 p'}{(2\pi)^3} V(p'-q) K_{\sigma\sigma'}^{ss'}(p', p-p').$$

Next, I integrated with respect to q on both sides of the equation and applied the approximation $V(p) \cong V$ to solve for the Green function in the case of $\sigma \neq \sigma'$,

$$K_{\sigma\sigma'}^{ss'}(p) = \int \frac{d^3 q}{(2\pi)^3} \frac{\delta_{\sigma's} \delta_{s'\sigma} \{n_{\sigma'}(p-q) - n_{\sigma}(q)\}}{\Sigma_{\sigma\sigma'}} + \int \frac{d^3 q}{(2\pi)^3} \frac{[n_{\sigma'}(p-q) + n_{\sigma}(q)]}{\Sigma_{\sigma\sigma'}} V K_{\sigma\sigma'}^{ss'}(p)$$

$$K_{\sigma\sigma'}^{ss'}(p) = \frac{\delta_{\sigma's} \delta_{s'\sigma} \int \frac{d^3 q}{(2\pi)^3} \frac{\{n_{\sigma'}(p-q) - n_{\sigma}(q)\}}{\Sigma_{\sigma\sigma'}}}{1 - V \int \frac{d^3 q}{(2\pi)^3} \frac{[n_{\sigma'}(p-q) + n_{\sigma}(q)]}{\Sigma_{\sigma\sigma'}}}. \quad 4.7$$

In this equation, I also made use of the relation

$$K_{\sigma\sigma'}^{ss'}(p) = \int \frac{d^3 q}{(2\pi)^3} K_{\sigma\sigma'}^{ss'}(q, p-q).$$

It can be seen from the above equation, that the only non-zero Green function for the case $\sigma \neq \sigma'$ is $K_{\sigma\sigma'}^{\sigma'\sigma}(p)$. This leads us to the solution of

$$K_{\sigma\sigma'}^{\sigma'\sigma}(p) = \frac{Q_{\sigma\sigma'}}{1 - V Q_{\sigma\sigma'}} \quad 4.8$$

Where I have defined

$$Q_{\sigma\sigma'}(p, 0) = \int \frac{d^3q}{(2\pi)^3} \frac{\{n_{\sigma'}(p-q) - n_{\sigma}(q)\}}{\Sigma_{\sigma\sigma'}}. \quad 4.9$$

Going back to look at the $\Sigma_{\sigma\sigma'}$ term, it is rewritten as

$$\Sigma_{\sigma\sigma'} = -2\beta H + \frac{1}{2m}(2p \cdot q - p^2) + V(N_{\sigma'} - N_{\sigma})$$

by assuming $E = 0$ and defining N_{σ} as the total number of electrons with spin σ . Now, 4.8 is rewritten by using the new form of $\Sigma_{\sigma\sigma'}$ as

$$Q_{\sigma\sigma'}(p, 0) = \int \frac{d^3q}{(2\pi)^3} \frac{\{n_{\sigma'}(p-q) - n_{\sigma}(q)\}}{-2\beta H + \frac{1}{2m}(2p \cdot q - p^2) + V(N_{\sigma'} - N_{\sigma})}.$$

Taking the integral over q-space at $T = 0$ and noting that the integral above is of the type

$$\int \frac{dx}{x^2 - a^2} = \begin{cases} \frac{1}{2a} \ln \frac{a-x}{a+x} + C & \text{for } |x| < |a| \\ \frac{1}{2a} \ln \frac{a+x}{a-x} + C & \text{for } |x| > |a| \end{cases},$$

leads to

$$\begin{aligned}
Q_{\uparrow\downarrow} &= Q_{\downarrow\uparrow} \\
&= \frac{3N}{8\epsilon_F} \left\{ (1+\xi)^{1/3} \frac{\epsilon + v\xi + x^2}{2x^2} - (1-\xi)^{1/3} \frac{\epsilon + v\xi - x^2}{2x^2} \right. \\
&\quad + \frac{(\epsilon + v\xi + x^2)^2 - 4x^2(1+\xi)^{2/3}}{8x^3} \ln \left| \frac{\epsilon + v\xi + x^2 - 2x(1+\xi)^{1/3}}{\epsilon + v\xi + x^2 + 2x(1+\xi)^{1/3}} \right| \\
&\quad \left. + \frac{(\epsilon + v\xi - x^2)^2 - 4x^2(1-\xi)^{2/3}}{8x^3} \ln \left| \frac{\epsilon + v\xi - x^2 + 2x(1+\xi)^{1/3}}{\epsilon + v\xi - x^2 - 2x(1+\xi)^{1/3}} \right| \right\}. \tag{4.10}
\end{aligned}$$

Where the following definitions have been used

$$x = \frac{p}{p_F}; \quad v = \frac{vN}{\epsilon_F}; \quad \xi = \frac{N_{\sigma'} - N_{\sigma}}{N}; \quad \epsilon = \frac{2\beta H}{\epsilon_F}. \tag{4.11}$$

Next, I calculated the Green function for the case $\sigma = \sigma'$. In this case, I was required to solve a system of equations of motion for the $\uparrow\uparrow$ and $\downarrow\downarrow$ cases and this leads to a more complicated looking Green's function,

$$K_{\sigma\sigma}(p, 0) = \sigma \frac{Q_{\sigma\sigma}(p, 0) + Q_{\sigma\sigma}(p, 0)Q_{-\sigma, -\sigma}(p, 0)}{1 - V^2 Q_{\sigma\sigma}(p, 0)Q_{-\sigma, -\sigma}(p, 0)}. \tag{4.12}$$

Where I have used the following definition,

$$Q_{\sigma\sigma}(p, 0) = \int \frac{d^3q}{(2\pi)^3} \frac{\{n_{\sigma}(p-q) - n_{\sigma}(q)\}}{-2\beta H + \frac{1}{2m}(2p \cdot q - p^2)}.$$

Finally, taking the integral over the above equation leads to

$$Q_{\uparrow\uparrow(\downarrow\downarrow)}(p, 0) = \frac{3N}{8\varepsilon_F} \left\{ \frac{x^2 - 4(1 \pm \xi)^{2/3}}{4x} \ln \left| \frac{x - 2(1 \pm \xi)^{1/3}}{x + 2(1 \pm \xi)^{1/3}} \right| + (1 \pm \xi)^{1/3} \right\} \quad 4.13$$

with + (−) for $\uparrow\uparrow$ ($\downarrow\downarrow$) case and using the same definitions in 4.10 as $Q_{\sigma\sigma'}(p, 0)$.

Using the definitions in 4.3, the Green's functions in momentum space can be calculated as

$$\phi_{xx}(p, 0) = \phi_{yy}(p, 0) = 2K_{\sigma\sigma'}^{\sigma'\sigma} = \frac{2Q_{\sigma\sigma'}(p, 0)}{1 - VQ_{\sigma\sigma'}(p, 0)}$$

$$\phi_{zz}(p, 0) = \frac{Q_{\uparrow\uparrow}(p, 0) + Q_{\downarrow\downarrow}(p, 0) + 2Q_{\uparrow\uparrow}(p, 0)Q_{\downarrow\downarrow}(p, 0)}{1 - V^2Q_{\uparrow\uparrow}(p, 0)Q_{\downarrow\downarrow}(p, 0)}$$

As a check on the validity of the equations, I looked at the case when the electrons are unpolarized, $\xi = 0$, and when no external magnetic field is applied to the sample, $\varepsilon = 0$. From these conditions, it is expected that the electrons will have no preferred direction of polarization.

$$Q_{\uparrow\uparrow}(p, 0) = Q_{\downarrow\downarrow}(p, 0) = \frac{3N}{8\varepsilon_F} \left\{ \frac{x^2 - 4}{4x} \ln \left| \frac{x - 2}{x + 2} \right| + 1 \right\} = Q(p, 0)$$

$$Q_{\uparrow\downarrow}(p, 0) = Q_{\downarrow\uparrow}(p, 0) = \frac{3N}{8\epsilon_F} \left\{ \frac{x^2}{2x^2} - \frac{-x^2}{2x^2} + \frac{x^4 - 4x^2}{8x^3} \ln \left| \frac{x^2 - 2x}{x^2 + 2x} \right| + \frac{x^4 - 4x^2}{8x^3} \ln \left| \frac{-x^2 + 2x}{-x^2 - 2x} \right| \right\}$$

$$= \frac{3N}{8\epsilon_F} \left\{ 1 + \frac{x^4 - 4x^2}{8x^3} \ln \left| \frac{x - 2}{x + 2} \right| + \frac{x^4 - 4x^2}{8x^3} \ln \left| \frac{x - 2}{x + 2} \right| \right\} = Q(p, 0)$$

$$\phi_{zz}(p, 0) = \frac{2Q(p, 0) + 2(Q(p, 0))^2}{1 - V^2(Q(p, 0))^2} = \frac{2Q(p, 0)(1 + Q(p, 0))}{(1 + Q(p, 0))(1 - Q(p, 0))} = \phi_{xx}(p, 0) = \phi_{yy}(p, 0).$$

It can be seen that the equations recreate the expected situation of incoherent electrons that have no preferred direction with respect to spin density when there is applied external magnetic field.

With the Green's function solved in momentum space, it is time to take the Fourier transform back to real space. I applied the asymptotic methods developed in Chapter 3 to be able get an expression that can be transformed back to real space.

The term I explored is the one in the denominator of the $\sigma \neq \sigma'$ (equation 4.9) case or the term $1 - VQ_{\sigma\sigma'}(x, 0)$. The strongest singularities arising from terms where $x \rightarrow 0$. There are also singularities due to the logarithmic terms, but these singularities are logarithmic in nature and very similar to 1.24. Therefore, these singularities are expected to produce the RKKY interaction part of the Hamiltonian. Focusing on the on the singularities arising from $x \rightarrow 0$ since they are expected to modify the Hamiltonian, the denominator in this case is approximated as

$$1 - VQ_{\sigma\sigma'}(x, 0) \approx a_s^2 + b_s^2 x^2$$

$$x \leq \varepsilon + v\xi,$$

where $a_s^2 = \frac{\varepsilon}{v\xi + \varepsilon}$ and $b_s^2 = \frac{v}{(v\xi + \varepsilon)^2} \left\{ 1 - \frac{2}{5(v\xi + \varepsilon)} [(1 + \xi)^{5/3} - (1 - \xi)^{5/3}] \right\}$. This calculation was performed by using the Taylor series expansion of

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots \text{ for } |x| \leq 1.$$

A similar expansion can also be performed on the numerator of 4.9. Keeping in mind the standard Fourier transform of the exponential decay function,

$$\int_{-\infty}^{\infty} dx e^{-a|x|} e^{-2\pi i x p} = \frac{2a}{a^2 + p^2},$$

a Fourier transform can be performed on the approximated expression to arrive at

$$\langle\langle \sigma_x(\vec{r}_i) | \sigma_y(\vec{r}_j) \rangle\rangle = \langle\langle \sigma_x(\vec{r}_i) | \sigma_y(\vec{r}_j) \rangle\rangle = \frac{\hbar N p_F^2 \xi (v\xi + \varepsilon)^2}{2\pi v \varepsilon_F} \frac{1}{|\vec{r}_i - \vec{r}_j|} e^{(-|\vec{r}_i - \vec{r}_j|/r_s)}.$$

Where I have used the definition of $\frac{1}{r_s} = p_F (v\xi + \varepsilon) \sqrt{\frac{\varepsilon}{v}}$.

The case of $\sigma = \sigma'$ are omitted from discussion as they did not yield any new singularities beyond the usual RKKY singularities.

The modified term for the effective Hamiltonian between spins for the polarized case of conduction electrons can be written in the following form

$$\mathcal{H}_{ij}^s = -J(|\vec{r}_i - \vec{r}_j|) \{ S_+^i S_-^j + S_-^i S_+^j \},$$

with

$$J(|\vec{r}_i - \vec{r}_j|) = \frac{A^2 N p_F^2 \xi (v\xi + \varepsilon)}{4\pi v \varepsilon_F} \frac{1}{|\vec{r}_i - \vec{r}_j|} e^{-(|\vec{r}_i - \vec{r}_j|/r_s)},$$

and

$$S_{\pm} = S_x \pm iS_y.$$

It can be seen that including electron-electron interaction with the usual exchange interaction will modify the form of the RKKY interaction with an additive term that exponentially decays with distance from the impurity. This decaying potential term has the same form as a screened Coulomb interaction and is commonly called a Yukawa potential. The addition of a screened Coulomb term is to be expected as the system being explored was being modified by the inclusion of electron-electron interactions. Therefore, the produced result justifies the technique for more complicated systems such as nanostructures.

CHAPTER 5

CONCLUSION

Introducing an impurity to a crystal alters periodic nature of the lattice and produces interesting phenomena. A non-magnetic impurity will alter the charge density of the conduction electrons that can be seen experimentally in the nuclear magnetic resonance of a dilute alloy. Inserting a magnetic impurity will produce a similar result but with variations of the spin density of the conduction electrons. A second magnetic impurity will “feel” the spin density variation produced. On the other hand, that second impurity will also produce variations in the spin density that the first impurity will “feel”. In this way, localized spins are coupled indirectly through the medium of conduction electrons.

The interaction between localized electrons and conduction electrons is represented in the s-d model exchange Hamiltonian. However, a similar interaction occurs between nuclear spins and conduction interaction when the contact part of the hyperfine interaction is considered. This similarity between interactions opens up the possibility of coupling not only localized electron moments to one another, but also nuclear spins to one another and a localized electron moment to a nuclear spin. All of these indirect coupling interactions are collectively known as the RKKY interaction.

The spin density variations from the RKKY interactions are driven by the exchange interaction of either a nuclear spin or localized electron moment with conduction electrons. However, RKKY interactions do not consider the electron-electron interactions of the conduction electrons. It is reasonable to expect the RKKY driven spin density of the conduction electrons to be altered even further when electron-electron interaction is considered.

The electron-electron interaction is taken into account by first constructing an effective Hamiltonian to describe the s-d model in terms of a retarded double time Green's function. From here, the chain of equations of motion for the Green's function is calculated. This chain of equations is truncated by using an approximation that is Hartree-Fock-like. The approximated equation of motion is then solved by taking the Fourier transform. Next, the Fourier transform must be performed asymptotically to get the Green's function back into the real space domain.

After the equation of motion is fully solved, the modification to the due to electron-electron interaction was found to be a decaying exponential. The interesting thing about the modification of the RKKY interaction Hamiltonian is the similarity to the Yukawa potential, which represents a screened Coulomb interaction. The final effective Hamiltonian ended up with a screened Coulomb potential to go with the RKKY terms which justifies the method employed in the paper.

The future direction of this research should be to apply the same Green's functions technique at different dimensions to find how the electron-electron interaction modifies the RKKY interaction at lower dimensions. The purpose of these findings would be to develop the technique for further use in the interaction of different nanostructures calculations. Next, the range of the screened of the Coulomb interaction can be compared to the oscillations of the RKKY effect in different alloys. There is a possibility of finding an alloy where the screened Coulomb effect is dominant when the spin density polarization goes to zero and it is expected to have calculable effects on the nuclear resonance of the material.

REFERENCES

- [1] C. Kittel, *Quantum Theory Of Solids*, (John Wiley & Sons, New York, 1963) pp.338-365.
- [2] N. Bloembergen, *J. Physique Rad.* **23**, 658 (1962).
- [3] J. Kondo, *Solid State Physics* vol. 23, *Theory Of Dilute Magnetic Alloys*, (Academic Press, New York, 1969).
- [4] G.D. Mahan, *Many-particle Physics*, 2nd ed. (Plenum, New York, 1990) pp. 58-60.
- [5] J.R. Schrieffer and P.A. Wolff, *Phys. Rev.* **149**, 2 (1966).
- [6] S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnár, M.L. Roukes, A.Y. Chtchelkanova, and D.M. Treger, *Science* **294**, 1488 (2001).
- [7] K. Yosida, *Phys. Rev.* **106**, 893 (1957).
- [8] M.A. Rudderman and C. Kittel, *Phys. Rev.* **96**, 1 (1954).
- [9] W.A. Harrison, *Solid State Theory*, (McGraw-Hill Book Company, New York, 1970), pp. 280-301.
- [10] Y. Yafet, *Phys. Rev. B* **36**, 7 (1987).
- [11] D.N. Zubarev, *Sov. Phys. Usp.* **3**, 3 (1960).
- [12] V.L. Bonch-Bruевич and S.V. Tyablikov, *The Green Function Method In Statistical Mechanics*, (North-Holland Publishing Company, Amsterdam, 1962).
- [13] S.V. Tyablikov, *Methods In The Theory of Quantum Magnetism*, (Plenum Press, New York, 1967).
- [14] M.S. Fullenbaum and D.S. Falk, *Phys. Rev.* **157**, 2 (1967)
- [15] M.J. Lighthill, *An Introduction to Fourier Analysis and Generalised Function*, 1st ed. (Cambridge University Press, Cambridge, 1964)

- [16] M. Rahman, *Application of Fourier Transforms to Generalized Functions*, 1st ed. (WIT Press, Southampton, 2011)
- [17] S.D. Silverstein, *Phys. Rev.* **132**, 3 (1963).

BIOGRAPHICAL INFORMATION

William Decker was born in Burleson, Texas in 1980. He received a BS in Physics and a BA in Mathematics from the University of Texas in Austin. From 2008 to current, he has worked at Bell Helicopter as an information analyst. In Spring 2012, he successfully defended his Master's Thesis in Physics and received his Master's degree in Physics in the Summer of 2012. The focus of his research has been on theoretical condensed matter.