

**DYNAMICAL MEAN FIELD APPROACH TO PHASE
TRANSITIONS IN FALICOV-KIMBALL MODEL**



A thesis submitted towards partial fulfilment of
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by

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Certificate

This is to certify that this thesis entitled "Dynamical mean field approach to phase transitions in Falicov-Kimball model" submitted towards the partial fulfilment of the BS-MS dual degree programme at the Indian Institute of Science Education and Research Pune represents original research carried out by Anees Ahmed at IISER Pune, under the supervision of Dr. Arijit Bhattacharyay during the academic year 2012-2013.

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Abstract

The Falicov-Kimball model is the simplest model of correlated electrons which shows long range order. The Falicov-Kimball model is exactly solvable in the limit of infinite dimensions through the use of Dynamical Mean Field Theory (DMFT). This thesis reviews the Hubbard model and Falicov Model in some detail, and details the DMFT formalism. The DMFT formalism is used to investigate continuous second order phase transitions in Falicov-Kimball model. It is seen that the model shows phase transitions for every non-zero value of the interaction strength.

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Chapter 1

Introduction

This chapter gives a brief overview of the Falicov-Kimball model and Dynamical Mean Field Theory. Selected papers are mentioned in order to trace out the history of developments in these fields. The next few chapters will develop the formalism for analysis of phase transitions in Falicov-Kimball model. Chapter 5 describes the results of some calculations. Long proofs and conventions employed can be found in Appendices A and B, respectively.

1.1 Strongly Correlated Systems

Strongly correlated systems are those in which the strength of the electron-electron interaction is comparable or larger than their kinetic energy. The key-phrase here is *strong correlations*. Correlation means that a quantity describing the many-particle system at position \mathbf{x} is affected by the property at \mathbf{y} . In the context of statistical physics, a quantity $Q(\mathbf{x})$ is correlated if

$$\langle Q(\mathbf{x})Q(\mathbf{y}) \rangle \neq \langle Q(\mathbf{x}) \rangle \langle Q(\mathbf{y}) \rangle.$$

$\langle \dots \rangle$ denotes the ensemble average. In some cases ignoring such correlations is a reasonable approximation, but not if the system under consideration has strong correlations in its properties. Strong electronic correlations are most commonly seen in materials with transition and rare-earth metals, i.e. in systems with partially filled d and f orbitals.

Such systems have been investigated since the 1960s with a variety of theoretical tools, but even now no systematic approach exists to deal with them. Perturbative approaches do not work well here, except when the interaction energy is far stronger than the kinetic energy, in which case the kinetic energy can be treated as a perturbation. In absence of exact solutions approximations are invoked but often it is difficult to ascertain whether

a given theoretical result is a genuine feature of the system or just an artefact of the approximation used. Computational methods can be employed too, such as the exact diagonalisation and quantum Monte Carlo methods. But these solutions suffer from two major disadvantages. Firstly, computational solutions do not always provide sufficient insight into the physics. Second is the lack of computational power to carry out realistic calculations.

The simplest model to describe such systems is the single-band Hubbard model,^[12] with the Hamiltonian given by

$$H = \sum_{ij,\sigma} t_{ij}^* c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1.1)$$

It is the simplest model of interacting quantum particles in a lattice. As will be seen in Chapter 2, where more details are provided, the model offers a highly intuitive picture of mobile fermions on a lattice. It should be mentioned at this stage that removal of the interaction term $U \sum_i n_{i\uparrow} n_{i\downarrow}$ from the Hubbard Hamiltonian essentially gives the tight-binding model, which has no electronic correlations.

1.2 Short History of the Falicov-Kimball Model

The Falicov-Kimball (FK) model was introduced by Falicov and Kimball in 1969^[6] to investigate metal-insulator phase transitions in rare-earth and transition metal compounds. In this thesis a spin-less version of the FK model will be considered. This model can be considered as an approximation to the Hubbard model. In the model one considers the σ variable of the Hubbard model to notate two species of spin-less particles, of which one does not hop and is frozen on the lattice. Essentially, the Hubbard Model is cast into a form where the one specie of particles is quantum in nature, while the other is classical. The rest of the section mentions some attempts at studying phase transitions in FK model.

The initial work based on FK model was targeted at analysing the thermodynamics of metal-insulator transition with a mean-field approach.^{[6], [18], [17]} The solutions with this approach showed both continuous and discontinuous phase transitions. In the 1970s this model was applied to other systems, and had both failures and successes.

In the 1980s it was realised that this is the simplest model of strongly correlated systems which shows long range order. It was shown that there always exists a finite transition temperature to a chessboard phase if the each particle concentration is $\frac{1}{2}$.^{[4], [5]} This transition can be identified as one from a high-temperature homogeneous fluid phase to a low-temperature ordered solid

phase. It was also proven that a phase transition takes place for any value of the interaction strength, given that the temperature is low enough.^{[13],[15]} In the 1990s various proofs of phase separation were submitted – one dimension and large interaction strength,^[14] one dimension and small interaction strength,^[8] arbitrary dimension and large interaction strength.^{[10],[9]}

1.3 Dynamical Mean Field Theory - A Briefing

1.3.1 Mean-Field Theories

In statistical mechanics a rough picture of a model can be obtained by using mean-field theories. Generally in a mean-field theory, a quantity describing the system is replaced by an averaged quantity, the *mean-field*, greatly simplifying all calculations. As with any other approximation scheme, the reliability of such a scheme should be well understood in every case of application. In some cases a parameter called the control parameter can be found, which, depending on its value, governs the accuracy of the scheme.

The most well known example of a mean-field theory is the Weiss theory for the Ising model. The theory replaces the detailed actual field of the system by an averaged field which is just a single number, constant in space and time. It can also be viewed as an effective *single-site* problem. This means that the mean-field approach can be viewed as replacing a system of particles by a single site embedded in an effective medium, with all the details of the surroundings being contained within the mean-field.

The control parameter for the Weiss theory is $1/Z$, Z being the coordination number of the lattice. In the limit $Z \rightarrow \infty$ or $1/Z \rightarrow 0$, the theory becomes exact. The small parameter $1/Z$ can be used to systematically improve the accuracy of the theory. A natural question arises - whether such an approximation is purely academic in nature without any practical implications. The answer is two-fold. First, a lot of naturally existing lattices have large coordination. In three dimensions, $Z = 6, 8$ and 12 for simple cubic, bcc, and fcc lattice resp. For the latter two, a mean field approach with $1/Z$ as the control parameter is expected to yield reasonably accurate results. This point will be supported quantitatively in Chapter 2. Secondly, even if the results of a mean-field theory in low dimensions are not quantitatively accurate, some qualitative results can be obtained to shed light on the physics.

1.3.2 Dynamical Mean Field Theory

The natural generalisation of Weiss mean-field theory, when dealing with quantum many-body systems, is Dynamical Mean Field Theory (DMFT). The essential idea, much like before, is to replace the system of particles on a lattice by a single-site quantum impurity model. This impurity model is contained within an effective medium which is determined self-consistently. This approach has the advantage that a lot of work has already been done in understanding impurity models.

A crucial feature of DMFT is that only the spacial fluctuations are frozen. Temporal fluctuations still exist and hence the name *dynamical*. As with the Weiss mean-field theory, DMFT becomes exact in the limit of large coordination number, and can be used both to calculate exact properties for materials with large coordination numbers or to gain valuable qualitative insight for smaller coordination numbers. In the $Z \rightarrow \infty$ limit it can be shown that the self-energy becomes local, i.e. it has no \mathbf{k} -dependence, and this result is behind the simplicity introduced in DMFT.

The origin of DMFT lies in the work of Metzner and Vollhardt (1989),^{Metzner89} with the realisation that the self-energy becomes local in large dimensions. Immediately after this, Brandt and Mielsch solved the Falicov-Kimball model exactly in large dimensions.^{[1],[2],[3]} In these three papers they also provided exact results for electronic phase transitions in the FK model and calculated the free energy.

1.3.3 Falicov-Kimball model and DMFT

There are two main reasons that make the use of DMFT of Falicov-Kimball model attractive. First, DMFT can be used at all interaction strengths. The only approximation used was the limit of infinite dimensions. Second, the Falicov-Kimball model is exactly solvable in large dimensions. By 'exactly solvable' it is meant that no quantum Monte Carlo is required to solve. Once the Green function is exactly known upon using DMFT, virtually any property can be calculated.

Chapter 2

DMFT of the Hubbard Model

This chapter introduces the Hubbard model and then describes the derivation of the DMFT equations for all Hubbard-like models.

2.1 A short introduction to the Hubbard Model

The Hubbard Hamiltonian is

$$H = \sum_{ij,\sigma} t_{ij}^* c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (2.1)$$

t_{ij}^* is called the *hopping amplitude* which is the probability of an electron to hop from site j to site i . The hopping amplitude is taken to be non-zero for nearest neighbour hopping only. This signifies that an electron has zero probability of jumping from site i to site j if i and j are not nearest neighbours. The hopping amplitude is a measure of the kinetic energy of the electron, and can be calculated as

$$t_{ij}^* = \langle i | \hat{T} | j \rangle \quad (2.2)$$

where \hat{T} is the one-body kinetic energy operator and $|i\rangle$ is a Wannier state. It is clear from definition of the hopping amplitude that the model is based on the tight-binding approach. The dispersion of momenta $\epsilon_{\mathbf{k}}$ is related to the hopping amplitude by a Fourier transform.

$$t_{ij}^* = \sum_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)} \epsilon_{\mathbf{k}} \quad (2.3)$$

Throughout this thesis the modelling will be done on a hyper-cubic lattice for which the nearest neighbour hopping amplitude can be represented by a

single constant: $t_{ij}^* = t^*$, if i, j are nearest neighbours, otherwise 0. Using (2.3) it can be shown that the dispersion in d -dimensions is

$$\epsilon_{\mathbf{k}} = 2t^* \sum_{i=1}^d \cos k_i \quad (2.4)$$

U is the *on-site* Coulomb interaction strength. Any site on the lattice can accommodate two electrons (of opposite spins) at maximum due to the exclusion principle. The interaction of such two electrons is quantified by U . The interaction part of the Hamiltonian contains only local terms $n_{i\uparrow}n_{i\downarrow}$, which guarantees that electrons on separate sites do not interact. In transition metal and rare-earth metals, where strong correlations are usually seen, the d -shell and f -shell is partially filled. As the electrons in these orbitals are strongly localised, it follows that the interactions between electrons of the same ion are much larger than those of different ones. This justifies the local nature of the interaction term. σ denotes the spin.

2.2 The limit of large dimensions

This section analyses Hubbard-type models in large dimensions. Hubbard-type models, for the purpose of this thesis, are those in which the hopping term is nearest neighbour only and the interactions are purely local. DMFT can be extended to more general cases of next-nearest neighbour hopping or nearest neighbour interactions but such *extended* Hubbard-type models are not discussed here.

2.2.1 Scaling of the hopping amplitude

This section investigates the limit of large dimensions for Hubbard-type models, following [16]. The interaction term is purely local for these models, and thus independent of the lattice structure and dimensions. It is the kinetic energy which depends on dimensionality and structure of lattice. Therefore only the kinetic energy is analysed in large dimensions. The non-interacting density of states (DOS) associated with dispersion $\epsilon_{\mathbf{k}}$ in d -dimensions is

$$D_d(\epsilon) = \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) \quad (2.5)$$

This expression can be considered to be the probability density for finding $\epsilon = \epsilon_{\mathbf{k}}$ for a random \mathbf{k} . In this interpretation $\epsilon_{\mathbf{k}}$ from (2.4) is a sum of d independent

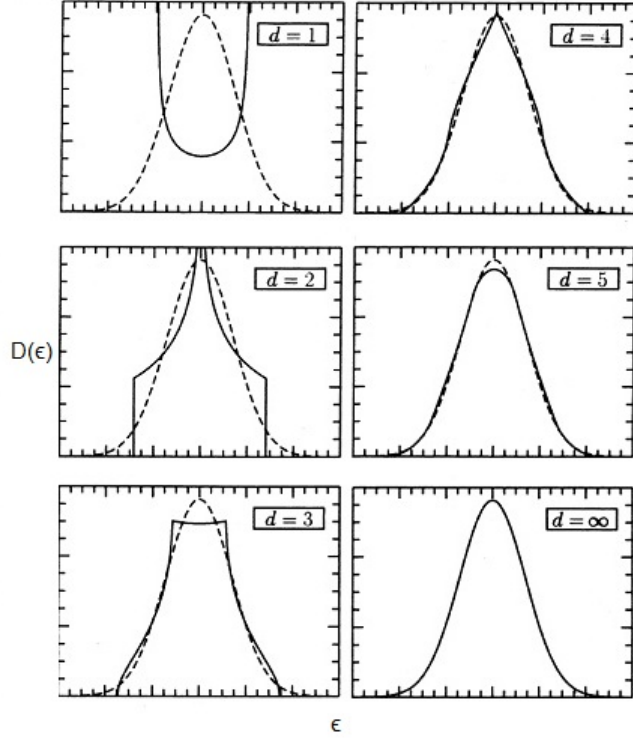


Figure 2.1: Comparison of DOS of dispersion $\epsilon_{\mathbf{k}}$ (2.4) for *small* dimensions $d=1,2,3,4$ and 5 (full lines) and $d = \infty$ (broken line). Notice that from $d = 4$ onwards the DOS begins to closely resemble the infinite dimensional DOS. From [19]

random numbers $2t^* \cos k_i$. In the limit $d \rightarrow \infty$ the central limit theorem yields

$$D_{\infty}(\epsilon) = \frac{1}{2t^*\sqrt{\pi d}} \exp \left[- \left(\frac{\epsilon}{2t^*\sqrt{d}} \right)^2 \right] \quad (2.6)$$

For large d this DOS becomes arbitrarily broad and flat, and only the following scaling saves it from being trivial

$$t^* = \frac{t}{2\sqrt{d}} \quad (2.7)$$

$$D_{\infty}(\epsilon) = \frac{1}{t\sqrt{\pi}} \exp \left[- \left(\frac{\epsilon}{t} \right)^2 \right] \quad (2.8)$$

t is a finite constant. Figure 2.1 compares some finite dimensional DOS with the infinite dimensional gaussian DOS. From $d = 4$ onwards the DOS begins to closely resemble the $d \rightarrow \infty$ one. Thus even for *small* dimensions

the calculations in the infinite dimension limit are expected to yield reliable results. For a brute-force approach to (2.7) and (2.8) see Appendix A. With this scaling the dispersion is

$$\epsilon_{\mathbf{k}} = \frac{t}{\sqrt{d}} \sum_{i=1}^d \cos k_i \quad (2.9)$$

2.2.2 Locality of Self-Energy

The most drastic consequence of the scaling (2.7) is that the self-energy becomes local in space, leading to great simplifications in the study of Hubbard-type models. The following results all hold true for Hubbard-like models, even though the Hubbard model is used explicitly throughout the discussion. The non-interacting kinetic energy is

$$KE = \frac{t}{2\sqrt{d}} \sum_{\langle i,j \rangle, \sigma} g_{ij,\sigma}^0 \quad (2.10)$$

where $g_{ij,\sigma}^0 = \langle c_{i\sigma}^\dagger c_{j\sigma} \rangle_0$ is the density matrix. It can be interpreted as the amplitude for hopping from site j to i . In d -dimensions, any site has $\mathcal{O}(d)$ nearest neighbours. Since an electron can move only to its nearest neighbour, $|g_{ij,\sigma}^0|^2$ is of the order $1/d$, which gives

$$g_{ij,\sigma}^0 \sim \frac{1}{\sqrt{d}}. \quad (2.11)$$

Also note that the kinetic energy as given in (2.10) is finite for infinite dimensions. Without the $1/\sqrt{d}$ scaling of the hopping amplitude, the kinetic energy would grow as \sqrt{d} . This is an independent corroboration of the said scaling. Now, the density matrix is just the single-particle non-interacting Green function in the limit $\tau \rightarrow 0^-$, which is defined as usual as

$$G_{ij,\sigma}^0(\tau) = -\langle \mathbb{T} \hat{c}_{i\sigma}(\tau) \hat{c}_{j\sigma}^\dagger(0) \rangle_0. \quad (2.12)$$

It follows that the Green function also follows the same scaling (2.11)

$$G_{ij,\sigma}^0 \sim \frac{1}{\sqrt{d}}, \quad (2.13)$$

for nearest neighbours i,j . For any arbitrary sites i and j , (2.13) can be used recursively to obtain

$$G_{ij,\sigma}^0 \sim \frac{1}{d^{(\|\mathbf{R}_i - \mathbf{R}_j\|)/2}}. \quad (2.14)$$

$\|\mathbf{R}\| \equiv \sum_{i=1}^d |R_n|$ is the length of vector \mathbf{R} in the New York metric.

Now, consider any self-energy diagram with two internal vertices i and j . A simple count argument will reveal a surprising feature of such self-energy diagrams. The self-energy Σ will have sums over both internal vertices i, j . Suppose the number of paths connecting i and j in the diagram is P . Each path connecting i and j will contribute a factor $(1/\sqrt{d})^{\|i-j\|}$, so that

$$\Sigma \sim \sum_{ij} \left(\frac{1}{\sqrt{d}} \right)^{P\|i-j\|}.$$

The sum over i, j could equally well be written as a sum over i and $R \equiv \|i - j\|$. The sum over i gives d^R , and the above relation becomes

$$\begin{aligned} \Sigma &\sim \sum_{R=0}^{\infty} d^R \left(\frac{1}{\sqrt{d}} \right)^{PR} \\ &= \sum_{R=0}^{\infty} d^{R(1-P/2)} \end{aligned}$$

For diagrams with $P \geq 3$ the term $d^{R(1-P/2)}$ vanishes in the limit $d \rightarrow \infty$, unless $R = 0$. Therefore only local terms, i.e. terms with $i = j$, contribute. Now, consider perturbation theory for the Hubbard model. The first order self-energy diagram is already local. For second and greater orders, $P \geq 3$. Thus the self-energy consists of terms which are local, and hence the self-energy itself is local. This fact leads to tremendous simplification when calculating Green functions, and is the basis of DMFT.

2.3 Construction of DMFT

There are multiple ways of deriving DMFT equations, each relying on the limit of infinite dimensions and the locality of self energy. One of the methods - the *cavity* method - involves calculation of Green function directly from the canonical or grand canonical partition function. In this section, DMFT for Hubbard model will be constructed using the cavity method following [11].

The basic idea of a cavity method is to focus on any one site of the lattice, say o and then integrate out the degrees of freedom on all other sites. This creates an *effective field* for the lattice. Up till now, this scheme is exact, that is, no approximation has been used. It is when this effective field is required to be the same as the actual field at site o (self-consistency), that the scheme becomes an approximation. The approximation becomes exact in

infinite dimensions, as will be seen in the derivation. The derivation begins with construction of the canonical partition function. In the path integral formulation with the Grassmann variables $\psi_{i\sigma}$ and $\bar{\psi}_{i\sigma}$ for the electrons.

$$Z = \int D[\psi_\sigma] e^{-S}, \quad (2.15)$$

$$S = \int_0^\beta d\tau \left(\sum_{i\sigma} \bar{\psi}_{i\sigma}(\tau) (\partial_\tau - \mu) \psi_{i\sigma}(\tau) + \sum_{ij,\sigma} t_{ij}^* \bar{\psi}_{i\sigma}(\tau) \psi_{j\sigma}(\tau) \right. \\ \left. + U \sum_i n_{i\downarrow}(\tau) n_{i\uparrow}(\tau) \right) \quad (2.16)$$

To calculate the effective action, all degrees of freedom except those at site o are integrated out.

$$\frac{1}{Z_{eff}} e^{-S_{eff}[\psi_{o\sigma}, \bar{\psi}_{o\sigma}]} = \frac{1}{Z} \int D^{(o)}[\psi_\sigma] e^{-S} \quad (2.17)$$

Here, $D[\psi_\sigma]$ and $D^{(o)}[\psi_\sigma]$ are shorthand notation for the path-integral measure and are explicitly written as

$$D[\psi_\sigma] = \prod_i D\bar{\psi}_{i\sigma} D\psi_{i\sigma}, \\ D^{(o)}[\psi_\sigma] = \prod_{i \neq o} D\bar{\psi}_{i\sigma} D\psi_{i\sigma} \quad (2.18)$$

The action S is split into three parts -

$$S_o = \int_0^\beta d\tau \left(\sum_\sigma \bar{\psi}_{o\sigma}(\tau) (\partial_\tau - \mu) \psi_{o\sigma}(\tau) + U n_{o\uparrow}(\tau) n_{o\downarrow}(\tau) \right), \quad (2.19)$$

$$\Delta S = \int_0^\beta d\tau \sum_{i\sigma} t_{io}^* (\bar{\psi}_{i\sigma}(\tau) \psi_{o\sigma}(\tau) + \bar{\psi}_{o\sigma}(\tau) \psi_{i\sigma}(\tau)) \quad (2.20)$$

and $S^{(o)} = S - S_o - \Delta S$. S_o is the action containing the degrees of freedom at site o , ΔS is the action for the interaction of site o with surroundings, and $S^{(o)}$ is the lattice action in presence of the cavity, i.e. with site o removed. Also, define a cavity partition function $Z^{(o)}$ as

$$Z^{(o)} = \int D^{(o)}[\psi_\sigma] e^{-S^{(o)}} \quad (2.21)$$

With this set-up the effective action in (2.17) becomes

$$\begin{aligned} \frac{1}{Z_{eff}} e^{-S_{eff}} &= \frac{1}{Z} e^{-S_o} \int D^{(o)}[\psi_\sigma] e^{-S^{(o)}} e^{-\Delta S} \\ &= \frac{Z^{(o)}}{Z} e^{-S_o} \langle e^{-\Delta S} \rangle^{(o)} \end{aligned} \quad (2.22)$$

where $\langle \dots \rangle^{(o)}$ denotes the trace with respect to the cavity partition function $Z^{(o)}$. Expanding the right hand side in Taylor series yields a series in $\langle (-\Delta S)^n \rangle^{(o)}$. Because of the presence of $\psi_{o\sigma}$ and $\bar{\psi}_{o\sigma}$ Grassmann variables in ΔS only terms with even n are non-vanishing. The second term in the expansion of $\langle e^{-\Delta S} \rangle^{(o)}$ is

$$\begin{aligned} \frac{1}{2} \langle (-\Delta S)^2 \rangle^{(o)} &= \int d\tau d\tau' \sum_{ij,\sigma} t_{io}^* t_{jo}^* \bar{\psi}_{o\sigma}(\tau') \psi_{o\sigma}(\tau) G_{ij,\sigma}^{(o)}(\tau - \tau') \\ &= T \sum_n \sum_{ij,\sigma} t_{io}^* t_{jo}^* \bar{\psi}_{o\sigma}(i\omega_n) \psi_{o\sigma}(i\omega_n) G_{ij,\sigma}^{(o)}(i\omega_n) \end{aligned} \quad (2.23)$$

which scales as

$$\langle (-\Delta S)^2 \rangle^{(o)} \sim \sum_{\langle ij,o \rangle} \frac{1}{d} \left(\frac{1}{\sqrt{d}} \right)^{\|i-j\|} \quad (2.24)$$

In the sum, i and j are both nearest neighbours of o . Therefore $\|i-j\|$ is either 0 or 2, depending on whether i and j are same or not. Plugging in these values gives the scaling for the second term as unity. The fourth term scales as

$$\langle (-\Delta S)^4 \rangle^{(o)} \sim \sum_{\langle ijkl,o \rangle} \frac{1}{d^2} \left(\frac{1}{\sqrt{d}} \right)^{\|i-j\|} \left(\frac{1}{\sqrt{d}} \right)^{\|j-k\|} \left(\frac{1}{\sqrt{d}} \right)^{\|k-l\|} \quad (2.25)$$

which simplifies to $1/d$. Further even terms are each smaller by $1/d$, and therefore in the infinite dimension limit, only the first of the even terms survives.

Now, the local action for site o surrounded by a bath, S_{eff} - the effective action, can be written as

$$S_{eff} = - \int_0^\beta d\tau d\tau' \sum_\sigma \bar{\psi}_{o\sigma}(\tau) \mathcal{G}_\sigma^{-1}(\tau - \tau') \psi_{o\sigma}(\tau') + U \int_0^\beta d\tau n_{o\downarrow}(\tau) n_{o\uparrow}(\tau) \quad (2.26)$$

$\mathcal{G}_\sigma(\tau - \tau')$ can be interpreted as the bare propagator for the local effective action, and is the amplitude for a particle to move from bath to site o at

time τ and then return back to the bath at time τ' . In contrast to the mean-field of Ising model, $\mathcal{G}_\sigma(\tau - \tau')$ is a function of time and devoid of any spatial fluctuations. In frequency space the kinetic part of S_o and the effective action S_{eff} read

$$S_{eff}^{kinetic} = -T \sum_n \sum_\sigma \bar{\psi}_{o\sigma}(i\omega_n) \psi_{o\sigma}(i\omega_n) \mathcal{G}_\sigma^{-1}(i\omega_n) \quad (2.27)$$

$$S_o^{kinetic} = -T \sum_n \sum_\sigma (i\omega_n + \mu) \bar{\psi}_{o\sigma}(i\omega_n) \psi_{o\sigma}(i\omega_n) \quad (2.28)$$

The interaction part is same for both S_{eff} and S_o . Therefore combining (2.22), (2.23), (2.27) and (2.28) along with the fact that only the second term in the expansion of $\langle e^{-\Delta S} \rangle^{(o)}$ contributes in the infinite dimension limit yields

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{ij} t_{io}^* t_{jo}^* G_{ij}^{(o)}(i\omega_n) \quad (2.29)$$

$G_{ij}^{(o)}$ is the Green function in presence of the cavity. To obtain the self-consistent equations of DMFT, the Green function of the original lattice G_{ij} is required. Relating $G_{ij}^{(o)}$ to G_{ij} is complicated for a general lattice. The proof will be omitted here, being quite extensive. The relation is

$$G_{ij}^{(o)} = G_{ij} - \frac{G_{io} G_{jo}}{G_{oo}} \quad (2.30)$$

Inserting (2.30) in (2.32) gives

$$\mathcal{G}^{-1}(i\omega_n) = \Sigma_n + G^{-1}(i\omega_n) \quad (2.31)$$

where, $G(i\omega_n) = \sum_{\mathbf{k}} G_{\mathbf{k}}(i\omega_n)$ is the local Green function. (Refer to Appendix A for detailed derivation.) This equation combined with Dyson's equation for homogeneous systems form the set of equations for DMFT.

2.3.1 DMFT on Bethe lattice

There is one lattice for which relating $G_{ij}^{(o)}$ and G_{ij} is very simple - the Bethe lattice. The Bethe lattice of connectivity z is a lattice in which each site is directly connected to z other sites, and any two sites are connected by only one path. The proof relies on the fact that once a cavity at site o has been introduced, the lattice separates into multiple disconnected lattices. Also note that the sum over site indices i, j in (2.29) is only over i, j which are nearest neighbours of the cavity site o . Combination of these two facts

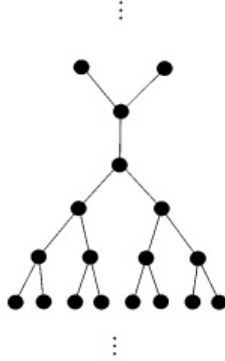


Figure 2.2: $z = 3$ Bethe lattice. From [11]

means that all the nearest neighbours of the cavity site are disconnected, and therefore the sum in (2.29) will have $i = j$.

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_i t_{io}^* t_{io} G_{ii}^{(o)}(i\omega_n) \quad (2.32)$$

In the infinite dimension limit, the local Green functions for lattice with and without cavity are equal, as removal of a single site does not make a difference. It should be cautioned that this statement does not hold for the non-local Green function G_{ij} . Also, for homogeneous phases, the local Green function G_{ii} is independent of i . Thus the above relation reduces to, upon introducing the scaling (2.7)

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G_{ii}(i\omega_n) \quad (2.33)$$

2.4 Summary

The Hubbard model has been briefly described in this chapter. It has been shown for Hubbard-type models in large dimensions that the density of states becomes trivial and the kinetic energy diverges, unless the hopping amplitude is scaled in a particular fashion. This scaling results in a simplification of the theory - the self-energy ceases being momentum-dependent, which has been proven using a simple power-counting argument. Employing the scaling the hopping amplitude and the locality of self-energy, the equations of DMFT have been derived. Finally, the form of bare propagator has been determined for Hubbard-like models on a Bethe lattice.

Chapter 3

DMFT of Falicov-Kimball Model

The Falicov-Kimball model is introduced in this chapter. Later the DMFT of FK model is formulated.

3.1 The Falicov-Kimball Model

As stated in Chapter 1, the FK model is a simplified version of the Hubbard. In this work, only the spin-less version of the FK model will be considered. The σ parameter of Hubbard model denotes not the spin in this case, but rather two species of particles c and f . The FK Hamiltonian can be written as

$$H = \sum_{ij} t_{ij}^* c_i^\dagger c_j + E \sum_i f_i^\dagger f_i + U \sum_i c_i^\dagger c_i f_i^\dagger f_i \quad (3.1)$$

Here, t_{ij}^* is the nearest neighbour hopping amplitude. Only the c -particles have an associated hopping amplitude and thus kinetic energy, and are appropriately called itinerant electrons. The f -particles occupy sites on the lattice with energy E and have no kinetic energy. These can either be considered to be localised electrons or ions. Thus, the model can be interpreted as having quantum c -particles (electrons) interacting with an external classical field (f -particles). As in the Hubbard model, the only interaction between electrons and ions occurs when they occupy the same site. In general, the chemical potentials associated with c and f particles μ and μ_f are unequal, unless the f -particles are also electrons.

FK model is essentially an independent-electron one, and thus appears to be a one-body model. The many-body aspects enter through the annealing average over all the possible configuration of ions. To understand this better, the Hamiltonian will be written in such a manner as to explicitly show the

classical nature of the ions.

$$H = \sum_{ij} t_{ij}^* c_i^\dagger c_j + E \sum_i W_i + U \sum_i c_i^\dagger c_i W_i \quad (3.2)$$

The set W_i is the configuration of ions, with W_i 1 (or 0) if site i is occupied (or unoccupied) by an ion. In calculating the partition function, the sum over all possible states will include a sum over all possible ion configurations. As can be seen from (3.2) the itinerant electrons do not interact with themselves, and it is only through the averaging over the ionic configurations does this model become a many-body model. This creates an effective long range interaction among the ions, and causes them to order or phase separate at low temperatures.

3.2 DMFT of the Falicov-Kimball model

The result from chapter 2 for the bare propagator \mathcal{G} (2.31) still holds here, as FK model is a Hubbard-type model too. The classical nature of f -particles makes the solution of the DMFT equations much easier in this case. Begin with the single particle Green function written in grand canonical ensemble

$$G_{ij}(\tau) = -\frac{1}{Z} Tr_{cf} \left[e^{-\beta(H - \mu N - \mu_f N_f)} \mathbb{T}_{c_i(\tau) c_j^\dagger(0)} \right] \quad (3.3)$$

where Tr_{cf} means the trace over both c and f degrees of freedom. N is the total electron number operator, while $N_f = \sum_i W_i$ is the total ion number. The Hamiltonian can be separated into two parts, one of which is ion-only - $H_f = EN_f$. With this division of the Hamiltonian the Green function can be written in path-integral formalism as

$$G_{ij}(\tau) = -\frac{1}{Z} Tr_f \left[e^{-\beta(H_f - \mu_f N_f)} \int D\psi D\bar{\psi} \psi_i(\tau) \bar{\psi}_j(0) e^{-S} \right] \quad (3.4)$$

where S is the action for FK Hamiltonian given by

$$S = \sum_i \int_0^\beta d\tau \bar{\psi}_i(\tau) (\partial_\tau + U W_i - \mu) \psi_i(\tau) + \sum_{ij} t_{ij}^* \int_0^\beta d\tau \bar{\psi}_i(\tau) \psi_j(\tau). \quad (3.5)$$

The action in frequency space reads

$$S = \sum_n S_n$$

$$S_n = \sum_{ij} t_{ij}^* \bar{\psi}_{in} \psi_{jn} + \sum_i (U W_i - i\omega_n - \mu) \bar{\psi}_{in} \psi_{in} \quad (3.6)$$

As before, the action is separated into three parts: $S_n = S_{on} + \Delta S_n + S_n^{(o)}$. One for degrees of freedom on the cavity site o , one for interaction of the site with the surroundings and one for the remaining lattice.

$$\begin{aligned} S_{on} &= (UW_o - i\omega_n - \mu)\bar{\psi}_{on}\psi_{on} \\ \Delta S_n &= \sum_j t_{jo}^* (\bar{\psi}_{jn}\psi_{on} + \bar{\psi}_{on}\psi_{jn}) \\ S_n^{(o)} &= S_n - S_{on} - \Delta S_n \end{aligned} \quad (3.7)$$

Then the local Green function at site o , $G_{oo,n}$, can be expanded exactly as for Hubbard model -

$$\begin{aligned} G_{oo,n} &= -T \frac{Z^{(o)}}{Z} Tr_f \left[e^{-\beta(H_f - \mu_f N_f)} \int D\bar{\psi}_o D\psi_o \psi_{on} \bar{\psi}_{on} \right. \\ &\quad \left. \times \exp \left(-T \sum_n S_{on} \right) \left\langle \exp \left(-T \sum_{n'} \Delta S_{n'} \right) \right\rangle^{(o)} \right] \end{aligned} \quad (3.8)$$

Only the second term in the Taylor expansion of $\langle e^{-T \sum_n \Delta S_n} \rangle^{(o)}$ survives in the limit of infinite dimensions. Associate with this term the Weiss field λ_n so that the Green function becomes

$$\begin{aligned} G_{oo,n} &= -T \frac{Z^{(o)}}{Z} Tr_f \left[e^{-\beta(H_f - \mu_f N_f)} \int D\bar{\psi}_o D\psi_o \psi_{on} \bar{\psi}_{on} \right. \\ &\quad \left. \times \exp \left(T \sum_{n'} (i\omega_{n'} + \mu - UW_o - \lambda_{n'}) \right) \right] \end{aligned} \quad (3.9)$$

The Weiss field λ_n , or equivalently it's Fourier transform $\lambda(\tau)$ is the mean-field of DMFT. As mentioned at the outset, this mean field is static in space and fluctuates in time. The term in the exponent is the effective action S_{eff} , to which can be associated a partition function

$$\begin{aligned} Z_{eff} &= Tr_f \left[e^{-\beta(H_f - \mu_f N_f)} \int D\bar{\psi} D\psi \right. \\ &\quad \left. \times \exp \left(T \sum_n (i\omega_n + \mu - UW_i - \lambda_n) \bar{\psi}_{on} \psi_{on} \right) \right]. \end{aligned} \quad (3.10)$$

The trace represents sum over all ion-configurations $\{W_i\}$. The trace has been evaluated in [4]

$$Z_{eff} = \exp \left[e^{i\omega_n 0^+} \sum_n \log \frac{A_n}{i\omega_n} \right] + e^{-\beta(E-\mu)} \exp \left[e^{i\omega_n 0^+} \sum_n \log \frac{A_n - U}{i\omega_n} \right] \quad (3.11)$$

The Green function (3.9) can be written as a derivative of the partition function.

$$G_{oo,n} = -\frac{1}{Z_{eff}} \frac{\partial Z_{eff}}{\partial \lambda_n} \quad (3.12)$$

Evaluating the derivative gives

$$G_{oo,n} \equiv G_n = \frac{w_0}{A_n} + \frac{w_1}{A_n - U}, \quad (3.13)$$

$$w_0 = \frac{1}{Z_{eff}} e^{-\beta(E-\mu)} \exp \left[e^{i\omega_n 0^+} \sum_n \log \frac{A_n - U}{i\omega_n} \right]$$

$w_1 (= 1 - w_0)$ can be interpreted as the probability of occupation of site o by an ion. Looking back at the effective action it is obvious that the inverse of $i\omega_n + \mu - \lambda_n \equiv A_n$ is the bare propagator, \mathcal{G}_n , for the effective action, i.e.

$$\mathcal{G}_n^{-1} = i\omega_n + \mu - \lambda_n \quad (3.14)$$

Using the result for Hubbard model (2.31)

$$\Sigma_n = \mathcal{G}_n^{-1} - G_n^{-1}$$

and combining it with (3.13) and (3.14), a quadratic equation in the self-energy Σ_n is obtained. Of the two solutions only one is analytic in $i\omega_n$, and it is

$$\Sigma_n = \frac{U}{2} - \frac{1}{2G_n} + \sqrt{\left(\frac{U}{2} - \frac{1}{2G_n}\right)^2 + w_1 \frac{U}{G_n}} \quad (3.15)$$

As seen in Appendix A, equation (A.7), the Green function for homogeneous systems is

$$G_n = \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_n} \quad (3.16)$$

Equations (3.15) and (3.16) form the set of DMFT equations for the Falicov-Kimball model. These equations are solved self-consistently, i.e. a guess is made for the Green function, which is used to evaluate the self-energy from (3.15). Then the self-energy is input in (3.16) to get another value of Green function. This process is repeated until the initial and final values of Green functions are sufficiently close.

3.3 Summary

In this chapter, the Falikov-Kimball model has been introduced. Thereafter, the DMFT equations for the model were derived using the cavity method. As the FK model is a Hubbard-type model, the DMFT equation derived in Chapter 2 also holds here, with one major difference. The simplicity of FK model as compared to the Hubbard model allows the expression of the self-energy as a very simple function of the Green function. This makes the model exactly solvable through DMFT, i.e. in the limit of large dimensions.

Chapter 4

Phase transitions

This chapter introduces the quantities and parameters needed to investigate phase transitions in Falicov-Kimball model and is based on [1] and [2]. As an introduction an intuitive understanding of phase transitions based on free energy will prove useful. A system will exist in that phase which minimises the free energy.

$$F = E - TS \tag{4.1}$$

The internal energy E has its origin in the Coulomb interaction between ions and electrons, represented in the FK model by the interaction strength U . The entropy is simply the measure of disorder in the system. For very large temperatures, the entropy S gives the major contribution minimisation of the free energy. This is why at large temperatures, systems exist in phases with maximum entropy, i.e. totally disordered ones. As temperature is lowered, the contribution from the entropy decreases and the effect of E becomes more prominent. This causes a phase transition to a more ordered phase. In case of the FK model, the first phase encountered, as temperature is decreased, is the *chessboard* phase. In this phase, as the name suggests, the ions are arranged in an alternating pattern like a chessboard, while the itinerant electrons move through this configuration.

With further decrease in temperature various other phases might be encountered. The last phase is the segregated phase, in which one half of the lattice is entirely occupied by the ions, whereas the itinerant electrons remain in the other half. This is a manifestation of the fact that at low temperatures E is the dominant factor, and a minimum E implies minimum interaction between the ions and itinerant electrons.

4.1 The Charge-density-wave susceptibility

Since phase transitions are a change in the ordering of the system, it is useful to define correlation functions that can quantify order. Begin by defining the density correlation function for c -particles.

$$\chi(\mathbf{R}_i - \mathbf{R}_j) \equiv \chi_{ij} = \langle (n_i - \langle n_i \rangle)(n_j - \langle n_j \rangle) \rangle \quad (4.2)$$

The charge-wave-density susceptibility is defined as the Fourier transform of the density correlation. To calculate the correlation, recall the definition of Green function (3.4). To the FK Hamiltonian add a time-independent field Λ which couples only to the itinerant electrons. Denote quantity A in presence of Λ by A^Λ .

$$\begin{aligned} H^\Lambda &= H + \sum_i \Lambda_i d_i^\dagger d_i \\ S^\Lambda &= S + \sum_i \Lambda_i \int_0^\beta d\tau \bar{\psi}_i(\tau) \psi_i(\tau) \\ &= S + \sum_i \sum_n \Lambda_i \bar{\psi}_{in} \psi_{in} \end{aligned} \quad (4.3)$$

As usual, G^Λ can be found by differentiating the partition function.

$$G_{ii}^\Lambda = T \sum_n G_{ii,n}^\Lambda = -\frac{1}{Z^\Lambda} \frac{\partial Z^\Lambda}{\partial \Lambda_i}$$

and

$$\frac{\partial G_{ii}^\Lambda}{\partial \Lambda_j} = G_{ii}^\Lambda G_{jj}^\Lambda - \frac{1}{Z^\Lambda} \frac{\partial^2 Z^\Lambda}{\partial \Lambda_i \partial \Lambda_j} \quad (4.4)$$

The density at site i $\langle n_i \rangle$ is just the Green function $G_{ii}(\tau)$ with $\tau \rightarrow 0^-$, i.e.

$$\begin{aligned} \langle n_i \rangle &= \lim_{\tau \rightarrow 0^-} G_{ii}^\Lambda(\tau) |_{\Lambda=0} \\ &= T \sum_n G_{ii,n}^\Lambda |_{\Lambda=0} \end{aligned}$$

Then it is clear that the first term in (4.4) corresponds to $\langle n_i \rangle \langle n_j \rangle$, and the second term corresponds to $\langle n_i n_j \rangle$. So,

$$\chi_{ij} = -T \frac{dG_{ii}^\Lambda}{d\Lambda_j} \Big|_{\Lambda=0} \quad (4.5)$$

Now observe that

$$\begin{aligned} -\frac{dG_{ii}^\Lambda}{d\Lambda_j} &= -\int d\bar{\mathbf{k}} \frac{dG_{\mathbf{k}}^\Lambda}{d\Lambda_j} \\ &= \int d\bar{\mathbf{k}} G_{\mathbf{k}}^\Lambda \frac{d(G_{\mathbf{k}}^\Lambda)^{-1}}{d\Lambda_j} G_{\mathbf{k}}^\Lambda \end{aligned}$$

where $(G_{\mathbf{k}}^\Lambda)^{-1}$ is the inverse of the momentum-dependent Green function. Switching to position-space changes the equation to

$$-\frac{dG_{ii}^\Lambda}{d\Lambda_j} = -\sum_{a,b} G_{ia,n}^\Lambda \left[\frac{d}{d\Lambda_j} (G_n^{-1\Lambda})_{ab} \right] G_{ai,n}^\Lambda \quad (4.6)$$

$(G_n^{-1\Lambda})_{ab}$ is the fourier transform of $(G_{\mathbf{k}}^\Lambda)^{-1}$ and not the inverse of the fourier transform of $G_{\mathbf{k}}^\Lambda$. Combining the explicit expression for $(G_n^{-1\Lambda})_{ab}$

$$(G_n^{-1\Lambda})_{ab} = (i\omega_n + \mu - \Sigma_{bb,n} - \Lambda_b) \delta_{ab} - t_{ab}^*$$

(which can be easily obtained by a fourier transform of $(G_{\mathbf{k}}^\Lambda)^{-1}$) and (4.6) gives

$$\frac{dG_{ii,n}^\Lambda}{d\Lambda_j} = G_{ij,n}^\Lambda G_{ji,n}^\Lambda + \sum_a G_{ia,n}^\Lambda G_{ai,n}^\Lambda \sum_m \frac{d\Sigma_{a,n}}{dG_{aa,m}^\Lambda} \frac{dG_{aa,m}^\Lambda}{d\Lambda_j} \quad (4.7)$$

Fourier transform of the above equation results in the expression for the charge-wave-density susceptibility $\chi_n(\mathbf{q})$.

$$\begin{aligned} \chi_n(\mathbf{q}) &= \chi_n^0(\mathbf{q}) \left[1 + \sum_m \frac{d\Sigma_n}{dG_m} \chi_m(\mathbf{q}) \right] \\ \chi_n(\mathbf{q}) &= -T^2 \sum_n \chi_n(\mathbf{q}) \end{aligned} \quad (4.8)$$

where, $G_{ii,n} \equiv G_n$, $\Sigma_{ii,n} \equiv \Sigma_n$. $\chi_n^0(\mathbf{q})$ is the fourier transform of $-G_{ij,n} G_{ji,n}$.

$$\begin{aligned} \chi_n^0(\mathbf{q}) &= -\sum_{ij} e^{-i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} G_{ij,n} G_{ji,n} \\ &= -\sum_{ij} e^{-i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \int d\bar{\mathbf{k}} d\bar{\mathbf{p}} e^{i(\mathbf{k}-\mathbf{p})\cdot(\mathbf{R}_i-\mathbf{R}_j)} G_{\mathbf{k},n} G_{\mathbf{p},n} \\ &= \sum_{ij} e^{-i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)} \int d\bar{\mathbf{k}} d\bar{\mathbf{k}}' e^{i\mathbf{k}'\cdot(\mathbf{R}_i-\mathbf{R}_j)} G_{\mathbf{k},n} G_{\mathbf{k}-\mathbf{k}',n} \\ &= \int d\bar{\mathbf{k}} G_{\mathbf{k},n} G_{\mathbf{k}-\mathbf{q},n} \end{aligned} \quad (4.9)$$

Consider Σ_n as a function of G_n and w_1 . Using the chain rule for the derivative of Σ_n in (4.8) gives

$$\chi_n(\mathbf{q}) = \frac{\chi_n^0(\mathbf{q})}{1 - \chi_n^0(\mathbf{q}) \frac{\partial \Sigma_n}{\partial G_n}} \left[1 + \frac{\partial \Sigma_n}{\partial w_1} \gamma(\mathbf{q}) \right] \quad (4.10)$$

where

$$\gamma(\mathbf{q}) = \sum_m \frac{dw_1}{dG_m} \chi_m(\mathbf{q}) \quad (4.11)$$

Combining (4.10) and (4.11) gives an equation explicitly devoid of $\chi_n(\mathbf{q})$

$$\gamma(\mathbf{q}) = \sum_n \frac{dw_1}{dG_n} \frac{\chi_n^0(\mathbf{q})}{1 - \chi_n^0(\mathbf{q}) \frac{\partial \Sigma_n}{\partial G_n}} \left[1 + \frac{\partial \Sigma_n}{\partial w_1} \gamma(\mathbf{q}) \right] \quad (4.12)$$

w_1 is a function of all A_n . This fact along with (2.31) can be used to express dw_1/dG_n by expanding through chain rule as

$$\frac{dw_1}{dG_n} = - \frac{dw_1}{dA_n} \frac{\frac{1}{G_n^2} - \left(\frac{\partial \Sigma_n}{\partial G_n} \right)_{w_1}}{1 - \sum_m \frac{dw_1}{dA_m} \left(\frac{\partial \Sigma_m}{\partial w_1} \right)_{G_m}} \quad (4.13)$$

Finally, defining

$$\begin{aligned} \eta_n(\mathbf{q}) &= \frac{G_n}{\chi_n^0(\mathbf{q})} - \frac{1}{G_n}, \\ \theta_n &= 1 - G_n^2 \left(\frac{\partial \Sigma_n}{\partial G_n} \right)_{w_1} \end{aligned} \quad (4.14)$$

and using (4.12) and (4.13), the expression for $\gamma(\mathbf{q})$ can be written as

$$\begin{aligned} \gamma(\mathbf{q}) &\left[1 - \sum_n \frac{dw_1}{dA_n} \left(\frac{\partial \Sigma_n}{\partial w_1} \right)_{G_n} \frac{\eta_n(\mathbf{q}) G_n}{\theta_n + \eta_n(\mathbf{q}) G_n} \right] \\ &= - \sum_n \frac{dw_1}{dA_n} \frac{\theta_n}{\theta_n + \eta_n(\mathbf{q}) G_n} \end{aligned} \quad (4.15)$$

$\chi_n(\mathbf{q})$ is a function of the wave vector \mathbf{q} . This wave vector, called the ordering vector, will serve as a guide into investigating phase transitions in FK model. Similar calculation can be done for density correlation between f particles, and between c and f -particles. The results are

$$\chi^{ff}(\mathbf{q}) = \frac{w_0 w_1}{1 - \sum_n \frac{dw_1}{dA_n} \left(\frac{\partial \Sigma_n}{\partial w_1} \right)_{G_n} \frac{\eta_n(\mathbf{q}) G_n}{\theta_n + \eta_n(\mathbf{q}) G_n}} \quad (4.16)$$

$$\chi^{cf}(\mathbf{q}) = \chi^{ff}(\mathbf{q})T \sum_n \frac{1 - \theta_n}{\theta_n + \eta_n(\mathbf{q})G_n} \quad (4.17)$$

The numerator in none of the cases diverges, while the denominator is the same for all three. This implies that phase transitions in the ions and electrons happens together.

4.2 Order parameter for Falicov-Kimball model in large dimensions

Define

$$X(\mathbf{q}) = \frac{1}{d} \sum_{i=1}^d \cos q_i. \quad (4.18)$$

The parameter X serves as the order parameter for continuous second order phase transitions in FK model. Different values of X correspond to different phases. $X = -1$ corresponds to the chessboard configuration, while $X = 1$ corresponds to the segregated phase.^{[1],[7]} The electron-electron bare susceptibility $\chi_n^0(\mathbf{q})$ can be written as a function of X .^[7]

$$\chi_n^0(X) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{1-X^2}} \int_{-\infty}^{\infty} dy \frac{e^{-y^2}}{i\omega_n + \mu - \Sigma_n - y} G \left(\frac{i\omega_n + \mu - \Sigma_n - Xy}{\sqrt{1-X^2}} \right) \quad (4.19)$$

$G(\mathfrak{z})$ was defined in Appendix A (A.9). With gaussian density of states the expression for $G(\mathfrak{z})$ is

$$G(\mathfrak{z}) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy \frac{e^{-y^2}}{\mathfrak{z} - y} \quad (4.20)$$

(From this point onwards, the hopping amplitude t is set to unity. The energy scale is thus defined in terms of t .) For $X = 0, \pm 1$ the bare susceptibility can be analytically derived. For other values of X , the integrations have to done numerically. Correspondingly, the value of $\eta_n(X)$ for these three values of X can also be calculated analytically. The values for $X = -1$ are

$$\chi_n^0(X = -1) = \frac{G_n}{i\omega_n + \mu - \Sigma_n} \quad (4.21)$$

$$\eta_n(X = -1) = \lambda_n \equiv i\omega_n + \mu - A_n \quad (4.22)$$

Assuming a continuous second order phase transition, the temperature at which $\gamma(X)$ diverges is the critical temperature. For all three susceptibilities, χ, χ^{ff} and χ^{cf} , the numerators never diverge. Any divergence will be a

result of the denominator approaching zero. The fact that all three susceptibilities have a common denominator, implies that phase transitions occur simultaneously for electrons and ions. Thus, the critical temperature is one that satisfies

$$\sum_n \frac{dw_1}{dA_n} \left(\frac{\partial \Sigma_n}{\partial w_1} \right)_{G_n} \frac{\eta_n(X)G_n}{\theta_n + \eta_n(X)G_n} = 1 \quad (4.23)$$

In general, for each value of X the susceptibility will diverge for a different temperature, i.e. to each X a critical temperature $T(X)$ can be associated. The critical temperature for transition from a homogeneous phase to a non-homogeneous one is, then, the greatest among these.

$$T_c = \max\{T(X)\} \quad (4.24)$$

Recall that the equations of DMFT derived in Chapter 3 are valid only for homogeneous phases, and will not hold for temperatures below T_c .

4.3 Summary

In this chapter a measure of the ordering, the charge-density-wave susceptibility $\chi(\mathbf{q})$, has been defined and calculated for a system based on Falicov-Kimball model. It has been shown that the two species of particles c and f have same critical temperatures. Using DMFT it has been shown that an ordering parameter can be defined.

Chapter 5

Results and discussion

In this chapter, the formalism developed in past chapters is put to use and phase transitions for small interaction strength U are analysed. In the last section future plans are described.

5.1 Phase transitions for small interaction strengths

It can be shown that critical temperature defined in (4.24) always corresponds to the chessboard phase ($X = -1$).^[2] This means that DMFT as developed in the previous chapters can be used only for calculating the transition from a homogeneous phase to the chessboard phase. The calculations are easiest for small interaction strength U . The relevant quantities to first order in U are

$$\begin{aligned}\Sigma_n &= w_1 U \\ \left(\frac{\partial \Sigma_n}{\partial G_n} \right)_{w_1} &= 0 \\ \left(\frac{\partial \Sigma_n}{\partial w_1} \right)_{G_n} &= U \\ \frac{dw_1}{dA_n} &= \frac{w_0 w_1 U G_n^2}{1 + U G_n} \\ \theta_n &= 1 \\ \eta_n(-1) &= i\omega_n + \mu - w_1 U - \frac{1}{G_n}\end{aligned}\tag{5.1}$$

Since the self-energy is just a constant, the Green function G_n (3.16) can be calculated directly without resorting to any numerical approach based on

self-consistency. Plugging in all these quantities in (4.15) gives

$$\begin{aligned} \gamma(X = -1) & \left[1 - w_0 w_1 U^2 \sum_n \frac{(i\omega_n + \mu - w_1 U) G_n^2 - G_n}{(1 + U G_n)(i\omega_n + \mu - w_1 U)} \right] \\ & = -w_0 w_1 U \sum_n \frac{G_n}{(1 + U G_n)(i\omega_n + \mu - w_1 U)} \end{aligned} \quad (5.2)$$

There are three possibilities for the behaviour of the critical temperature to the chessboard phase T_c as a function of U .

1. $T_c > 0$ for all $U \geq 0$. In particular, there is a non-zero T_c even for zero interaction.
2. $T_c = 0$ for $U = 0$, and $T_c > 0$ for $U > 0$.
3. $T_c = 0$ for $U < U_0$, and $T_c > 0$ for $U > U_0$. U_0 is a positive number.

It is easy to check that possibility 1 is wrong. For $U = 0$, $\gamma = 0$, and $\chi = \chi^0$. The bare susceptibility χ^0 in this case is simply $\sum_n G_n / (i\omega_n + \mu)$ which does not diverge for any finite value of temperature. Thus there is no phase transition in absence of interactions. This is also intuitively obvious - without any interactions to counter it, the entropy of the system will keep the system in a disordered homogeneous phase.

To check possibilities 2 and 3, consider a half-filled lattice, i.e. $w_0 = w_1 = 1/2$.

$$\gamma(X = -1) = -\frac{U \sum_n \frac{G_n}{(1 + U G_n)(i\omega_n + \mu^*)}}{4 - U^2 \sum_n \frac{(i\omega_n + \mu^*) G_n^2 - G_n}{(1 + U G_n)(i\omega_n + \mu^*)}} \quad (5.3)$$

Here $\mu^* = \mu - U/2$ is the reduced chemical potential. The numerator is always finite, except for $U = 0$, and hence it suffices to calculate the temperature at which the denominator vanishes. Explicit numerical calculation shows that possibility 2 is the correct one. Figure 5.1 shows the variation of critical temperature with U , with the chemical potential set at 0.5. Thus, to every non-zero value of U , corresponds a non-zero critical temperature.

$$\begin{aligned} U = 0 & \Rightarrow T_c = 0 \\ U > 0 & \Rightarrow T_c > 0 \end{aligned} \quad (5.4)$$

The critical temperature T_{cs} for the segregated phase ($X = 1$) is always lesser than the critical temperature T_c for the chessboard phase ($X = -1$). It follows that a zero interaction T_{cs} is also zero.

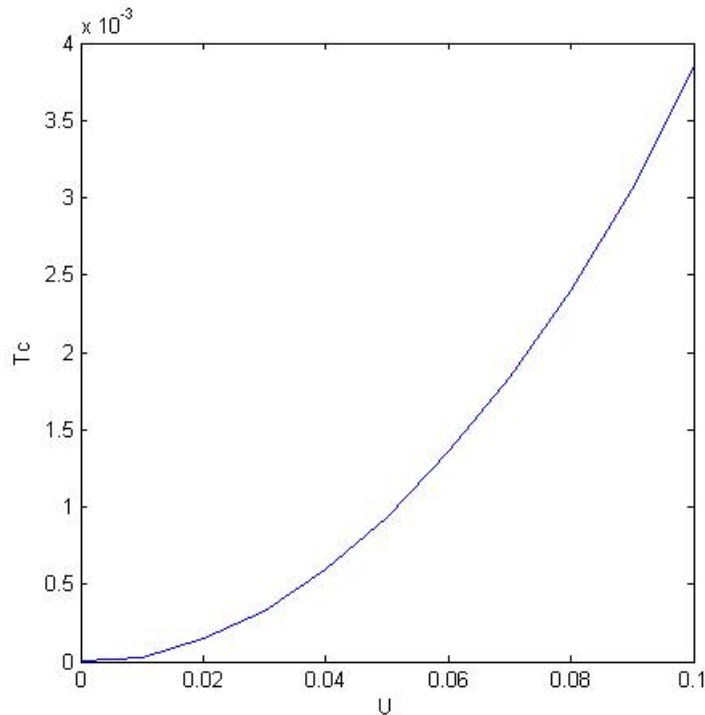


Figure 5.1: Critical temperatures for transition from a homogeneous to chess-board phase in weakly interacting systems . $\mu = 0.05$

5.2 Discussion and future research plan

In the last section it was seen that phase transitions will not occur if and only if the interaction strength U is zero. This result implies that at zero interaction strength the segregated phase cannot be the dominant phase regardless of the temperature. This is in complete contrast to the zero temperature phase diagram in [7] (refer to Fig 5.2), where the segregated phase was shown to be stable for some range of electronic concentrations even for zero interaction. In the said diagram, the segregated phase is stable at zero interaction for some range of electronic concentration. It should be remembered at this point that the DMFT formalism developed in previous chapters is valid only for homogeneous phases. This gives a clue to the possible reason behind this discrepancy. The author of [7] has used the DMFT formalism for homogeneous phases to analyse phases at temperatures lower than the highest critical temperature. In shorter terms, the formalism for homogeneous phases has been erroneously applied to heterogeneous phases in [7].

The result of last section was based on a calculation which assumed small

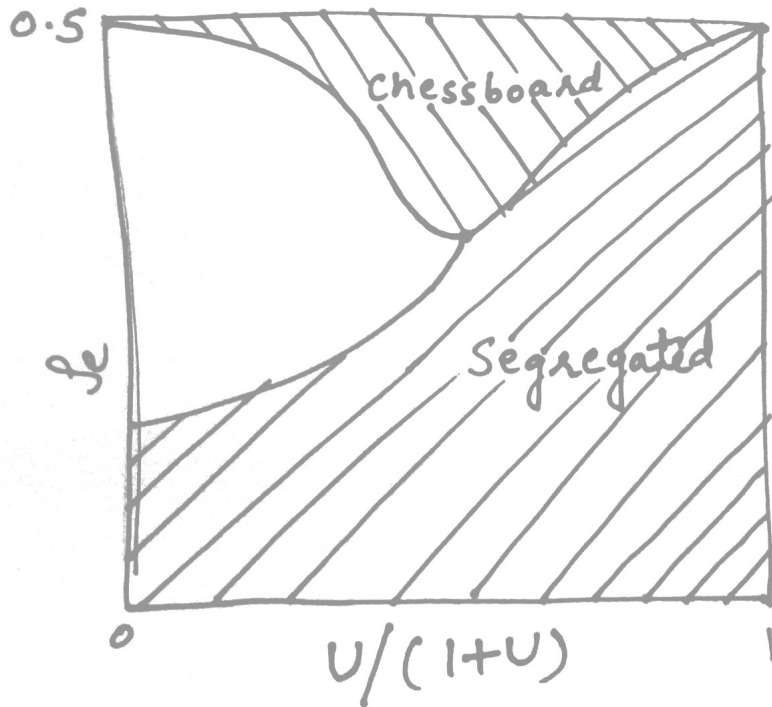


Figure 5.2: Phase diagram for the symmetric case, with regions of stabilities indicated by respective names.

interaction strength U . This restriction to U makes the calculation a lot simpler, but severely restricts the scope of the result. It is intended that the restriction is removed, and the calculation is done for any arbitrary U . Also, for more general analysis, the current DMFT formalism which holds only for homogeneous phases, has to be extended for heterogeneous phases. With this extension, it will be possible to probe critical temperatures other than just the highest one (corresponding to the chessboard phase).

Appendix A

Long derivations

A.1 Density of states in large dimensions

This section derives the gaussian density of states (DOS) in large dimensions by explicit summation. The DOS is

$$D_d(\epsilon) = \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}) \quad (\text{A.1})$$

and the dispersion is

$$\epsilon_{\mathbf{k}} = -2t^* \sum_{i=1}^d \cos k_i. \quad (\text{A.2})$$

Converting the sum in (A.1) to an integral over the first Brillouin zone gives

$$\begin{aligned} D_d(\epsilon) &= \int d\bar{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}}), \quad d\bar{\mathbf{k}} = \prod_{i=1}^d \frac{dk_i}{2\pi} \\ &= \int d\bar{\mathbf{k}} \int_{-\infty}^{\infty} dx e^{ix(\epsilon - \epsilon_{\mathbf{k}})} \\ &= \int_{-\infty}^{\infty} dx e^{ix\epsilon} \left[\int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{i2t^*x \cos k} \right]^d \end{aligned}$$

Denote the integral inside the brackets $[...]^d$ by $F(2t^*x)$. By explicit Taylor expansion it can be shown that

$$F(x) = 1 - \frac{x^2}{4}, \quad x \ll 1. \quad (\text{A.3})$$

It is clear that for finite t^*x , $\lim_{d \rightarrow \infty} [F(2t^*x)]^d$ either vanishes or blows up. The only way it remains finite is if t^* approaches zero at the same rate as

$1/\sqrt{d}$ does. In this case $t^* = t/2\sqrt{d}$ and (A.3) can be used, which implies that in the limit $d \rightarrow \infty$

$$\begin{aligned} [F(2t^*x)]^d &= \left(1 - \frac{t^2x^2}{4d}\right)^d \\ &= e^{-t^2x^2/4} \end{aligned} \quad (\text{A.4})$$

Finally,

$$D_\infty(\epsilon) = \int_{-\infty}^{\infty} dx e^{ix\epsilon} e^{-t^2x^2/4} \quad (\text{A.5})$$

which returns the same result as (2.8). It is clear that any scaling $t^* = t/c\sqrt{d}$, c being a finite constant would work equally well. $c = 2$ is nothing more than a convenience.

A.2 Self energy for the Hubbard Model

The bare propagator $\mathcal{G}(i\omega_n)$ was calculated in (2.29), and the Green function in presence of the cavity $G_{ij}^{(o)}$ in (2.30). Combining the two gives

$$G_n^{-1} = i\omega_n + \mu - \sum_{ij} t_{io}^* t_{jo}^* G_{ij,n} + \frac{1}{G_{oo,n}} \left(\sum_i t_{io}^* G_{io,n} \right)^2 \quad (\text{A.6})$$

To evaluate (A.6), first calculate $G_n = \sum_{\mathbf{k}} G_{\mathbf{k},n}$, with

$$G_{\mathbf{k},n} = \frac{1}{i\omega_n + \mu - \epsilon_{\mathbf{k}} - \Sigma_n} \quad (\text{A.7})$$

which is just the Dyson equation for homogeneous phases. Thus the entirety of work built upon this equation holds only for homogeneous phases. Note that the self-energy Σ_N is local in space, i.e. has no momentum dependence. This result was arrived at in Chapter 2 in the limit of infinite dimensions.

$$\begin{aligned} G_n &= \int_{-\infty}^{\infty} d\epsilon \frac{\sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}})}{i\omega_n + \mu - \epsilon - \Sigma_n} \\ &= \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{i\omega_n + \mu - \epsilon - \Sigma_n} \end{aligned} \quad (\text{A.8})$$

$D(\epsilon)$ is the density of states, which in the infinite dimensional limit is a gaussian. (A.8) can also be written in the following manner, with \mathfrak{z} replacing the variable $(i\omega_n + \mu - \Sigma_n)$ -

$$G(\mathfrak{z}) = \int_{-\infty}^{\infty} d\epsilon \frac{D(\epsilon)}{\mathfrak{z} - \epsilon} \quad (\text{A.9})$$

Thus, the Green function is just the Hilbert transform of the density of states. (A.6) in momentum-space reads

$$\mathcal{G}_n^{-1} = i\omega_n + \mu - \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^2 G_{\mathbf{k},n} + \frac{(\sum_{\mathbf{k}} \epsilon_{\mathbf{k}} G_{\mathbf{k},n})^2}{\sum_{\mathbf{k}} G_{\mathbf{k},n}} \quad (\text{A.10})$$

which in terms of the density of states is

$$\mathcal{G}_n^{-1} = \Sigma_n + \mathfrak{z} - \int d\epsilon D(\epsilon) \frac{\epsilon^2}{\mathfrak{z} - \epsilon} + \frac{\left(\int d\epsilon D(\epsilon) \frac{\epsilon}{\mathfrak{z} - \epsilon} \right)^2}{\int d\epsilon D(\epsilon) \frac{1}{\mathfrak{z} - \epsilon}} \quad (\text{A.11})$$

Using the fact that the density of states is even function of ϵ in the limit of infinite dimensions, the above equation simplifies to

$$\mathcal{G}_n^{-1} = \Sigma_n + G_n^{-1} \quad (\text{A.12})$$

Appendix B

Conventions

B.1 Units

Throughout this thesis natural units are used.

$$\hbar = k_B = 1 \tag{B.1}$$

The lattice spacing is also set to unity.

B.2 Fourier transform

The discrete position-momentum fourier transform and its inverse are defined as

$$f_i = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} f_{\mathbf{k}} \tag{B.2}$$

$$f_{\mathbf{k}} = \sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i} f_i \tag{B.3}$$

Each component of the momentum \mathbf{k} is restricted to

$$k_j = \frac{2\pi m_j}{N} \quad m_j \in \left(-\frac{N}{2}, \frac{N}{2} \right] \tag{B.4}$$

N is the number of sites on the lattice. The work in this thesis is modelled upon an infinite lattice, $N \rightarrow \infty$, and the Fourier relations read

$$f_i = \int_{-\pi}^{\pi} d\bar{\mathbf{k}} e^{i\bar{\mathbf{k}}\cdot\mathbf{R}_i} f_{\mathbf{k}} \tag{B.5}$$

$$f_{\mathbf{k}} = \sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i} f_i \tag{B.6}$$

where, $d\bar{\mathbf{k}} = \prod_j \frac{dk_j}{2\pi}$. Throughout this thesis, even if momentum to position Fourier transform is written as a sum, it actually means an integral .

B.3 Imaginary time formalism

A Fourier transform of a function in imaginary time is given by

$$F(i\omega_n) \equiv F_n = \int_0^\beta d\tau e^{i\omega_n\tau} F(\tau) \quad (\text{B.7})$$

$\omega_n = (2n + 1)\pi T$ are the Matsubara frequencies. The reverse transformation is

$$F(\tau) = T \sum_{n=-\infty}^{\infty} d\tau e^{-i\omega_n\tau} F_n. \quad (\text{B.8})$$

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