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A Theoretical Study of Phase Separation in Strongly Correlated Electron Systems with Wide and Narrow Bands

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ABSTRACT

Using the theoretical formalism of A. O Sboychakov[6] and R. Schaffer *et al*.[7], we have theoretically studied the phase separation in strongly correlated electron systems with wide and narrow bands. We observed the following facts;

(1) In this paper, the spinless Falicov-Kimball model on the simple cubic lattice is analyzed. The analysis is performed with the help of Hubbard-I and dynamical mean field (DMFT) approximations. We have obtained the Matsubara and real frequency itinerant Green's function, the evolution of the system with doping and the range of phase separation is evaluated in thesr two approximations.
(2) We observed that at large values of the on-site Coulomb repulsion in both approximations gives similar results. It was observed that both approximations coincide in the narrow band limit W—0.
(3) It was also seen that the system remains unstable towards the phase separation even at finite band width.
(4) The analysis also reveals the fact that the phase separation is the inherent feature of Hubbard like models with wide and narrow bands.

Keywords: Strongly correlated electron system, Hubbard-I model, DMFT model, Heavy fermion compounds, High T_C cuprates, t-J model, Phase separation phenomenon, On-site Coulomb repulsion.

INTRODUCTION

Strongly correlated electron systems are those systems, where the interactions between electrons are larger than their kinetic energy. Heavy fermion compounds, high T_C cupeates, magnetic oxides such as Manganites, Cobaltites and many others belong to these class of materials. In theoretical study, the Hubbard model and its modifications such as t-J model and others are widely used to explain the complex behavior of strongly correlated materials. The main problem arising in the analysis of the Hubbard –like Hamiltonians is the absence of reliable analytical methods at large electron-electron interactions. The numerical studies as Monte-Carlo simulations and exact diagonalization on small clusters have large computational costs. On the other hand, there exists a huge number of different approximate methods not requiring time consuming calculations. However, each of these methods have restricted range of applicability and it is not always clear whether the results obtained by this or that approximation reveal an actual physics or just reflect the features of initial assumptions.[1-4]

The simple model of correlated electrons is the Failcov-Kimball model[5.] This model is helpful to describe metal to insulator transitions in rare-earth and transition metal compounds. It includes both itinerant and localized electrons with on-site interaction between them. This model exhibits many interesting features such as non-Fermi liquid behavior for any value of coupling constant U, charge density wave phase and phase separation. The FK model has been studied both numerically with Monte Carlo simulations and exact diagonalization and by using different approximations. Several exact results have been obtained also, such as the existence of the phase separation at large coupling constant.

In this paper using the theoretical formalism of A. O. Shoychakov[6] and R a Schaffer *et al.*[7],we have theoretically evaluated Real and Imaginary part of energy as a function of Matsubara frequency ω_n by taking different values U/W, E_f/W and n^f under two approximations Hubbard –I and dynamical mean field theory (DMFT). We have evaluated dependence of n^d and n^f on n. Our theoretically evaluated results show that both n^d and n^f increase with n. Our theoretically results of real and imaginary part of the energy increase with frequency. Our theoretical evaluated results are in good agreement with other theoretical workers[8-10]

MATHEMATICAL FORMULA USED IN THE STUDY

One uses FK model Hamiltonian[5] to study electron correlated sustem which is written as

$$H = -\Sigma_{ij}(t_{ij}d^{\dagger}{}_i d_j + H.c) - \in_f \Sigma_i n^f{}_i + U\Sigma_i n^d{}_i n^f{}_i - \mu\Sigma_i(n^d{}_i + n^f{}_i) \quad (1)$$

Here, $n^d{}_i = d^{\dagger}{}_i d_i$ and $n^f{}_i = f^{\dagger}{}_i f_i$ and $d^{\dagger}{}_i(d_i)$, $f^{\dagger}{}_i(f_i)$ are creation (annihilation) spinless fermion operators for the bound and localized electrons respectively. The first term of equation

(1) describes the kinetic energy of band electrons, the second term controls the position of the localized level with respect to the centre of the conduction band while the third term corresponds to the on site interaction between the band and localized electrons. Here, one considers attractive interaction U>0

The evaluation is done with the help of two approximation Hubbard I and DMFT approximation. The Hubbard-I approximation is based on the decoupling in the system of equation for the electron Green's function. The use of Matsubara Green's function is more convenient to study the system at finite temperature. It also allows simply comparing the Hubbard-I and DMFT approximations. DMFT deals with one-particle Matsubara frequency.

DISCUSSION OF THE RESULTS

Using the theoretical formalism of A O Sboychakov[6] and R Schaffer etal[7], we have theoretically studied phase separation in strongly correlated electron system with wide and narrow bands. In tableT1, we have shown the evaluated results of real part of self-energy as a function of $\frac{\omega_n}{W}$. Here W is the band width and frequency is Matsubara frequency. We have kept parameter (U/W)=0.1, n^f =0.4, (E_F/W)=0.1 and (T/W)=0.1. The evaluation is done with the help of DMFT model and Hubbard I model. Our theoretically evaluated results indicate that real part of self-energy increase with $\frac{\omega_n}{W}$ for both the approximations. In Table T2, we repeated the calculation for the value U/W =5 and all the other parameters are kept same as in table T1. In this case also our evaluated results indicate that real part of self-energy increase with $\frac{\omega_n}{W}$. In tableT3, we have evaluated imaginary part of the self energy as a function of $\frac{\omega_n}{W}$ keeping the value of U/W=0.1 and all the other parameters are same. In this case, we observed that imaginary part of the self energy also increase negatively with $\frac{\omega_n}{W}$. Results obtained from both the approximations are identical in trend. In table T4, we repeated the calculation of imaginary part of the self-energy as a function of $\frac{\omega_n}{W}$ for the value of U/W =5 and all other parameters are the same. Similar results were obtained in this case also. In table T5, we have shown the dependence of n^d and n^f as a function of n. Our theoretically evaluated results show that these two parameters decrease and increase with n.

Table T1

An evaluated result of Re(Σ_n) as a function of $\frac{\omega_n}{W}$ calculated for (U/W) =0.1. others parameter is n^f=0.4, (E_f/W) =0.1 and (T/W) =0.1. Calculation were performed in two approximation DMFT and Hubbard-I

(ω_n / W)	DMFT Approx.	Hubbard I Approx
0.0	0..024	0.022
0.5	0.026	0.024
1.0	0.028	0.026
1.5	0.030	0.028
2.0	0.032	0.030
2.5	0.034	0.032
3.0	0.035	0.033
3.5	0.036	0.034
4.0	0.037	0.035
4.5	0.038	0.036
5.0	0.042	0.037

Table T2

An evaluated result of Re(Σ_n) as a function of $\frac{\omega_n}{W}$ calculated for (U/W) =5. others parameter is n^f=0.4, (E_f/W) =0.1 and (T/W) =0.1. Calculation were performed in two approximation DMFT and Hubbard-I

(ω_n / W)	DMFT Approx.	Hubbard I Approx
0.0	0.0	0.0
2.o	0.8	0.87
4.0	0.9	0.92
5.0	1.0	1.02
6.0	1.1	1.12
7.0	1.2	1.15
8.0	1.3	1.16
10	1.4	1.17
12	1.5	1.18
14	1.6	1.19
16	1.8	1.20

Table T3

An evaluated result of Im(Σ_n) as a function of (ω_n / W) calculated for (U / W) =0.1. other parameters are (E_F / W) =0.1, (T / W) =0.1, n^f=0.4. Calculations were performed using DMFT model and Hubbard I model

$\frac{\omega_n}{W}$	Im(Σ_n)	
	DMFT	Hubbard I
0.0	-0.10	-0.009
0.5	-0.008	-0.007
1.0	-0.007	-0.006
1.5	-0.006	-0.005
.2.0	-0.005	-0.004
2.5	-0.004	-0.003
3.0	-0.003	-0.002
3.5	-0.002	-0.001
4.0	-0.001	-0.0008
4.5	-0.0008	-0.0007
5.0	-00007	-0.0006
5.5	-0.0005	-0.0005
6.0	0.000	0.000

Table T4

An evaluated result of Im(Σ_n) as a function of (ω_n / W) calculated for (U / W) =4.0. others parameters are (E_F / W) =0.1, (T / W) =0.1, n^f=0.4. Calculations were performed using DMFT model and Hubbard I model

(ω_n / W)	Im(Σ_n)	
	DMFT	Hubbard I
O	-0.72	-0.89
2	-0.63	-0.78
4	-0.55	-0.65
6	-0.50	-0.56
108	-0.40	-0.48
12	-0.32	-0.37
14	-0.20	-0.28
16	-012	-0.19
18	-0.008	-0.13
20	-0.007	-0.10
22	-0.005	-0.008
24	-0.003	-0.006
26	0.000	-0.004

Table T5
An evaluated result of dependence of n^d and n^f on n. others parameter are same as in previous tables

n	n^d	n^f
0.0	0.00	0.00
0.10	0.10	0.02
0.20	0.15	0..04
0.30	0.20	0.06
0.40	0.23	0.10
0.50	0.27	0.15
0.60	0.32	0.25
0.70	0.31	0.32
0.80	0.30	0.38
0.90	0.25	0.47
1.00	0.26	0.58
1.10	0.20	0.67
1.20	0.15	0.78
1.30	0.09	0.83

CONCLUSION

From above theoretical investigation and analysis, we have come across the following conclusions:

In this paper, the spinless Falicov-Kimball model on the simple cubic lattice is analyzed. The analysis is performed with the help of Hubbard-I and dynamical mean field (DMFT) approximations. We have obtained the Matsubara and real frequency itinerant Green's function, the evolution of the system with doping and the range of phase separation is evaluated in thesr two approximations.

We observed that at large values of the on-site Coulomb repulsion in both approximations gives similar results. It was observed that both approximations coincide in the narrow band limit W—0.

It was also seen that the system remains unstable towards the phase separation even at finite band width.

The analysis also reveals the fact that the phase separation is the inherent feature of Hubbard like models with wide and narrow bands.

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