Density matrix renormalization group study of a three-orbital Hubbard model with spin-orbit coupling in one dimension

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Abstract

In this report, the results of our recent study of a three-orbital Hubbard model with spin-orbit coupling is discussed [1]. We used the density matrix renormalization group (DMRG) technique to solve the mentioned model in one dimension. The focus of this work was to create the λ (spin-orbit coupling strength) vs. U (Coulomb repulsion) phase diagram for doping(n)=4. The importance of this work lies in the fact that this was the first exact study of three-orbital Hubbard model with spin-orbit coupling using DMRG. Apart from providing a full phase diagram, the presence of an Excitonic condensate in both at intermediate U and in the strong coupling region was the main finding of this work.

1. Introduction and Motivation

Materials with large atomic spin orbit coupling have recently gained attention from the condensed matter community. The spin orbit coupling increases as we move down in the periodic table as an order of Z^2 for the outer shell electrons, where Z is the atomic number, and it can play an important role in transition metals having 4d, and 5d orbitals as outer shells. At the same time, the Coulomb repulsion between the outer shell electrons decreases because the size of the wavefunction grows. In general, 4d and 5d materials have λ of order of 0.1-0.3 eV and 0.1-1.0 eV respectively. The Coulomb repulsion is of order of 0.5-3 eV and 0.4-2 eV in 4d and 5d compounds., respectively.

One of the initial transition-metal oxides where the effect of spin-orbit coupling was appreciated was Sr_2IrO_4 (5d). This material has Ir^{4+} (d^5) surrounded by six oxygen atoms leading to large octahedral crystal field splitting and has been studied extensively using experimental techniques and Ab-initio studies [2,3,4]. LDA (without SOC) calculations have shown that the bandwidth of the t_{2g} sector is nearly 4eV, while LDA+SOC (λ~0.4eV) leads to much narrower bands coming from j_{eff}=3/2 and j_{eff}=1/2 manifolds, where j_{eff}=1/2 is half-filled and has bandwidth ($W_{J=1/2}$) of value 1.5 eV. Using Constrained Random Phase Approximation, the effective on-site Coulomb interaction (U) in Sr_2IrO_4 is shown to be order of 2 eV (i.e. $U/W_{J=1/2} \sim 1.3$). This coupling stabilizes the Mott Insulating phase with a Neel temperature (T_N) of ~240K. Ba_2IrO_4 also belongs to the same class of Sr_2IrO_4 with large $T_N \sim 240$K.

Recently there have been some interesting studies performed regarding the material Sr_2YIrO_4[5]. This compound has Ir^{5+} which results to d^4 doping. In the atomic limit because of large SOC all 4 electrons fully fill the j_{eff}=3/2 states, and if one turns on the hopping this system becomes band insulator. At this point, naturally the question arises of what will be the effect of Coulomb interaction on this system? Experimental studies lead by G.Cao et al.[5] suggests that Sr_2YIrO_4 (SYIO) shows antiferromagnetic(AFM) ordering at low temperature with T_N~1.3K. The antiferromagnetism for d^4 system in presence of SOC was predicted by G.Khillauin [6] in strong coupling limit by formation of excitonic condensate.

First-principles calculations on SYIO have also found AFM ordering [10], Generalized gradient approximation (without SOC and U) for SYIO shows the bandwidth of t_{2g} sector to be nearly 2eV [10]. If we take $U = 2eV$ and $\lambda = 0.4eV$ as in the case of Sr_2IrO_4 , then U/W and λ/W are order of 1.0 and 0.2 respectively for Sr_2YIrO_4.

We take a different route by considering full 3-orbital Hubbard model with SOC, and use DMRG to solve it exactly; this way we can solve this model in the strong coupling limit and intermediate coupling limit as well, where perturbation theory does not work. In section-2 we discuss the model we used for this study, and in section-3 we show the results.

2. Model

We use one dimensional three-orbital Hubbard model. The Hamiltonian contains a tight-binding term, an on-site Hubbard interaction, and a spin-orbit coupling as shown below in the standard notation for fermionic creation and destruction operators, etc:

$$H_{\text{kin}} = \sum_{i,\alpha,\beta,\sigma} -t_{\alpha\beta}\left(c^{\dagger}_{i,\alpha,\sigma}c_{i+1,\beta,\sigma} + h.c\right) + \sum_{i,\alpha} \Delta_{\alpha}\, n_{i,\alpha}$$

$$H_{SOC} = \lambda \sum_{i,\alpha,\beta,\sigma,\sigma'} \langle\alpha|\boldsymbol{L}_i|\beta\rangle.\langle\sigma|\boldsymbol{S}_i|\sigma'\rangle\, c^{\dagger}_{i,\alpha,\sigma}c_{i,\beta,\sigma'}$$

$$H_{int} = U\sum_{i,\gamma} n_{i\uparrow\gamma}n_{i\downarrow\gamma} + (U' - J_H/2)\sum_{i,\gamma<\gamma'} n_{i\gamma}n_{i\gamma'}$$
$$-2J_H \sum_{i,\gamma<\gamma'} \boldsymbol{S}_{i\gamma}.\boldsymbol{S}_{i\gamma'} + J_H \sum_{i,\gamma<\gamma'} (P^{\dagger}_{i\gamma}P_{i\gamma'} + h.c.)$$

3. Main Results:

In Fig-1 we show the full phase diagram. In weak coupling limit (U/W<0.2) we found a metal to band insulator transition, as expected. We also found a nontrivial Block phase and Ferromagnetic phase in intermediate and strong coupling region, respectively. Both these phases are well studied in the literature [7,8,9]. An important result in our effort is that we identified the Excitonic Condensate phase by calculating the pair-pair correlation between excitons i.e $\Delta^{\tilde{j},m}_{j,m}(i) = a^{\dagger}_{i,\tilde{j},m}a_{i,j,m}$ where $\tilde{j} = \frac{3}{2}, j = \frac{1}{2}$, and flavor of the exciton is decided by choosing

m(±1/2). In the excitonic phase we found staggering order in pair-pair correlation as shown in Fig-2, which was always accompanied by antiferromagnetic ordering in spin degree of freedom.

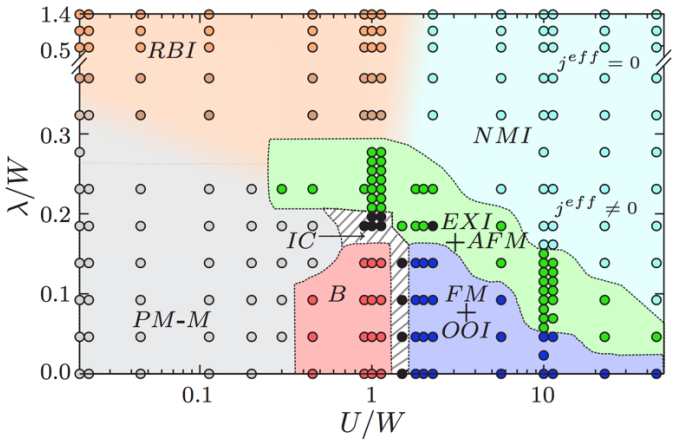

Fig-1. In above figure we show λ/W vs U/W phase diagram. RBI, PM-M, B, FM, OO, IC, EXI, AFM, and NMI stands for relativistic band insulator, paramagnetic metal, block phase, ferromagnetic, orbital ordering, incommensurate, excitonic insulator, antiferromagnetic, and nonmagnetic insulator, respectively.

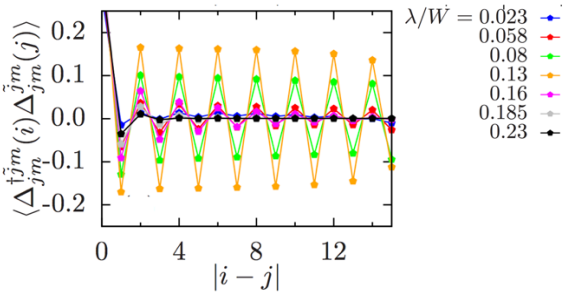

Fig-2. Above figure shows pair-pair correlation for U/W=10 for various λ/W.

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