Slave rotor approach to exciton condensation in a two-band system

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1. Introduction

The Coulomb screening between the conduction band electron and the valence band hole, under certain conditions, causes the formation of bound state leading to a non-conducting state: the exciton. This excitonic phase has been predicted theoretically for small, direct or indirect band-gap semiconductors or semi-metals in which the exciton binding energy is larger than the electronic band gap. In this case, excitons form spontaneously and can condense into a new insulating ground state. A plethora of theoretical and experimental work has been performed for decades to explore the physics of the excitons in a variety of systems [1–7] and still remains alive and engrossing [8–11]. This is due to their application potential and also a deep connection to the understanding of semiconductors [5], the charge density order via excitonic fluctuations in transition metal dichalcogenides [12], novel superconductors [13], electronic ferroelectricity [14–16] and so on.

In an idealised system where the number of electrons in the valence and conduction bands is separately conserved,
the excitonic condensation breaks this symmetry and fixes the relative phase of valence and conduction electrons. An inter-band hybridization or correlated-hopping terms in the Hamiltonian, which mix the valence and conduction bands, inevitably exist in real materials, the excitonic condensation in this sense is always an approximation. The closest realization of this idealized exciton condensate (EC) can be found in the bi-layer systems. The exciton condensation in semiconductor-bi-layer systems exploits the strategy of hosting electrons in the first layer and holes in the second layer by means of electric gates which allow separate contacts to the layers. The spacer between the two quantum wells suppresses the inter-layer tunneling and therefore the exciton recombination, but it is sufficiently thin to provide strong inter-layer Coulomb interaction [17]. Exciton condensation takes place under suitable conditions including small inter-layer distance, so that inter-layer electron–electron interaction is sufficiently strong, has large enough intra-layer electron mobility so that sufficiently high $T_c$ can be achieved, and a matching doping such that the electron concentration in one layer closely matches the hole concentration on the other layer. Two types of structures have been studied: 2D quantum well systems in a perpendicular magnetic field. The idea here is to use the formation of Landau levels and, in particular, the dependence of the number of quantum states per Landau level on the magnetic field as a means to achieve the desired electron and holes concentrations [18]. Another bi-layer system that has been extensively studied is the composite of two graphene layers separated with a dielectric where EC is predicted to take place at room temperature [19, 20].

The Falicov–Kimball model (FKM) was introduced to explain semiconductor to metal transition and has been extensively used to describe valence transitions in heavy fermion compounds. Its original version contains a dispersive band of itinerant electrons interacting with localized orbitals through local Coulomb interaction. Of late, this has also been used to study excitonic fluctuations in systems like $\text{Ta}_x\text{NiSe}_5$, transition metal dichalcogenides [12] and $\text{GdI}_2$ [21] in the limit of small but finite hybridization between the two bands. Possible electronic ferroelectricity has also been studied in FKM [15, 22–24] where the two participating orbitals have odd and even parity respectively. Sham and coworkers [15] using the self-consistent mean-field (BCS-like) theory found that the exciton condensate made of holes and electrons may spontaneously break the lattice inversion symmetry and lead to a ferroelectric phase transition of electronic origin. Importantly, their excitonic condensate also existed in the absence of hybridization among two species of electrons, suggesting spontaneous symmetry breaking in the ground state. This result was challenged by subsequent theoretical studies [25] and refuted such possibility of spontaneous symmetry breaking in an FKM. Such systems are often modelled by the Falicov–Kimball Hamiltonian, which, in its extended incarnation, takes into account the strong inter-band Coulomb interaction and hybridization among them. Hybridization between the bands, however, is not the only way to develop excitonic coherence between the two bands. Any dispersion of the localized band can also induce it [10, 26]. A strong hybridization, however, can lead to a gap in the density of states leading to the so-called excitonic insulator (EI) phase. If the Coulomb correlation is weak (in comparison to the kinetic energy), the magnitude of the single-particle gap, up to a constant, is given by the excitonic order parameter (EOP). A mean-field description works fairly well in this regime. On the other side, for strong Coulomb interactions, the Mott physics becomes increasingly relevant and the exciton formation and coherence scales move away from each other, the latter goes down with correlation while the former increases. Excitonic fluctuations become increasingly dominant in this regime till the excitonic insulating phase appears through a Mott transition. This transition is beyond the usual treatment of excitons using mean-field theory and calls for methods designed to address strong coupling physics.

Several numerical schemes, Hartree–Fock (HF) mean-field [15, 16, 27, 28], variational cluster approximation [29], constrained path Monte-Carlo [30], projector based renormalization method [31] and cluster perturbation theory (CPT) [32] have been brought to bear on this problem in the past and the efforts renewed during the last decade. A weak-coupling HF theory of excitonic condensation is analogous to the BCS theory of superconductivity. The role of the pairing glue is played by the inter-band Coulomb interaction, which favours formation of bound electron–hole pairs: the excitons and has been worked out long-time ago [33]. Majority of the theoretical considerations on excitons is still based on mean-field theories. The advent of dynamical mean-field theory (DMFT) has provided a consistent and capable theoretical framework for strongly correlated electronic systems, and models like the single- and multi-band Hubbard model have been studied with a good degree of success using DMFT and its various extensions. It (with its various impurity solvers) is essentially based on numerical solutions of the relevant impurity model to which the original correlated models are mapped [34–36]. The FKM is, in fact, exactly solved by using DMFT in the infinite dimension [37–40].

A mean-field approach, the slave-rotor mean field theory (SRMF), based on the idea of nominal charge-spin separation provides a fast and semi-analytical means for investigating Mott transition in a variety of situations, particularly in the strong coupling limit where the charge-spin separation scenario appears to work. In this approach, the Hilbert space of the physical electronic degrees of freedom is enlarged in terms of separate chargon and fermion Hilbert spaces. The unphysical states are then eliminated by enforcing local constraints on the enlarged Hilbert space. In this formulation, the rotor sector and spinon sector are coupled to each other by self-consistency equations, and the rotor Hamiltonian is solved for a finite number of sites self-consistently coupled to an order parameter bath (rest of the lattice). The limitation of this finite-site mean field theory is that it is coupled to a static bath, the phase fluctuations are ignored. In the strong coupling limit, the lattice problem maps on to the problem of interacting slave particles self-consistently coupled to a gauge field. The gauge fluctuations, being weak, provide a framework for studying the Mott–Hubbard physics at intermediate to large coupling [41, 42]. In a straightforward
extension to a two orbital systems [43], the orbital degrees are also included and the physics of spin, orbital and charge are treated accordingly. SRMF has been applied to a variety of strongly correlated electron systems such as the Hubbard model (and its multi-orbital extension [43, 44]) with competing magnetic orders in two dimensions, Anderson model [41], superconductivity [42] and metamagnetism [45] on bipartite and non-bipartite lattices. This semi-analytical method is useful for discussing correlation effects on the symmetry breaking or single-particle excitation spectra, especially in the insulating state. Owing to disparate charge and spin (or orbital) degrees, it is capable of handling the spin (or orbital)-liquid like states in frustrated systems [41, 42]. The main advantage of the two-site cluster mean field theory lies in that the short range correlation functions of the rotors is properly taken care of. Although a few studies on Hubbard model using SRMF exist, FKM has not been discussed in this context so far. To the best of our knowledge, this is for the first time the ground state properties ($T = 0$) of an extended FKM has been studied using a slave-rotor (SR) approach. We show here that the physics (like identifying an extended FKM has been studied using a slave-rotor (SR) approach. We show here that the physics (like identifying a symmetry making an order parameter) becomes identical to a single band Hubbard model in the pseudospin space. When $t_a \neq t_b$ one can get an asymmetric Hubbard model.

(ii) With $t_a = -t_b$ and $V = 0$, the corresponding model mapped onto a Hubbard model with an attractive interaction. The corresponding mapping is achieved by the particle-hole transformation in one of the bands: $c_{\beta \text{l}} = c_{\beta \text{l}}^\dagger$ and reversing the sign of interaction $U \rightarrow -U$.

(iii) If $t_b = 0$, $V = 0$, this model describes an original FKM [40, 46–48]. This Hamiltonian commutes with $n_{\beta}$, in which case local occupancy of electron in band-$\beta$ is either 0 or 1. This renders the model ‘solvable’, albeit numerically, by annealing over the localized electron configurations [51]. No coherence between electrons from the two bands is possible in this situation.

(iv) The inter-orbital hybridization between two bands, $V$, or a finite dispersion of $\beta$-electron, $t_b$ breaks the local $U(1)$-symmetry which is prohibited by Elitzur’s theorem [49, 50] but preserves independently the number of $\alpha$ and $\beta$ electrons which still preserves the global $U(1)$-symmetry making an order $\langle c_{\alpha \text{l}}^\dagger c_{\beta \text{l}} \rangle$ possible. One can study exciton formation and condensation in this limit, essentially an excitonic insulator phase.

3. Formulation

In this section, we briefly review the formulation of the SRMF for the above described two-level model. The electronic Hilbert space at a single lattice site has four states: $|0\rangle$, $|\alpha\rangle$, $|\beta\rangle$, $|\alpha\beta\rangle$. In the SR representation, the electronic charge and the orbital degrees are described by a charged rotor and a fermion carrying the pseudospin (orbital) index respectively. The direct product space of the rotor and fermion states contains the four physical states at every site, with additional, unphysical states in an enlarged Hilbert space which is mapped back onto the physical one via a local constraint acting like a gauge term. In the SR representation, the electron number is equal to the fermion number $\langle n_e \rangle = \langle \sum n_{\beta \text{l}} \rangle$. The electron annihilation operators for two corresponding bands, for example, are written in the SR representation as

$$c_{\alpha \text{l}} \equiv f_{\alpha \text{l}} \exp(i\theta); c_{\beta \text{l}} \equiv f_{\beta \text{l}} \exp(i\theta) \right).$$

In terms of decoupled spinon creation (annihilation) operator $f_{\alpha \text{l}}^\dagger$, $f_{\beta \text{l}}^\dagger(f_{\alpha \text{l}}, f_{\beta \text{l}})$ and rotor creation (annihilation) operator $\exp(i\theta)$ and $\exp(-i\theta)$ operators, this model can be written as (following [41, 42]).
\[
H_{SR} = -\sum_{\langle ij \rangle} t_{ij} \phi_i^{\dagger} \phi_j e^{-i\theta} + \frac{U}{2} \sum_i n_i^0 (n_i^0 - 1) \\
+ V \sum_i \phi_i^{\dagger} \exp(-i\theta) \phi_j \exp(i\theta) + \sum_{ij} \mu_{ij} \phi_i^{\dagger} \phi_j.
\]

The chargon density operator is defined as \( n_i^0 \) and spinon density is given by \( n_i^f \).

SRMF theory decouples the Hamiltonian for the rotor and auxiliary fermion sectors as:

\[
H_i = -\sum_{\langle ij \rangle} t_{ij} B_{ij} \phi_i^{\dagger} \phi_j + \sum_i \mu_{ij} n_i^0 + V \sum_i (\phi_i^{\dagger} \phi_i + \text{h.c.})
\]

and

\[
H_\theta = -2 \sum_{\langle ij \rangle} t_{ij} \chi_i \phi_j e^{-i(\theta_j - \theta_i)} + U/2 \sum_i (n_i^0)^2 - \mu_0 \sum_i n_i^0
\]

where, \( B_{ij} = \langle e^{-i\theta} \phi_j \phi_i \rangle_\theta \) is the rotor kinetic energy and the spinon kinetic energy is defined as \( \chi_i = \langle \phi_i^{\dagger} \phi_i \rangle_f \). \( \mu_0 \), \( \mu_f \) are chemical potentials used to control \( n_i^0 \) and \( n_i^f \) for the local number operator constraint: \( \sum_i n_i^0 + n_i^f = 1 \). The Hamiltonian for the rotor part is diagonalized numerically, \( B_{ij} = \langle e^{-i\theta} \phi_j \phi_i \rangle_\theta \) is calculated from the ground state eigenfunctions and fed back to \( H_i \) to get \( \chi \). This \( \chi \) is then put in \( H_\theta \) and the process is repeated till convergences in \( \chi \), \( \phi \) and \( B_{ij} \) are reached. In a homogeneous situation considered here, these site and bond order parameters become independent of the site indices and these are henceforth dropped.

### 3.1. Single-site analysis

The idea of mean-field theory is to focus on a finite cluster of sites and treat the influence of the sites outside the cluster (‘the bath’) using a mean-field order parameter. In single site mean-field theory, the chargon kinetic energy \( B_{ij} \) is decoupled as \( B_{ij} = \langle e^{-i\theta} \phi_j \phi_i \rangle \), where \( i \) is the cluster and \( j \) is the bath. For single site approximation, \( B_{ij} = \Phi \phi_j \), with \( \Phi = \langle e^{i\theta} \phi_j \rangle \), hence, rotor kinetic energy is represented as \( B = \Phi \phi \). The rotor kinetic energy acts as the quasiparticle (QP) weight (\( Z \)) for the fermions. If \( \Phi \phi \) vanishes, charge fluctuation is quenched and the system goes into an insulating state. The single-site rotor Hamiltonian now reads as:

\[
H_\theta = -4 (t_\alpha \phi_\alpha + t_\beta \hat{\phi}_\beta) \phi (e^{-i\theta} + e^{i\theta}) + U/2 (n_\theta)^2 - \mu_0 n_\theta.
\]

The order parameter for electron–hole bound state is defined as,

\[
\Delta = \langle \phi_i^{\dagger} \phi_i \rangle_f.
\]

In this way, the rotor sector \( H_\theta \) and free-fermion sector \( H_i \) are coupled and the rotor Hamiltonian is solved on a single site cluster. The order parameter bath (rest of the lattice). However, the single-site theory has its limitations. It fails to identify the long range correlation (the pseudospin exchange) and underestimates the Mott scale. It is very similar to the Gutzwiller approximation in a sense that the double occupancies are completely eliminated along with the Mott transition. A minimum cluster of two sites is then required to incorporate these.

### 3.2. Two-site analysis

Intersite correlations are captured in the two-site extension. The rotor Hamiltonian under site extension becomes

\[
H_\theta = -\sum_i t_i (\chi_i (e^{-i\theta} \phi_2 + \text{h.c.)}) + U/2 \sum_i (n_i^0)^2 + U/2 (n_\theta)^2 - \mu_0 (n_i^0 + n_i^f).\]

For a two-site extension, the inter-site correlation is accounted by considering a bond connecting two sites; along with the site interaction terms. This two-site extended mean-field Hamiltonian is again diagonalized numerically to obtain the eigenvalues and the ground state wave function of the rotor part in a two-site basis \( |n_i^0, n_i^f \rangle \), where, \( B = \Phi \phi \) gives the rotor kinetic energy corresponding to site interaction and \( B_{ij} = \langle e^{-i\theta} \phi_j \phi_i \rangle \) for intersite or bond contribution. When \( \Phi \) goes to 0 (i.e. the insulating phase), unlike the single-site case, the nearest neighbor inter-site correlation could assume a non-vanishing value in this approximation. The first term in the above equation gives a finite rotor kinetic energy \( \sim \frac{1}{N} \). A bond approximation approach, therefore, recovers the inter-site exchange correlation \( \sim \frac{1}{N} \). The cluster mean field theory focuses on sites and treats the influence of the sites outside the cluster (‘the bath’) via a mean field order parameter. A larger cluster size yields much better results for \( \Phi \) and \( B_{ij} \). It is indeed likely that larger clusters will improve the accuracy further and recover longer range interaction scales. The qualitative change and new physics that emerge going from one- to two-site is our main point. There are qualitative differences between the results obtained from the single-site mean field theory and the two-site extension of SRMF: in single-site theory, the rotor kinetic energy \( B_{ij} \) is the square of the order parameter i.e. \( \Phi \phi \). When it vanishes, Mott insulating phase sets in. This amounts to neglecting all density fluctuations within the Mott phase, too crude an approximation close to the Mott transition. By contrast, the cluster mean field theory captures the short distance correlation. The main advantage of the cluster mean field theory is that the short range correlation functions of the rotor are properly taken care of. In contrast to the HF mean-field theory, SRMF provides an exact treatment of the quartic interactions in the above Hamiltonian.

### 4. Results

#### 4.1. Symmetric case (Hubbard model)

When \( t_\alpha = t_\beta = t \) and \( V = 0 \), Hamiltonian (1) corresponds to the Hubbard model, which shows a metal–insulator transition (MIT) driven by local correlation. We reproduce the one-site and cluster (two-site) results for this model for
The non-local correlations are accounted for in the two-site calculation, the critical value of \( U \) at which metal-insulator transition occurs, gets a lower value. Figure 1 shows that when \( \Phi \) vanishes an MIT occurs at 6.483\( t \) and 6.219\( t \) for single and two-site cases respectively, these values of \( U_c \) match exactly with earlier results [42, 45]. We note that the obtained value of \( U_c \) from a two-site cluster is in good agreement with the C-DMFT prediction of \( U_c^2 = 6.05t \) [35]. It preserves Hubbard bands in the insulator, and a ‘preformed’ Mott spectral gap opens up discontinuously at the transition, as in DMFT [36]. Both in the single-site and two-site analysis, Mott transitions follow Brinkman–Rice scenario [33]. The QP weight \( Z = \Phi^2 \) goes to zero at critical Hubbard \( U_c \) in a continuous fashion and the effective mass diverges, where, \( Z \) scales with \( (1 - (U/U_c)^2) \). The inter-site correlation term \( B_{ij} \) (inset, figure 1) signifies that the non-local fluctuation remains finite even in the insulating phase and approaches zero in the \( U/t \to \infty \) limit.
When one of the two-spin components in the Hubbard model goes to zero, it reduces to the well-known FKM. If the hybridization term \( H_v = \sum V(\epsilon_{\alpha i}^c \epsilon_{\beta j}^c + \text{h.c.}) \) between these two bands are included in the Hamiltonian, the local \( U(1) \) symmetry of the \( \beta \)-electrons is lifted. The same happens for an extended FKM with finite \( \beta \)-electron dispersion: \( (\sum_{\langle ij \rangle} -t_\beta(\epsilon_{\beta i}^c \epsilon_{\beta j}^c)^\dagger + \text{h.c.}), \) has been considered in section 4.4.

We check \( U_c \) for the FKM at which the rotor K.E. \( (\Phi) \) vanishes, suggesting an MIT, it is found that as for an FKM, the required \( U(=U_c) \) at which \( \Phi \) goes to zero just becomes half of the \( U_c \)-value for the Hubbard model. Figure 2 shows that \( U_c \) for single-site and two-site are 3.24\( t \) and 3.105\( t \) respectively. It shows the variation of excitonic order parameter with hybridization strength \( V \); as \( U \) increases the critical value of \( V \) at which excitonic insulating state appears is shifted towards left. Similarly, an increase in \( V \) also leads to MIT at a critical \( V_c \) which goes down as \( U \) increases (panel (b), figure 2). For small values of \( U \), it is obvious that a hybridization will not change the low-energy nature of the metallic phase qualitatively. The rotor kinetic energy vanishes at a small \( U \) as we increase \( V \), which is again associated with the electron–hole pair (exciton) formation and condensation. For a large \( U \), the gap is robust and less affected by the hybridization \( V \). A large \( V \) also makes the system gapped and the value of the gap is of the order of \( 2V \); giving rise to a metal-insulator transition. Expectedly, at a critical \( V \) (\( V_c \)), the EOP saturates with a first order jump. Well below \( V_c \), there is a co-existence of metallic as well as excitonic phases; where at \( V_c \) the system goes over to an excitonic insulator phase with a first order jump in the EOP.

Figure 3 shows a 3D plot of excitonic parameter in the \( U-V \)-plane for single as well as two-site extension. The mean-field behaviour has salient differences for single-site and two-site extended theory. The low-\( U \) limit, both single and two-site results show a continuous change in the order parameter. This regime can be compared to earlier results obtained using HF mean field [16]. As we see \( \Delta \) increases with \( V \) and as well as with \( U \) and saturates after a certain \( V \). To see the differences between HF mean-field theory in the weak-coupling regime, and the treatment using SRMF, one compares the variation of \( \Delta \) in the \( U-V \) plane (figure 3) with earlier study [16]. The jump in EOP seen in SRMF is absent in the HF mean-field. The large-\( U \) regime, better captured in the SRMF theory, shows deviations from HF as well as between single and two-site approximations. In the single-site case, with increasing \( U \), excitonic order shows a first order jump and goes to its saturation value quickly with increasing \( U \). On the other hand, two-site results show second order nature through a weakly first order at intermediate \( U \). Figure 4 corroborates the same as shown in figure 3 in detail. It shows the behaviour of EOP with \( V \) for several correlation strength \( U \) and a metamagnetic transition is clearly visible at large \( U \) side in the left panel (one-site case) and a weakly first order character is obtained for two-site approximation.

The phase diagram in figure 5 details the nature of phase transition in single as well as in two-site case. The transition from the metal+exciton mixed state to excitonic insulator (EI) is of first order in nature. In the two-site case, even when \( \Phi \sim 0 \), \( \Delta \) does not reach the saturation value, still varies with \( V \) and reaches a saturation value when \( B_p \) goes to zero. The (green) dashed line in figure 5 shows \( B_p \). There are several differences between the earlier BCS mean-field result. The exciton formation leads to the insulating state in the earlier treatment while a co-existing exciton metallic state appears.
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In the SRMF, in addition, the non-zero $B_{ij}$ beyond $\Phi = 0$, signifies a region analogous to the spin-liquid in the Hubbard model [41]. In the bond approximation a new scale $t^2/U$ emerges signifying the appearance of long-range inter-orbital excitonic fluctuations, analogous with the anti-ferromagnetic exchange in the Hubbard model at half-filling [45].

### 4.3. Intersite excitonic order parameter

The excitonic order parameter $\Delta$ is a local one or an on-site order parameter which means that the participating electron and hole are from the same site or position. But one can also have a non-local binding as well. In order to incorporate such an excitonic order we extend our calculation with an additional term in the Hamiltonian, $\sum_{ij} V'(\epsilon_{\alpha i} c_{\beta j}^\dagger + \text{h.c.});$ here, $j$ corresponds to the nearest neighbours on a square lattice. If a cross-hopping is possible between two bands a non-local order parameter could be defined and after the slave-rotor transformation the extended excitonic order takes the form, $\Delta_e = \langle f_{\alpha i} f_{\beta j} \rangle$.

We calculate this intersite excitonic order parameter as $V$ and $U$ are varied. It increases with $V$ initially and then decreases for large $V$ as shown in figure 6. The effect of $U$ is also different in this case, the value of $\Delta_e$ reduces with

![Figure 4](image-url). Mean-field results for exciton order parameter as a function of hybridization strength $V$ for different sets of $U$ for single-site (left panel) as well as two-site case (right panel). In the left panel, the order parameter rises from zero steeply with $V$ for $U \sim U_c$.

![Figure 5](image-url). Phase diagram showing EOP with hybridization strength $V$ for $U = 2.5$. Left (right) panel shows single (two)-site results. The metal + exciton region gets enhanced in a two-site analysis. The transition from the mixed state (metal+exciton state) to EI is first order for single site case. EOP takes over exactly when $\Phi$ vanishes for a single site case. But in two-site approximation, the transition is weakly first order (at $U = 2.5$) as one incorporates the inter-site correlation $B_{ij}; \Delta$ has finite value even when $\Phi = 0$ and saturates as $B_{ij}$ goes to zero (shown by a dashed green line).
U. On the other hand, the on-site excitonic order parameter $\Delta$ increases with $V$ as well as $U$; this order saturates when $\Delta_e$ vanishes. In the large $U$-limit, the behaviour of $\Delta_e$ follows that of $B_{ij}$ and vanishes in the large-$U$ limit. Clearly, $\Delta_e$ vanishes as $V' \to 0$. Since the same electrons and holes are involved in the extended excitonic order ($\Delta_e$) and the local excitonic order ($\Delta$), one has to delete while the other builds up. For low $V$, both of these order parameters increase, while as $V$ becomes larger $\Delta_e$ drops off rapidly and $\Delta$ increases as expected. Besides, the extended order parameter is severely affected by the approaching incompressibility as $U$ increases. As charge fluctuation gets quenched, the intersite order also decreases following $B_{ij}$, while the pseudo-spin fluctuation builds up enhancing $\Delta$. In the presence of on-site hybridization, the extended FKM can be mapped onto an XXZ model with the hybridization term appearing like a transverse field in the $XY$-plane. Moreover, in the pseudospin space, the non-local hybridization $V'$ favors staggered Ising-type ordering along the $x$ direction, while $V$ favors a uniform polarization along the $x$ direction and the staggered Ising-type ordering along the $y$ direction.

4.4. Effect of finite $t_3$

As it is seen from above results, a finite hybridization between two bands can induce electron–hole pairing. Moreover, analytical and numerical studies [28, 30, 31, 52, 53] showed that a finite localized-electron bandwidth can also induce electron–hole coherence in an FKM. Indeed, it was found, that the localized-band (e.g. $\beta$-electron hopping) of the opposite parity than the itinerant-band, stabilizes the excitonic phase, but only in the dimension $D > 1$ [30]. We have also considered an EFKM with different hopping terms and parity in the two involving bands. The left panel in figure 9 shows a tight-binding dispersion for a square lattice with opposite parities of the participating bands ($t_\alpha/t_\beta < 0$) and with different hopping terms ($t_\alpha \neq t_\beta$) and also in the presence of hybridization $V$. The right panel is for same parity bands ($t_\alpha/t_\beta > 0$) with different hopping terms in the presence of hybridization $V$. It is evident from the tight-binding bands that a gap opens up which is driven by $V$ and the magnitude of gap is exactly same as the applied $V$; this gap is mediated by the excitons formed in the system driven by hybridization and hence known as an excitonic band insulator. For an asymmetric hopping between $\alpha$ and $\beta$, an increase in $t_\beta$, the $\beta$-fermion kinetic energy increases hence the critical $U$ for metal-insulator transition increases. On the other hand, the excitonic order parameter goes down as the probability of formation of electron–hole bound state at a site reduces with increased $\beta$-electron hopping. In addition to that, steps appear (absent for $t_3 = 0$) in the $\Delta$ versus $V$ curves and the step-size increases with the value of $t_3$.

Steps appear (see the right panels of figures 7 and 8, and figure 10) when both the spins has same parity ($t_3/t_\alpha > 0$), no steps for the opposite parity ($t_3/t_\alpha < 0$) case. The step-size increases if we incorporate inter-site correlation $B_{ij}$. In the two-site approximation, the effect of hopping becomes interesting. When $U \simeq U_c$, $t_3 = 0$ (FKM limit), it is found that the $\Delta - V$ curve is almost continuous, but as we see from figure 8, the order parameter $\Delta$ becomes first order with the inclusion of $t_3$. One can go from weakly second order to first order by tuning $t_3$. The excitonic order always reduces with $t_3$, the probability of formation of excitonic bound state becomes less and less. Figure 10 shows how the excitonic order reduces with increasing $t_3$. Therefore, in the absence of $U$, the system can open a gap; driven by $V$, known as excitonic gap which is exactly equal to $2\Delta$. At low $U$, large $V$ is required to make $\Phi$ zero, consequently one enters an insulating phase. This is
a band-insulator driven by $V$. On the opposite, large $U$ limit, even a small $V$ opens a gap. Here a correlated insulator is realized.

In the strong-coupling regime, the EFKM ($V \neq 0$) can be mapped onto the spin-1/2 Ising XXZ model with a transverse magnetic field [10]. In that case, the spontaneous excitonic order corresponds to the spontaneous magnetization in the $XY$ plane. Therefore, the excitonic order in EFKM is like the metamagnetism in the half-filled Hubbard model: the variation in the magnetization with external applied magnetic field. This is reflected in $\Delta - V$ behaviour. The Zeeman term in the metamagnetism in Hubbard model couples to the $z$-component of spin, while $V$ term in the EFKM is like a transverse field.
An extended FKM was studied using HF mean-field theory [16], which works reasonably well for the ground state in the low-\(U\) regime. The single-site SRMF theory, however, captures the physics of the ground state at large-\(U\) better and in its two-site version even the exchange scale is resolved. The difference between the mean-field and SRMF results can be compared to the difference between mean-field calculations and Gutzwiller theory in the Hubbard model. Using a cluster (minimal two-site) extension to SR formalism, we unravel the ground state (\(T = 0\)) properties of exciton in a two-band system in the strongly correlated regime. The inclusion of hybridization among these levels gives rise to an electron–hole bound state defined by the local and extended order parameters \(\Delta\) and \(\Delta_e\). \(\Delta\) increases with \(V\) for all \(U\) as expected.

5. Conclusions

Figure 9. Tight-binding bandstructure of a square lattice in the presence of hybridization \(V\) with different hopping terms \(t_{\alpha}/t_{\beta} < 0\) (left panel) and \(t_{\alpha}/t_{\beta} > 0\) (right panel).

Figure 10. The variation of EOP (\(\Delta\)) with \(t_{\beta}\) for \(V = 0.1\) for two cases when \(t_{\beta}/t_{\alpha} > 0\) and \(t_{\beta}/t_{\alpha} < 0\).
The behaviour of $\Delta_e$ is somewhat different. A metal-insulator transition can be tuned by $V$ also, it is found that for low $U_e$ a large $V$ is required to make the rotor kinetic energy zero. The value of $U_e$ (MIT scale) moves down with increasing $V$. After a certain critical correlation $U_e$ or $V$, there is a first-order jump in the excitonic order parameter associated with an MIT. The two-site analysis gives $t^2/U$-scale in the calculation and correctly describes the metallic and insulating phases. There is coexistence of metallic and excitonic phases and after a certain hybridization, electrons are completely localized and an EI state follows.

In the large-$U$ limit, the gap (proportional to excitonic OP) is less affected by the magnetic field or the hybridization $V$; whereas in the weak-coupling regime, a gap opens up with the inclusion of $V$ and its value is same as the excitonic order parameter $\Delta$ (dictated by $V$). The effect of $t_3$ is also interesting, the behaviour of $\Delta$ depends on the sign of $t_3$; steps appear when $t_3/t_0 > 0$. The excitonic order parameter reduces with increasing $t_3$.

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