

Effect of Strong Orbital Magnetic Field on the Exciton Condensation in an Extended Falicov Kimball Model

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Abstract. A spinless, extended Falicov-Kimball model in the presence of a perpendicular magnetic field is investigated employing a self-consistent mean-field theory in two dimensions. In the presence of the field the excitonic average $\Delta = \langle d_i^\dagger f_i \rangle$ is modified: the exciton responds in subtle different ways for different values of the magnetic flux. We examine the effects of Coulomb interaction and hybridization between the localized and itinerant electrons on the excitonic average, for rational values of the applied magnetic field. The excitonic average is found to get enhanced exponentially with the Coulomb interaction while it saturates at large hybridization. The orbital magnetic field suppresses the excitonic average in general, though a strong commensurability effect of the magnetic flux on the behaviour of the excitonic order parameter is observed.

1. Introduction

The Falicov-Kimball model (FKM), involving a dispersive d -electron band, an atomic-like f -electron state and an on-site Coulomb interaction U between them, is perhaps the simplest lattice model to study many-body effects. Since its introduction in 1969 [1], to describe valence or metal-insulator transition in some transition metal oxides, the model has been successful in describing several correlation effects [2], e.g., metal-insulator transition [3], mixed-valence [4], the formation of ionic crystals [5, 6] and orbital [7] and charge-density waves (CDW)[8]. Brandt and Schmidt [9] and Kennedy and Lieb [8] showed that on a bipartite lattice at half-filling ($n_d = n_f = 0.5$), the f -electrons order in the checkerboard pattern. Portengen *et al.* [10, 11] introduced a k -dependent hybridization between d and f -bands and the resulting bound state between d -electrons and f -holes underwent a Bose Einstein condensation (BEC) of $d-f$ ‘excitons’. As d and f -states differ by an odd parity, this could lead to an ‘electronic ferroelectricity’. In the weak-coupling mean-field theory, the formation of an order parameter and the condensation thereof are concomitant. The Coulomb interaction U gives rise to a nonvanishing $d-f$ coherence $\langle d_i^\dagger f_i \rangle \neq 0$ even in the limit of $V \rightarrow 0$ [10]



in the presence of a putative homogeneous ground state under the HF approximation. Czycholl [12] showed later that $\langle d_i^\dagger f_i \rangle \rightarrow 0$ as $V \rightarrow 0$, i.e., there is no spontaneous symmetry breaking, consistent (but not contradictory at $T = 0$ though, where Elitzur's theorem does not forbid an order) with the local $U(1)$ gauge symmetry at $V = 0$. For a small non-zero V , the inhomogeneous (CDW) phase is stable, and the EOP is finite. Similar conclusions were then reached for a triangular lattice as well [13]. Indeed the Coulomb interaction between the conduction band electron and the valence band hole causes the formation of an excitonic bound state in some materials.

Recently, there is report of possible transition to an excitonic insulating state in the quasi-1D Ta_2NiSe_5 due to BEC of these bound states [14]. A moot question is what happens to such an excitonic condensate in the presence of orbital field. This kind of gauge-field can be experimentally realised in ultracold particles (fermions and bosons) in optical lattices. Moreover, of late, there are proposals for the realization of FKM in optical lattices with mixtures of light atoms in the correlated, disordered environment of heavy atoms [15, 16]. Therefore, it is quite pertinent to appraise an extended Falicov-Kimball model (EFKM) in optical lattices in the presence of artificial gauge fields. In a spinful situation, strong magnetic field may cause the two Zeeman-split bands to move sufficiently apart, and at low filling only the lower band is relevant, effectively reducing it to a spinless problem. We implement a self-consistent mean-field calculation to study the effect of a perpendicular magnetic field in the spinless model. We first examine the case without a magnetic field and then study the effect of the field on the exciton condensation. Results for commensurate and incommensurate magnetic fluxes are discussed.

2. An extended Falicov Kimball model

We consider an EFKM, a model system with spinless electrons arising from d and f orbitals on every site on a square lattice

$$H = - \sum_{\langle ij \rangle} (t_{ij} d_i^\dagger d_j + h.c.) + U \sum_i d_i^\dagger d_i f_i^\dagger f_i + E_f \sum_i f_i^\dagger f_i + \sum_i V (d_i^\dagger f_i + h.c.) \quad (1)$$

where $\langle i, j \rangle$ are nearest-neighbour site indices on a square lattice (lattice constant $a = 1$), d_i (f_i) are itinerant (localized) electron annihilation operators at site i . The first term represents the kinetic energy of d -electrons while the second term represents on-site Coulomb interaction between d (density $n_d = \frac{1}{N} \sum_i d_i^\dagger d_i$) and f -electrons (at E_f , with density $n_f = \frac{1}{N} \sum_i f_i^\dagger f_i$; N being the number of sites). The fourth term stands for the hybridization between them. We set the hopping integral t to 1 and all energies are defined in units of t . For $V = 0$, the Hamiltonian commutes with $\hat{n}_{f,i}$, in which case $n_{f,i}$ is a good quantum number. It can be 'solved' numerically by annealing over the f -electron positions. For $V \neq 0$ the local $U(1)$ gauge symmetry is removed and the Hamiltonian is no longer exactly solvable, albeit in the above sense. We, therefore, take recourse to the usual self-consistent mean-field approximation to obtain the excitonic

average $\Delta = \langle d_i^\dagger f_i \rangle$. The inhomogeneous mean-field theory discussed below allows for local excitonic order parameter (EOP) and involves diagonalizing the mean-field Hamiltonian matrix followed by calculation of the EOP. The new EOP's are then fed back in to the Hamiltonian and the process continues till convergence (up to $10^{-7}\%$) in all the EOP's is reached.

3. Effect of perpendicular magnetic field

For $B \neq 0$, the spinless, mobile fermions 'see' the field via the canonically conjugate momentum. The field then couples to the 'orbital degrees' only. With the choice of Landau gauge $\vec{A}(r) = B(0, x, 0)$ for a uniform magnetic field B perpendicular to the plane of the lattice, the hopping integral does not change in x -direction while along the y -direction it gets a 'Peierls phase' $t_{ij} = -t \exp(\pm ie/\hbar \int_j^i A(\vec{r}) d\vec{r}) = -t \exp(\pm 2\pi i m \frac{\phi}{\phi_0})$. Here, $\phi = Ba^2$ is the flux per plaquette of a square lattice. This represents the gain of phase by an electron, hopping along a closed path around the plaquette. We consider only rational magnetic flux, i.e., $\phi = \frac{p}{q}\phi_0 = \alpha\phi_0$ with p, q co-prime integers and ϕ_0 , the Dirac flux quantum. As is customary, the lattice is discretized by $(x, y) = (ma, nb)$ - each site is then indexed by two integers " (m, n) " along (x, y) -directions (m, n now stand for the x, y coordinates in this discrete geometry) respectively. Peierls phases leave the Hamiltonian invariant only for such translations that are in the magnetic translation group [17]. This group is associated with a magnetic unit cell q times larger than the original unit cell, so as to enfold an integer flux $p\phi_0$. With the choice of a Landau gauge, the hopping in y -direction is associated with a phase which again depends on the x -component of the position vector " m ". Therefore, to accommodate a magnetic flux $B = \frac{2\pi}{L}$, the resultant magnetic supercell will have to be a strip of length L [18] (we use maximum $L = 36$). We work in the half-filled limit ($n_f + n_d = 1$), in the particle-hole symmetric case at zero temperature. In the non-interacting limit, the problem reduces to the original Hofstadter model (as the f -electrons do not enter in the problem now) and shows the well-known energy spectrum: a self-similar structure in which widths and gaps open and close depending on the values of the magnetic flux [19, 20].

4. Results and discussions

To check our numerical procedure we start with the extended ($V \neq 0$) FKM in the symmetric case ($E_f = 0$ and $n_d = n_f = 0.5$) without the transverse field. We study the effect of Coulomb interaction on the stability of excitons. It is evident from Fig. 1 that $\Delta = 0$ in the $V \rightarrow 0$ as expected on symmetry grounds. For a finite V , there is a nonvanishing Δ that is strongly enhanced as U increases. As we increase hybridization between d and f electrons, for a fixed Coulomb correlation, we find an enhancement in the EOP. In the $V \rightarrow 0$ limit we find a CDW ground state, which melts on increasing V . Moreover, we study the effect of Coulomb interaction: the effect of U is more for small- V regime: the EOP is exponentially enhanced with U as expected. These results are in complete agreement with previous results in a wide parameter regime [12, 13].

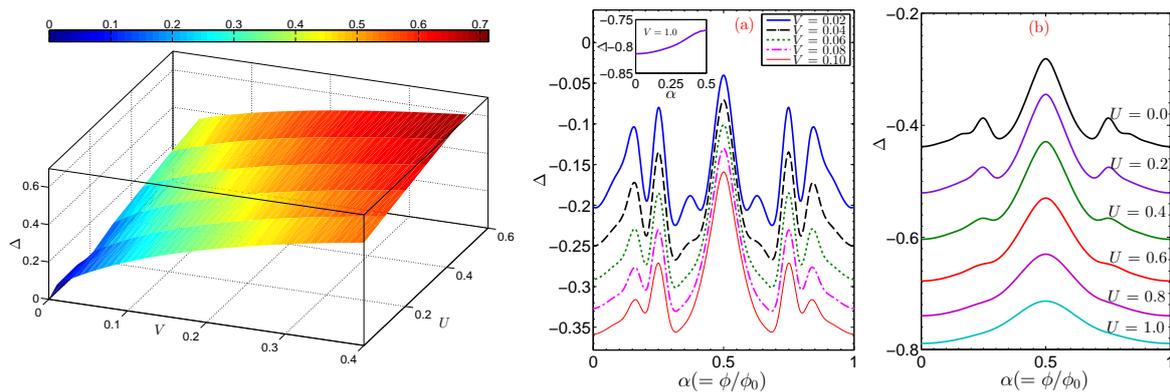


Figure 1. The mean-field behaviour of $\Delta = \langle d_i^\dagger f_i \rangle$ in the UV plane in the zero-field limit. **Figure 2.** (a) Δ versus α for different V (inset: $V = 0.1$) at constant $U = 0.2$. (b) EOP with α for different U at fixed $V = 0.20$.

The effect of orbital magnetic field on the evolution of excitons is a question we address next. With flux $\alpha \neq 0$ per plaquette, the hopping term is associated with a phase which affects the exciton formation. In Fig. 2, the EOP is suppressed by the field (note the negative sign of the EOP, so it increases downwards) and a prominent peak at $\alpha = 0.25$ and a dip at $\alpha = 1/3$ can be seen for $U = 0$. There is a large peak at $\alpha = 0.5$; signifying the value of α at which Δ is a minimum: same is the case for all the U . The large oscillations of Δ reduce with larger U . As the Hamiltonian is symmetric, between α and $1 \pm \alpha$, Fig. 2 is symmetric about $\alpha = 0.5$ and displays typical Hofstadter characteristics like the non-interacting limit. The variation of Δ with V more or less follows the same pattern as in the absence of magnetic field (see Fig. 3(a)). However, for a fixed U , the general tendency is that the excitonic average reduces with increase in magnetic field. However, it is also possible to get an enhancement in the excitonic average in a region where hybridization and correlation effects are quite weak (see Fig. 3(b)) for special (here $1/3$) values of the flux. This is likely to be related to the extra stabilization in the band energy at special flux values, also observed in the Hofstadter spectrum [19].

In the presence of field, there is serious commensurability effect on the excitonic average. For certain values of $d - f$ correlation and hybridization, the system is essentially in the homogeneous state. From Fig. 4, we see that for some magnetic flux values, the magnetic unit cell is commensurate with the lattice size (in the present study on a 24×24 lattice, $1/24, 2/24, 3/24, \dots, 12/24$ and so on, represent commensurate fluxes) and the excitonic average is uniform throughout the lattice. With increase in the value of the commensurate flux, magnitude of Δ decreases and the EOP is uniform. On the other hand, the EOP varies in a quite different way when the magnetic flux is incommensurate. In this case, the excitonic average exhibits a one-dimensional modulation and the modulation length changes with the flux (Fig. 4(b), (c)).

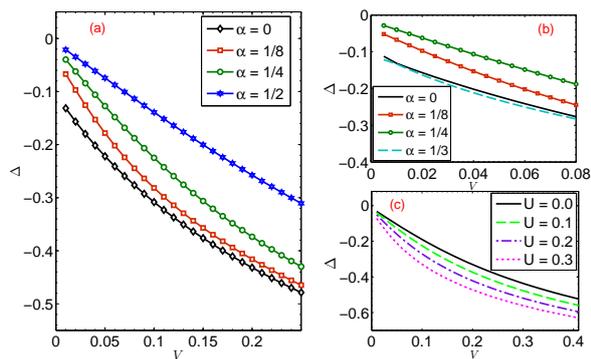


Figure 3. (a) EOP with V for several α at $U = 0.20$. (b) $\alpha = 1/3$ (dashed line). (c) Δ vs V at different U with $\alpha = 0.25$.

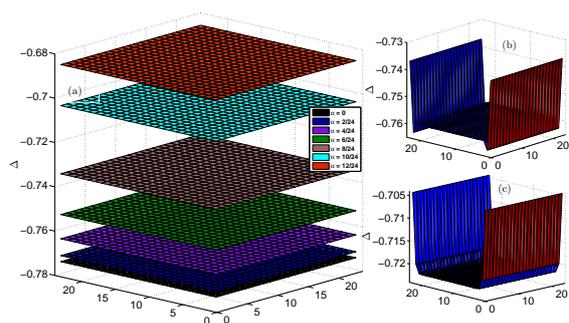


Figure 4. The EOP on a 2D lattice plane for α (a) commensurate (b) 0.1, (c) 0.37. At $U = 1.0$ and $V = 0.2$.

5. Summary and conclusion

We observe the competition between magnetic field and Coulomb correlation in a prototype correlated lattice model. The Coulomb interaction exponentially enhances the excitonic average while the orbital magnetic field has a localizing effect on mobile d -electrons, affecting the excitonic coherence: a drop in the value of excitonic average (hence electronic ferro-electricity) with both commensurate and incommensurate flux. In the small V limit, there is a special value ($\alpha = 1/3$) of the field which gives extra stability to the exciton. These observations open up the possibility of tuning ferro-electricity via applied magnetic field.

6. References

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