International Journal of Modern Physics B
Vol. 19, Nos. 1, 2 & 3 (2005) 525–527

World Scientific
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ELECTRONICALLY DRIVEN FERROELECTRICITY IN THE EXTENDED FALICOV-KIMBALL MODEL

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Received 9 June 2004

We calculate the quantum phase diagram of an extended Falicov-Kimball model in the intermediate coupling regime using a constrained path quantum Monte Carlo technique. The mixed-valence regime is dominated by a Bose-Einstein condensation of excitons with a built-in electric polarization.

Keywords: Electron correlations; ferroelectricity.

Recently, one of us demonstrated[1] that a novel ferroelectic state[2] is realized in the strong-coupling, mixed-valence regime of an extended Falicov-Kimball model (FKM)[3]. This new ferroelectric state is based upon a purely electronic mechanism of an essential *quantum* nature. A spontaneous phase-coherent hybridization between the two local orbitals in the same unit cell providing these orbitals possess different parity under spacial inversion, leads to finite electric polarization. The electronic origin of this novel ferroelectric state is driven by strong Coulomb repulsion. The interplay between the orbital and the spin flavors of the electronic degrees of freedom make this novel state suitable for new technological applications.

The FKM for sinless fermions that contains the electronic ferroelectricity can be exactly mapped on an asymmetric Hubbard model with a Zeeman term [1]:

$$H = e_d \sum_{\mathbf{i},\sigma} n_{i\sigma} + \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} t_\sigma (c^\dagger_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma} c_{\mathbf{i}\sigma}) + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow} + B_z \sum_{\mathbf{i}} \tau^z_i, \quad (1)$$

where $\tau_{\mathbf{i}}^{\alpha} = \frac{1}{2}\sum_{\nu,\nu'} c_{\mathbf{i}\nu}^{\dagger}\underline{\sigma}^{\nu\nu'}c_{\mathbf{i}\nu'}$, with $\alpha = \{x, y, z\}$, $e_d = \frac{1}{2}(\epsilon_d + \epsilon_f)$, $t_{\uparrow} = t_d$, $t_{\downarrow} = t_f$, and $B_z = \epsilon_d - \epsilon_f$, where ϵ_d, ϵ_f and t_d, t_f represent positions of $d-$ and $f-$bands and overlap integrals between neighboring Wannier orbitals of the original FKM respectively [1]. Hamiltonian in Eq. 1 is $U(1)$ invariant, its symmetry is generated by the total magnetization along the z axis $M^z = \sum_{\mathbf{i}} \tau_{\mathbf{i}}^z$. This symmetry corresponds to the conservation of the difference between the total number of particles in each band of the original FKM.

At half filling, the ground state of H exhibits two possible magnetic orderings in the strong coupling limit: Ising-like antiferromagnetism and xy-like ferromagnetism for $\gamma = -t_{\downarrow}/t_{\uparrow} > 0$ [1]. The Ising-like phase corresponds to staggered orbital ordering (SOO) in the original FKM and the xy-like ferromagnetism corresponds to a Bose-Einstein (BE) condensate of excitons with a built-in electric polarization [2]:

$$\vec{P} = \frac{\vec{\mu}}{\Omega}\sum_{\mathbf{i}}(c_{\mathbf{i}\uparrow}^{\dagger}c_{\mathbf{i}\downarrow} + c_{\mathbf{i}\downarrow}^{\dagger}c_{\mathbf{i}\uparrow}) = \frac{2\vec{\mu}}{\Omega}M^x, \tag{2}$$

where $\vec{\mu}$ is the inter-band dipole matrix element and Ω is the volume of the system. The electrical polarization is given by the in-plane pseudo-spin magnetization.

In Fig. 1, we present the 2D quantum phase diagram of H at half-filling as a function of γ and B_z, calculated using the constrained path quantum Monte Carlo (CPMC) technique [4]. The diagram shows the three phases which are exactly obtained in the strong coupling limit [1]. For $B_z = 0$, the ground state is an Ising-like antiferromagnet or a staggered orbital ordered (SOO) phase in the FKM language. At a critical value of $|B_z| = B_z^{c1}$ there is a transition from the SOO phase to a phase with a long-range order in xy plane measured by the pseudspin-pseudospin correlation function $S^x(0,0)$:

$$S^x(\mathbf{q}) = \frac{1}{N_s^2}\sum_{\mathbf{i},\mathbf{j}}\langle\tau_{\mathbf{i}}^x\tau_{\mathbf{j}}^x\rangle e^{i\mathbf{q}\cdot(\mathbf{r_i}-\mathbf{r_j})}. \tag{3}$$

The scaling of $S^x(0,0)$ is shown in Fig. 1. (Note, that SOO phase is given by a finite $S^z(\pi,\pi)$). This second phase is also characterized by a non-zero uniform magnetization along the z axis. When $|B_z|$ reaches a second critical value, B_z^{c2}, M^z saturates and a new gap opens. In terms of our original language, this is the transition from a mixed valence to non-mixed valence regime in which one band is full and the other one is empty. This is also transition from an excitonic insulator to a band insulator.

To calculate B_z^{c1}, we have scaled the calculated gap of the SOO phase for different chain sizes up to $N_s = 14 \times 14$ (N_s is the number of sites). A typical scaling is shown in Fig. 1 for four different values of γ. The value of $B_z^{c1}(\gamma = 0)$ was calculated exactly. Note in Fig. 1 that the values of $B_z^{c1}(\gamma)$ calculated with the CPMC method converge to the exact value when γ approaches zero. The other special value, $\gamma = 1$, corresponds to the $SU(2)$ critical point for which the pseudospin correlations along the three different axis are the same. In the strong coupling limit the gap of the SOO phase closes exponentially [1], as γ approaches one. The transition from the SOO to

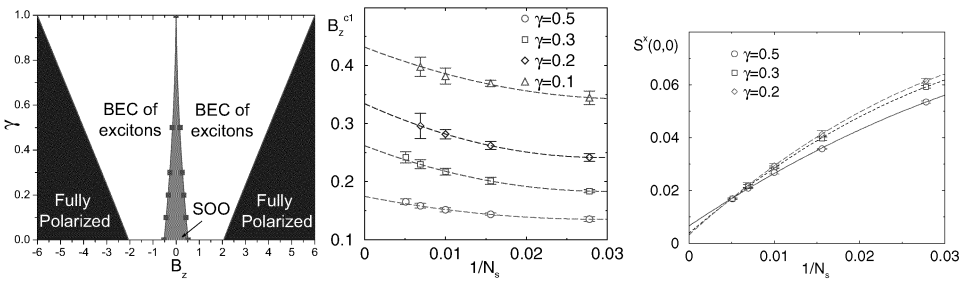

Fig. 1. Left: two dimensional phase diagram of the extended FKM. The circles are the calculated points and the full lines are guides to the eye. The error bars are smaller than the symbol sizes. Middle: scaling of B_z^{c1}. Right: scaling of $S^x(0,0)$ computed at $M^z = N_s/4$. All figures are computed at $U = 2$ and $t_\uparrow = 1$.

the ferroelectric BE condensate of excitons is a first order valence transition because the relative population between the two bands, M^z, changes discontinuously.

We have presented the quantum 2D phase diagram of the extended FKM in the intermediate coupling limit. The insulating phase obtained at half filling undergoes a transition at B_z^{c2} from a non-mixed valence to a mixed valence regime as a function of B_z or in the language of the original FKM, as a function of the difference of positions of $d-$ and $f-$ bands. At this transition the system changes from a band insulator to an excitonic insulator which is a BE condensate of electron-hole pairs. This phase is characterized by a finite in-plane pseudo-spin correlation function which furthermore possesses *ferroelectric order*. If B_z is further decreased, there is a first order valence transition at B_z^{c1} from the BE condensate of excitons to a state with staggered orbital ordering and no ferroelectric order. Recent calculations show, that the inclusion of small hybridization between the $d-$ and $f-$ bands stabilizes the ferroelectric phase [5].

Acknowledgements

J.B. acknowledges the financial support of Slovene MESS under grant P1-0044. This work was in part sponsored by the US DOE under contract W-7405-ENG-36. H.Q. Lin is partly supported by RGC Project CUHK 4037/02P.

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