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Combined effects of local and nonlocal hybridization on formation and condensation of excitons in the extended Falicov-Kimball model

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ABSTRACT

We study the combined effects of local and nonlocal hybridization on the formation and condensation of the excitonic bound states in the extended Falicov-Kimball model by the density-matrix-renormalization-group (DMRG) method. Analysing the resultant behaviours of the excitonic momentum distribution $N(q)$ we found, that unlike the local hybridization V, which supports the formation of the q=0 momentum condensate, the nonlocal hybridization V_n supports the formation of the $q=\pi$ momentum condensate. The combined effect of local and nonlocal hybridization further enhances the excitonic correlations in q=0 as well as $q=\pi$ state, especially for V and V_n values from the charge-density-wave (CDW) region. Strong effects of local and nonlocal hybridization are observed also for other ground-state quantities of the model such as the f-electron density, or the density of unbound d-electrons, which are generally enhanced with increasing V and V_n. The same calculations performed for nonzero values of f-level energy E_f revealed that this model can yield a reasonable explanation for the pressure-induced resistivity anomaly observed experimentally in $TmSe_{0.45}Te_{0.55}$ compound.

1. Introduction

The formation of excitonic quantum condensates is an intensively studied continuous problem in condensed matter physics [1-4]. Whilst theoretically predicted a long time ago [5], no conclusive experimental proof of the existence of the excitonic condensation has been achieved yet. However, the latest experimental studies of materials with strong electronic correlations showed that promising candidates for the experimental verification of the excitonic condensation could be $TmSe_{0.45}Te_{0.55}$ [6], $1T-TiSe_2$ [7], Ta_2NiSe_5 [8], or a double bilayer graphene system [9]. In this regard, the mixed valence compound $TmSe_{0.45}Te_{0.55}$ was argued to exhibit a pressure-induced excitonic instability, related to an anomalous increase in the electrical resistivity [6]. In particular, the detailed studies of the pressure-induced semiconductor-semimetal transition in this material (based on the Hall effect, electrical and thermal (transport) measurements) showed that excitons are created in a large number and condense below 20 K. On the other hand, in the layered transition-metal dichalcogenide $1T-TiSe_2$, a BCS-like electron-hole pairing was considered as the driving force for the periodic lattice distorsion [7]. Moreover, quite recently, the excitonic-insulator state was probed by angle-resolved photoelectron spectroscopy in the semiconducting Ta_2NiSe_5 compound [8]. At present, it is generally accepted that the minimal theoretical model for a description of excitonic correlations in these materials could be the Falicov-Kimball model [10] and its extensions [11-20].

The original Falicov-Kimball model describes a tight-binding system of itinerant d electrons interacting via the on-site Coulomb repulsion with localized f electrons (the spin degrees of freedom of the d and f electrons are not included):

$$H_0 = -t_d \sum_{\langle i,j\rangle} d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i, \quad (1)$$

where f_i^+, f_i are the creation and annihilation operators for an electron in the localized state at lattice site i with binding energy E_f and d_i^+, d_i are the creation and annihilation operators of the itinerant spinless electrons (with the nearest-neighbor d-electron hopping constant t_d) in the d-band Wannier state at site i. In what follows we consider t_d=1 and all energies are measured in units of t_d.

Since the local f-electron number $f_i^+ f_i$ is strictly conserved quantity, the d-f electron coherence cannot be established in this model. One way to overcome this shortcoming is to include an explicit local hybridization $H_V = V\sum_i d_i^+ f_i + f_i^+ d_i$ between the d and f orbitals. This model has been extensively studied in our previous work [20]. The numerical analysis of the excitonic momentum distribution $N(q) = \langle b_q^+ b_q \rangle$ (with $b_q^+ = (1/\sqrt{L}) \sum_k d_{k+q}^+ f_k$, where L denotes the number of lattice sites) showed that this quantity diverges for q=0, signalizing a massive condensation of preformed excitons at this momentum. The stability of the zero-momentum (q=0) condensate against the f-electron hopping has been studied in our very recent paper [21]. It was found that the negative values of the f-electron hopping integrals t_f support the

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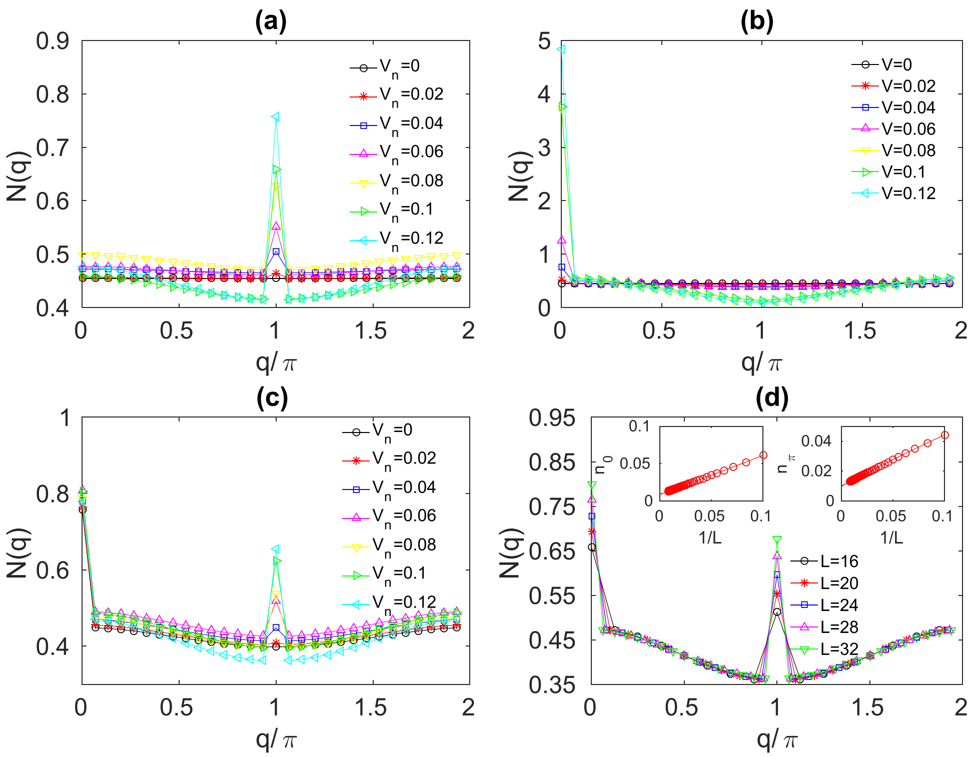

Fig. 1. The DMRG results for the excitonic momentum distribution $N(q)$ calculated for different model parameters. (a) $N(q)$ calculated for $V=0$, $U=4$, $E_f=0$, $L=30$ and different values of V_n. (b) $N(q)$ calculated for $V_n=0$, $U=4$, $E_f=0$, $L=30$ and different values of V. (c) $N(q)$ calculated for $V=0.04$, $U=4$, $E_f=0$, $L=30$ and different values of V_n. (d) $N(q)$ calculated for $V=0.04$, $V_n=0.12$, $U=4$, $E_f=0$ and different values of L. The insets show the densities of q=0 and $q=\pi$ momentum excitons as functions od $1/L$ calculated for the same values of model parameters.

formation of zero-momentum condensate, while the positive values of t_f have the fully opposite effect. Moreover, it was shown that the fully opposite effects on the formation of condensate exhibit also the local and nonlocal hybridization with an inversion symmetry. The first one strongly supports the formation of condensate, while the second one destroys it completely. However, in the real d-f systems, the on-site hybridization V is usually forbidden for parity reasons [22], and therefore the fact that the nonlocal hybridization with an inversion symmetry does not support the formation of excitonic condensate strongly limits the class of materials, where this phenomenon can be observed. In this situation, the most promising candidates for studying this phenomenon seem to be the systems with equal parity orbitals, where the nonlocal hybridization H_n can be written as:

$$H_n = V_n \sum_{\langle i,j \rangle} (d_i^+ f_j + H.c.). \tag{2}$$

In such systems, the local hybridization V is allowed, and thus one can examine the combined effects of the local and nonlocal hybridization within the unified picture. The weak ($U<1$) and strong ($V \ll U$ and $V_n \ll U$) coupling limits of the model Hamiltonian $H_0+H_V+H_n$ have been analyzed recently by Zenker et al. in [23], and the corresponding mean-field quantum phase diagrams were presented as functions of the model parameters U, V, V_n and E_f for the half-filed band case $n_f+n_d=1$ and D=2. Moreover, examining effects of the local V and nonlocal V_n hybridization they found that in the pseudospin space ($c_{i\uparrow}^+ = d_i^+$, $c_{i\downarrow}^+ = f_i^+$) the nonlocal hybridization V_n favors the 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.

In the current paper we examine model for arbitrary V and V_n and unlike the paper of Zenker et al. [23] we focus our attention primarily on a description of process of formation and condensation of exitonic bound states. For this reason we calculate (by the DMRG method) various ground state characteristics of the model such as the excitonic momentum distribution $N(q)$, the density of zero momentum excitons $n_0 = \frac{1}{L} N(q=0)$, the total exciton density $n_T = \frac{1}{L}\sum_q N(q)$, the total d-electron density n_d and the total density of unbound d electrons $n_d^{un} = n_d - n_T$, and analyze their bahaviours as functions of the local/nolocal hybridization and the f-level position E_f. It should be noted that such a study could be very valuable from the point of view of real materials, since taking into account the parametrization between the external pressure and the position of the f level ($E_f \sim p$), one could deduce from the E_f dependencies of the ground state characteristics also their p dependencies, at least qualitatively [24]. As shown at the end of this paper a simple model based on the above mentioned parametrization can yield a reasonable explanation for the pressure-induced resistivity anomaly observed experimentally in $TmSe_{0.45}Te_{0.55}$ compound [6].

2. Results and discussion

To examine combined effects of the local V and nonlocal V_n hybridization on the formation and condensation of excitonic bound states in the extended Falicov-Kimball model we have performed exhaustive DMRG studies of the model Hamiltonian $H=H_0+H_V+H_n$ for a wide range of the model parameters V, V_n and E_f at the total electron density $n=n_d+n_f=1$ (the half-filled band case). In all examined cases we typically keep up to 500 states per block, although in the numerically more difficult cases, where the DMRG results converge slower, we keep up to 1000 states. Truncation errors [25], given by the sum of the density matrix eigenvalues of the discarded states, vary from 10^{-6} in the worse cases to zero in the best cases.

Let us start a discussion of our numerical results for the case E_f=0. The typical examples of the excitonic momentum distribution $N(q)$ calculated for the representative values of V, V_n and U are summarized