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Suppression of Nearest Neighbour Electron Hopping in FeSe-Based Superconductors

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In this paper, we evaluate the fitting parameters for the hopping model for the d_{xy} and d_{xz} bands within the Γ–M cut for different FeSe-based superconductors. Comparison of these parameters for DFT calculations and for experimentally obtained data reveals a dramatic change of hopping probability between the nearest neighbours. This change is much bigger than the expected band renormalization and can be explained by the appearance of an antiferromagnetic-like ordering.

Key words: FeSe, electronic structure, iron-based superconductors, intercalated systems, FeSe films.

У статті оцінено параметри моделю перескоків для апроксимації d_{xy}- та d_{xz}-зон у Γ–M-перерізі для різних надпровідників на основі FeSe. Порівняння значень цих параметрів для експериментально одержаних і розрахованих методою ТФГ електронних дисперсій показує зменшення ймовірности перескоку між найближчими сусідами. Такі зміни можуть бути пояснені появою певного виду впорядкування.

Ключові слова: FeSe, електронна структура, залізні надпровідники, інтеркальовані системи, плівки FeSe.

В статье оценены параметры модели перескоков для аппроксимации d_{xy}- и

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d_{xz}-зон в Г–М-сечении для разных сверхпроводников на основе FeSe. Сравнение значений параметров для экспериментально полученных электронных дисперсий и рассчитанных с помощью метода ТФП показало снижение вероятности перескоков между ближайшими соседями. Такие изменения можно объяснить возникновением некоторого упорядочения.

Ключевые слова: FeSe, электронная структура, железные сверхпроводники, интеркалированные системы, плёнки FeSe.

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1. INTRODUCTION

Iron-based superconductors is a new class of high-temperature superconductors, which was discovered in 2008 [1–3]. Fermi surface topology of iron-based superconductors have been predicted by numerous density functional theory (DFT) calculations and confirmed by many experiments [1–5]. However, there are some differences between the results of calculations and experimentally obtained data.

First of all, it is strong renormalization of bands, which differs for distinct bands and different compounds. However, these differences can be explained by dynamical mean-field theory (DMFT) calculations [6, 7].

Another difference is a shrinking of experimentally obtained Fermi surfaces in comparison to DFT calculated ones. Such a shrinking is supposed to be a result of the shifts of bunches of the hole and electron bands in the opposite directions in the centre and at the corner of the Brillouin zone [8–10].

There are several explanations for such shifts in opposite directions. In Ref. [11], it is supposed that such shifts are fully consistent with the enhancement of the Pomeranchuk $s^{\pm}$-susceptibility predicted by the analytical renormalization group technique. Another mechanism considers these differences as a result of self-energy corrections due to exchange of the spin fluctuations between the hole and electron pockets. In this case, the band shifts are supposed to be orbital-dependent ones [12–14].

In this paper, we analyse experimentally obtained ARPES data and DFT calculations of different FeSe-based superconductors in terms of hopping parameters [15, 16]. It is shown that characteristic shifts of the experimentally obtained bands can be naturally explained by blocking of hopping between the nearest neighbours.

2. EVALUATION OF HOPPING PARAMETERS

Taking into account the hopping between up to three nearest neigh-

bours, the dispersion in the Γ–M direction for the 2-Fe unit cell is given by formula:

$$\varepsilon(k) = \varepsilon_0 + t_1\cos(k_x a) + t_2\cos(2k_x a) + t_3\cos(3k_x a),$$

where t_1, t_2, and t_3 are the hopping integrals, which are proportional to probabilities of hopping between the nearest neighbours, next nearest, and next-next nearest neighbours, respectively. The hopping integrals obtained by fitting the experimental and DFT dispersions to this formula for different FeSe-based (Figs. 1–3) compounds are presented in Tables 1–3. In this case, we pay attention only on two bands, whose positions have been obtained experimentally.

It is supposed that the band structure in the range 0–1 eV is renormalized with some factor of renormalization. The value of the renormalization factor differs for distinct compounds and bands. Different papers give different renormalization factor values ranging from 2 to almost 17 [9, 17–19], but it is more probable that for FeSe-based superconductors these factors are near 3 [4]. Such variety may be explained by the various methods for determination of the renormalization parameters. The value of these parameters can be obtained by comparing the velocities (first derivatives with respect to **k** of the electronic dispersions) or masses (second derivatives) in different points of the Brillouin zone. These methods work properly within the 'rigid' band, but the band shifts in opposite directions make determination of these parameters ambiguous.

In terms of the hopping model, the renormalization factors can be

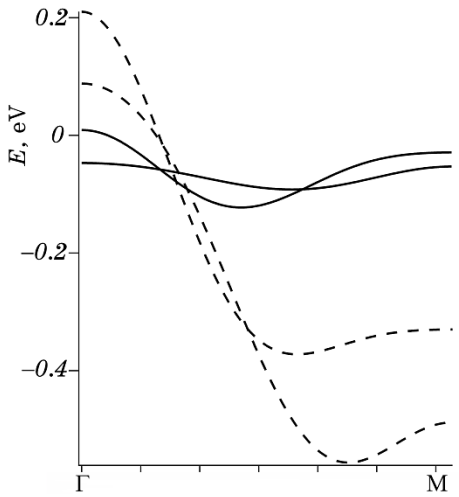

Fig. 1. Fit of calculated (dashed lines) and experimentally obtained (solid lines) d_{xz} (in Γ-point upper band) and d_{xy} (in Γ-point lower band) for FeSe.

determined by various ways. For example, $d\varepsilon/dk \approx -ka^2(t_1 + 2t_2 + 3t_3)$ in the vicinity of Γ-point, and $d\varepsilon/dk \approx -a(t_1 - 3t_3)$ for $k = \pi/(3a)$.

If the renormalization is related with the enhancement of quasi-

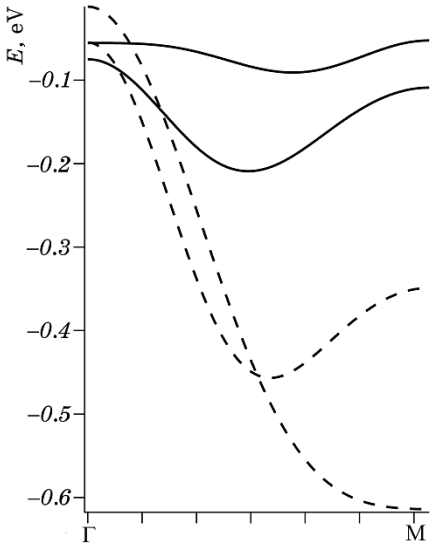

Fig. 2. Fit of calculated (dashed lines) and experimentally obtained (solid lines) d_{xy} (in Γ-point upper band) and d_{xy} (in Γ-point lower band) for KFeSe.

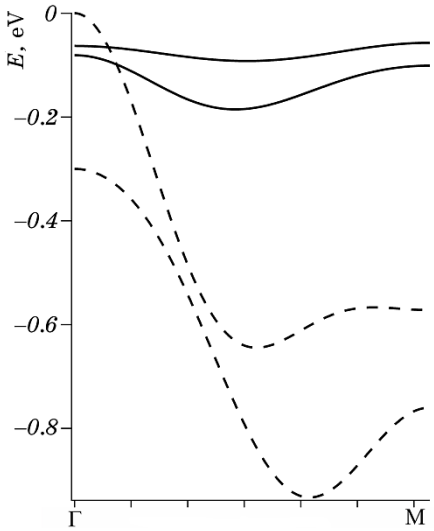

Fig. 3. Fit of calculated (dashed lines) and experimentally obtained (solid lines) d_{xz} (in Γ-point upper band) and d_{xy} (in Γ-point lower band) for monolayer FeSe film on STO substrate.

particle mass, $d^2\varepsilon/dk^2 = -a(0.5t_1 - 2t_2 - 3t_3)$ for $k = \pi/(3a)$ and $d^2\varepsilon/dk^2 = -a(t_1 + 4t_2 + 9t_3)$ for Γ-point.

So, direct comparison of the experimental and the calculated dispersions cannot be made due to changes of renormalization factor with respect to ways of its definition and due to the shift of the bands in opposite directions. Thus, the most reliable way to compare the experimental and calculated dispersions is to evaluate the ratio between hopping integrals of each.

Since the DFT calculations do not take into account the band renormalization due to electronic correlations, the obtained values of hopping parameters for the calculated and experimentally obtained bands differ essentially but related by a 'renormalization coefficient'. For t_2 and t_3, the ratio between coefficients of fitting for the calculated and

TABLE 1. Fitting parameters for FeSe.

FeSe	ε_0		t_1		t_2		t_3	
d_{xz}(calc/exp)	–0.209	–0.063	0.233	0	0.149	0.053	0.037	0.019
d_{xy}(calc/exp)	–0.302	–0.067	0.322	0.005	0.102	0.019	–0.034	–0.008

TABLE 2. Fitting parameters for KFeSe.

KFeSe	ε_0		t_1		t_2		t_3	
d_{xz}(calc/exp)	–0.209	–0.15	0.123	0.007	0.126	0.058	0.024	0.01
d_{xy}(calc/exp)	–0.385	–0.07	0.299	0.006	0.072	0.016	0.002	–0.0075

TABLE 3. Fitting parameters for monolayer FeSe film on STO substrate.

FeSe(Monolayer)	ε_0		t_1		t_2		t_3	
d_{xz}(calc/exp)	–0.195	–0.141	0.221	0	0.179	0.053	0.065	0.019
d_{xy}(calc/exp)	–0.406	–0.076	0.276	0	0.146	0.016	0.029	–0.003

TABLE 4. Ratio between hopping integrals for calculated and experimentally obtained electronic dispersions for FeSe, KFeSe, and single layer FeSe film on STO substrate.

	t_1(calc)/t_1(exp)		t_2(calc)/t_2(exp)		t_3(calc)/t_3(exp)	
	d_{xz}	d_{xy}	d_{xz}	d_{xy}	d_{xz}	d_{xy}
FeSe	∞	64	2.8	5.4	2.05	4.25
KFeSe	17	50	2.2	4.5	2.4	0.26
FeSe (single layer)	∞	∞	3.4	9.125	3.4	9.6

experimental obtained bands is close to the renormalization factor of the band (*e.g.*, for FeSe, it is 2–3 for d_{xz} band and 4–5 for d_{xy} band; Table 4). An important difference is that t_1 for experimentally obtained bands for all compounds is much smaller than for results of DFT calculations. For all compounds and all bands, t_1 becomes zero or its value is near zero. As have been proposed in this article, changes of t_1 are equivalent to decreasing of probability or complete blocking of the nearest neighbour hopping that can be result of appearance of some kind of ordering.

3. CONCLUSIONS

In this paper, the hopping parameters for the d_{xy} and d_{xz} bands for the Γ–M cut of different FeSe-based superconductors have been obtained. As shown, the hopping integral for the nearest neighbours based on experimentally obtained data undergoes significant depletion comparing to the DFT calculated data. This depletion cannot be explained by simple band renormalization, but rather by decreasing of probability of nearest neighbour hopping, that can be a consequence of an antiferromagnetic-like ordering.

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