Magnetism in Parent Iron Chalcogenides: Quantum Fluctuations Select Plaquette Order

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Magnetism in parent Fe-chalcogenides: quantum fluctuations select a plaquette order

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We analyze magnetic order in Fe-chalcogenide $Fe_{1+y}Te$ – the parent compound of high-temperature superconductor $Fe_{1+y}Te_{1-x}Se_x$. Experiments show that magnetic order in this material contains components with momentum $Q_1 = (\pi/2, \pi/2)$ and $Q_2 = (\pi/2, -\pi/2)$ in Fe-only Brillouin zone. The actual spin order depends on the interplay between these two components. Previous works assumed that the ordered state has a single-Q (either Q_1 or Q_2). In such a state, spins form double stripes along one of diagonals breaking the rotational C_4 symmetry. We show that quantum fluctuations actually select another order – a double Q plaquette state with equal weight of Q_1 and Q_2 components, which preserves C_4 symmetry. We argue that the order in $Fe_{1+y}Te$ is determined by the competition between quantum fluctuations and magnetoelastic coupling.

Introduction. The analysis of magnetism in parent compounds of iron-based superconductors (FeSCs) is an integral part of the program to understand the origin of superconductivity in these materials [1–12]. Parent compounds of Fe-pnictides are moderately correlated metals, [5, 13] whose magnetic order can be reasonably well understood within itinerant scenario [7–9, 14, 16] The locations and the shapes of the Fermi surfaces (FSs) select two possible ordered state with momenta $(0, \pi)$ and $(\pi, 0)$– in the Fe-only Brillouin zone (BZ) [9].

In each of these two states spins are ordered in a stripe fashion – ferromagnetically along one direction in 2D Fe-plane and antiferromagnetically in the other. Such an order breaks C_4 lattice rotational symmetry and causes pre-emptive spin-nematic order [15]. The same magnetic order is selected in the strong coupling approach, based on $J_1 - J_2$ model of localized spins with nearest and second-nearest neighbor spin exchange [17, 18]. The actual coupling in Fe-pnictides is neither truly small nor strong enough to cause Mott insulating behavior [13], which makes it extremely useful that the two descriptions agree.

There is one family of FeSCs - 11 Fe-chalcogenides $Fe_{1+y}Te_{1-x}Se_x$, in which smooth evolution between parent and optimally doped compounds does not hold. Magnetism in these materials changes considerably between $x = 0$ and $x \sim 0.5$, where the T_c is the largest. Near optimal doping magnetic fluctuations are peaked at or near $(0, \pi)$ and $(\pi, 0)$, as in Fe-pnictides, while magnetic order in a parent compound $Fe_{1+y}Te$ has very different momenta $\pm(\pi/2, \pm\pi/2)$ [19–23]. Upon doping, the spectral weight at $\pm(\pi/2, \pm\pi/2)$ decreases, and the spectral weight at $(0, \pi)$ and $(\pi, 0)$ increases [20]. The transport properties of $Fe_{1+y}Te$ are also quite different from those of parent compounds of Fe-pnictides: the resistivity, $\rho(T)$, of $Fe_{1+y}Te$ does not show a prominent increase with increasing T, but instead remains flat and even shows a small increase as T decreases [24]. ARPES studies of $Fe_{1+y}Te$ show that low-energy spectra are very broad [25], consistent with the notion that electrons are not propagating. These observations lead several groups to suggest that parent Fe-chalcogenides are more correlated than parent Fe-pnictides, and magnetism in $Fe_{1+y}Te$ can be understood by assuming that electrons are "almost" localized and interact magnetically via a Heisenberg exchange [26–29]. This model is indeed only an approximation as even for $Fe_{1+y}Te$ the localized scenario only works at low $T \leq 10K$, while some electronic itineracy is needed to describe the system at room temperature [22]. It has been suggested [30–32] that in all FeSc, a certain percentage of electronic states are localized and phase separated from itinerant electrons, and the percentage of localized states varies between different materials being the largest in parent Fe-chalcogenides. An alternative scenario for FeTe, which we don't discuss here, is orbital order [33].

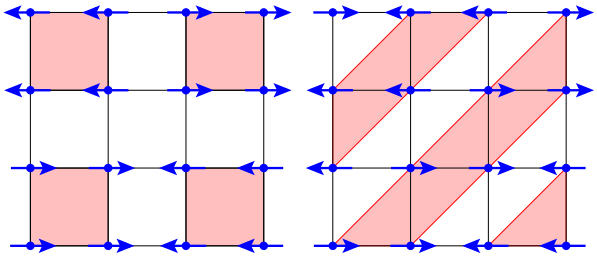

FIG. 1: The two possible collinear configurations for the $J_1 - J_2 - J_3$ model: (a) orthogonal double stripe (ODS) and (b) diagonal double stripe (DDS).

In this communication we apply the localized electron scenario to $Fe_{1+y}Te$ and verify whether the observed commensurate $\pm(\pi/2, \pm\pi/2)$ order can be obtained in a Heisenberg model with exchange interactions up to third neighbors. Classically, $\pm(\pi/2, \pm\pi/2)$ order is unstable with respect to a spiral order for any non-zero first neighbor exchange, unless one artificially breaks C_4 symmetry and sets interactions to be spatially anisotropic [21, 30]. We analyze the isotropic quantum Heisenberg model and show that quantum fluctuations do stabilize a commensurate order in some range of parameters. This, however, does not uniquely determine spin configuration as

a generic commensurate $\pm(\pi/2, \pm\pi/2)$ order is a superposition of two different $Q-$vectors: $\mathbf{Q}_1 = (\pi/2, -\pi/2)$, and $\mathbf{Q}_2 = (\pi/2, \pi/2)$: $\mathbf{S}(\mathbf{r}) = \mathbf{\Delta}_1 \cos \mathbf{Q}_1\mathbf{r} + \mathbf{\Delta}_1^{'} \sin \mathbf{Q}_1\mathbf{r} + \mathbf{\Delta}_2 \cos \mathbf{Q}_2\mathbf{r} + \mathbf{\Delta}_2^{'} \sin \mathbf{Q}_2\mathbf{r}$, with $|\mathbf{\Delta}_i| = |\mathbf{\Delta}_i^{'}| = \Delta$ and $\mathbf{\Delta}_1 \cdot \mathbf{\Delta}_2 = \mathbf{\Delta}_1^{'} \cdot \mathbf{\Delta}_2^{'} = 0$. In Fig. 1 we show two prototypical commensurate spin configurations – a single Q bi-collinear, diagonal double stripe (DDS) order ($\mathbf{\Delta}_1 = \mathbf{\Delta}_1^{'} = \mathbf{\Delta}$, $\mathbf{\Delta}_2 = \mathbf{\Delta}_2^{'} = 0$), which breaks C_4, and a double Q plaquette, or orthogonal double stripe (ODS) order ($\mathbf{\Delta}_1^{'} = \mathbf{\Delta}_2 = \mathbf{\Delta}$, $\mathbf{\Delta}_1 = \mathbf{\Delta}_2^{'} = 0$), which preserves C_4 symmetry, but breaks Z_4 translational symmetry (four plaquette states are obtained by moving a shaded square in Fig. 1a by one lattice site in either x or y direction [34]). The real-space configuration for both orders is "up-up-down-down" along both directions.

Most of previous theoretical and experimental works assumed that the commensurate order is DDS [10] and studied in detail the feedback from this order on electrons [21]. We argue that quantum fluctuations of spins actually select ODS order as a stable collinear state for a finite nearest-neighbor exchange J_1, while DDS state is unstable for any non-zero J_1.

There are several numerical and experimental evidence in support of our result. The ODS order has been found in exact diagonalization studies of $J_1 - J_2 - J_3$ model on clusters up to 36 spins [35] and in the mean-field studies of the $t - J$ model in Fe-chalcogenide $K_{0.8}Fe_{1.6}Se_2$ [36]. The authors of [22] argued that the form of the static structure factor $S(q)$ in the paramagnetic phase in $Fe_{1+y}Te$ shows that the system tends to order into ODS state. Another argument is the absence of a monoclinic distortion in $Fe_{1+y}Te$ above T_N, which would be expected (by the same reasons as in Fe-pnictides [15]) for DDS order as the latter breaks rotational in-plane C_4 symmetry. Furthermore, for $y > 0.12$, magnetic transition occurs at a higher temperature than the structural transition [37]. At the same time, below the structural transition the two diagonals in the ab plane becomes inequivalent, what lowers the energy of the DDS phase. We argue below that spin order in $Fe_{1+y}Te$ is determined by the competition between quantum fluctuations, which favor ODS state, and magnetoelastic effects. We present the results in one Fe cell in which is more convenient to distinguish between different spin configurations. The actual unit cell contains two Fe atoms because of non-equivalence of Fe on even add odd sites with respect to locations of Te. In two Fe cell, $(\pi/2, \pi/2)$ and $(\pi/2, -\pi/2)$ order becomes $(\pi, 0)$ and $(0, \pi)$ order, respectively.

Model. We follow earlier works and model magnetic interactions in $Fe_{1+y}Te$ by a $J_1 - J_2 - J_3$ Heisenberg model [27, 28, 35, 38]:

$$H = \sum_{n=1}^{3} J_n \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_{i+n} \qquad (1)$$

where J_1, J_2, and J_3 are antiferromagnetic exchange couplings between first-, second-, and third-nearest neighbors. For $Fe_{1+y}Te$ the values of J_1, J_2, and J_3 have been estimated in [27] and found to be in the range $J_3 > \frac{J_2}{2} \gg J_1$. In this limit, the classical ground state of (1) is a spiral with the pitch vector $\mathbf{Q} = (\pm q, \pm q)$, where $q = \arccos(\frac{-J_1}{2J_2+4J_3})$ [39]. At $J_1 = 0$, the model has an extensive degeneracy, and any order with momentum $\pm(\pi/2, \pm\pi/2)$ is the classical ground state, including DDS, ODS, and an infinite number of other four-sublattice states (Fig. 2). Quantum fluctuations lift degeneracy within sublattices made of even and odd spins, much like it happens in the well-known $J_1 - J_2$ model at $J_2 > J_1/2$ [40]. DDS and ODS states survive this selection, however for each of these two states some of classical "zero modes" are lifted by quantum fluctuations, and only true Goldstone modes remain.

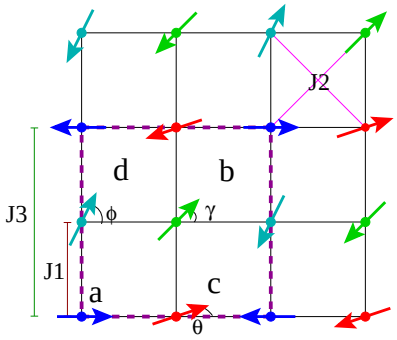

FIG. 2: Spin order in the classical $J_1 - J_2 - J_3$ model at $J_1 = 0$. Classically degenerate configurations form four sublattices, labeled as a, b, c, and d. A configuration with arbitrary γ, θ, and ϕ is a ground state.

We consider here what happens in the quantum model at a finite J_1. We show that quantum fluctuations modify the phase diagram and select classically unstable ODS state to be the ground state in some range of J_1, before a spiral order sets in, while DDS state remains unstable. The reason why ODS state is selected is related to how J_1 term couples low-energy excitations. In a classical case, any non-zero J_1 give rise to imaginary excitations near zero modes in both ODS and DDS states, what makes both of them unstable. In a quantum case, for DDS state, the modes, which are coupled by J_1, are the true Goldstone modes, which are not lifted by quantum fluctuations. As a result, DDS state remains unstable at $J_1 \neq 0$ in the quantum case as well. On the other hand, for ODS state classically unstable modes are accidental zero modes, whose energies are lifted by quantum fluctuations. As a result, perturbation theory in J_1 is not singular, and ODS state remains stable in a finite range of J_1. We verified that ODS state is the ground state in this range.

Large-S spin-wave calculations. We consider large value of spin S and study the role of quantum fluctuations within $1/S$ expansion. The computational steps

are presented in [41]. For $J_1 = 0$, spins on even and odd sites form two non-interacting sublattices, each described by $J_2 - J_3$ model. This model is identical to "$J_1 - J_2$" model, with diagonal hopping J_2 playing the role of "J_1" and third-neighbor hopping J_3 playing the role of "J_2". We use this analogy and borrow the results of the quantum analysis of "$J_1 - J_2$" model [40]. For $J_3 > J_2/2$ (which holds in $Fe_{1+y}Te$), quantum fluctuations select stripe configurations within each sublattice, i.e. the angle γ in Fig.2 is locked at $\gamma = 0$ or $\gamma = \pi$, and the angle θ is locked at $\theta = \phi$ or $\theta = \pi + \phi$. The states with $\gamma = 0$ and $\gamma = \pi$ are equivalent up to an interchange of X and Y directions, and below we set $\gamma = 0$. The collinear DDS and ODS states belong to the manifold of selected states and correspond to different locking of the angle ϕ between the nearest-neighbor spins: DDS state corresponds to $\phi = 0, \theta = \pi$ or $\phi = \pi, \theta = 0$, while ODS corresponds to $\phi = \theta = 0$ or $\phi = \theta = \pi$.

To analyze whether a generic state selected by quantum fluctuations at $J_1 = 0$ remains stable at a finite value of J_1, we need to know its excitation spectrum. At $J_1 = 0$, spins on even and odd sites are decoupled, each sublattice is described by its own bose field ($\alpha_{\mathbf{k}}$ for even sites and $\beta_{\mathbf{k}}$ for odd sites), and spin-wave excitations are described by

$$H_{sw} = S(\Omega_{\alpha\mathbf{k}}\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}} + \Omega_{\beta\mathbf{k}}\beta^\dagger_{\mathbf{k}}\beta_{\mathbf{k}}), \tag{2}$$

The classical spin-wave spectrum is the same for all selected states

$$\Omega_{\mathbf{k}} = S(A^2_{\mathbf{k}} - B^2_{\mathbf{k}})^{1/2},\ A_{\mathbf{k}} = 4J_3 + 2J_2\cos(k_x + k_y),$$
$$B_{\mathbf{k}} = 2J_3(\cos 2k_x + \cos 2k_y) + 2J_2\cos(k_x - k_y). \tag{3}$$

This spectrum contains nodes at $\pm(\pi/2, \pm\pi/2)$, but some of them are not symmetry-related and are lifted by quantum fluctuations. For the sublattice made of even sites, the order has momentum $\pm(\pi/2, -\pi/2)$ (Fig. 2 b), hence the true nodes are located only at these momenta, while the ones at $\pm(\pi/2, \pi/2)$ must be lifted. For the sublattice made out of spins at odd sites, the order has momentum $\pm(\pi/2, \pi/2)$ if we take $\theta = \phi$, like in the ODS, and $\pm(\pi/2, -\pi/2)$ if we take $\theta = \pi + \phi$, like in the DDS. Quantum fluctuations then must lift the nodes at $\pm(\pi/2, -\pi/2)$ and at $\pm(\pi/2, \pi/2)$ for the ODS and the DDS state, respectively. We computed quantum corrections to the spectrum in Eq. (3) within perturbation theory to order $1/S$ and indeed found that accidental nodes are lifted by quantum fluctuations and only true Goldstone modes remain [41].

We next set J_1 to be small but finite and consider which of stripe states, if any, remain stable. The qualitative reasoning is the following: a non-zero J_1 couples the two sublattices and adds to the Hamiltonian (2) the terms in the form $\alpha^\dagger_{\mathbf{k}}\beta_{\mathbf{k}}$ and $\alpha_{\mathbf{k}}\beta_{\mathbf{k}}$. For the DDS state (or, more accurately, for the DDS family of states as we keep ϕ as a parameter) the stripes on even and odd sites are directed parallel to each other, and the dispersions of $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ fields are identical, including $O(1/S)$ terms. The two dispersions are then gapless at the same momenta $\mathbf{k} = \pm(\pi/2, -\pi/2)$. Around these $\mathbf{k}$ points, the perturbation theory in J_1 is singular, as there is no symmetry requirement which would force the coupling to vanish at $\pm(\pi/2, -\pi/2)$. As a result, the excitations become purely imaginary close enough to $\pm(\pi/2, -\pi/2)$, which implies that the DDS states are unstable at any non-zero J_1. On the other hand, for the ODS family of states, the dispersions $\Omega^\alpha_{\mathbf{k}}$ and $\Omega^\beta_{\mathbf{k}}$ have nodes at different momenta, $\pm(\pi/2, -\pi/2)$ and $\pm(\pi/2, \pi/2)$, respectively. Because of this disparity, perturbation theory near either $\pm(\pi/2, -\pi/2)$ or $\pm(\pi/2, \pi/2)$ is not singular, and corrections in J_1 only gradually shift the values of spin-wave velocities thus keeping ODS states stable.

We verified this reasoning by explicit calculations. We obtained the J_1-induced interaction in terms of the original Holstein-Primakoff bosons and re-expressed it in terms of $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ bosons from Eq. (2), which are related to the original ones by Bogoliubov transformation. The $u_{\mathbf{k}}v_{\mathbf{k}}$-coefficients of this transformation dress up the interaction terms. For DDS states, expanding the Hamiltonian near the true Goldstone points at $(\pi/2, -\pi/2)$ as $\mathbf{k} = (\pi/2, -\pi/2) + \tilde{\mathbf{k}}$ we obtain $H_{DDS} = H_{sw} + \delta H_{DDS}$, where H_{sw} is given by (2) with

$$\Omega^\alpha_{\tilde{\mathbf{k}}} = \Omega^\beta_{\tilde{\mathbf{k}}} \approx 4S\sqrt{J_3(2J_3 + J_2)}(\tilde{k}^2_x + \tilde{k}^2_y - 2a\tilde{k}_x\tilde{k}_y)^{1/2}, \tag{4}$$

where $a = \frac{J_2}{2J_3} < 1$, and

$$\delta H_{DDS} = \Delta^{DDS}_{\tilde{\mathbf{k}}}(\alpha^\dagger_{\tilde{\mathbf{k}}}\beta_{\tilde{\mathbf{k}}} + \alpha_{\tilde{\mathbf{k}}}\beta_{-\tilde{\mathbf{k}}} + h.c) \tag{5}$$

where

$$\Delta^{DDS}_{\tilde{\mathbf{k}}} = \frac{J_1 S}{2}\left(\frac{2J_3 + J_2}{J_3}\right)^{1/2}\frac{\tilde{k}_y - \tilde{k}_x}{(\tilde{k}^2_x + \tilde{k}^2_y - 2a\tilde{k}_x\tilde{k}_y)^{1/2}} \tag{6}$$

The coupling term remains finite when $\tilde{k}_{x,y}$ tends to zero, except for special directions. Diagonalizing (5) we find that at low enough $\tilde{k}$ one of the two solutions is $E^2_{\tilde{k}} \approx -2\Omega^{\alpha(\beta)}_{\tilde{\mathbf{k}}}|\Delta^{DDS}_{\tilde{\mathbf{k}}}|$. A negative $E^2_{\tilde{k}}$ implies that fluctuations around a DDS state grow exponentially with time and make this family of states unstable. Note that the sign of J_1 does not matter – DDS state is unstable for both $J_1 > 0$ and $J_1 < 0$.

For the ODS states the situation is different because near any of the points $\pm(\pi/2, -\pi/2)$ or $\pm(\pi/2, \pi/2)$, the zero in one of the spin-wave branches is lifted by quantum fluctuations. For example, near $(-\pi/2, \pi/2)$ expanding of the Hamiltonian again gives $H_{ODS} = H_{sw} + \delta H_{ODS}$, however now only $\Omega^\alpha_{\tilde{\mathbf{k}}}$ is gapless, while $\Omega^\beta_{\tilde{\mathbf{k}}}$ is gapped with the gap of the order $1/S$. The interaction term δH_{ODS} has the same form as in (5), but with

$$\Delta^{ODS}_{\tilde{\mathbf{k}}} = 2J_1S^2(2J_3 + J_2)\frac{\tilde{k}_y - \tilde{k}_x}{(\Omega^\alpha_{\tilde{k}}\Omega^\beta_{\tilde{k}})^{1/2}} = O\left(J_1S^{3/2}|\tilde{k}|^{1/2}\right). \tag{7}$$

Diagonalizing H_{ODS} we find two solutions,

$$E^2_{1,2} = \frac{1}{2}\Big((\Omega^{\alpha}_{\tilde{k}})^2 + (\Omega^{\beta}_{\tilde{k}})^2 \pm \sqrt{((\Omega^{\alpha}_{\tilde{k}})^2 - (\Omega^{\beta}_{\tilde{k}})^2)^2 + 16(\Delta^{ODS}_{\tilde{\mathbf{k}}})^2\Omega^{\alpha}_{\tilde{k}}.\Omega^{\beta}_{\tilde{k}}}\Big). \quad (8)$$

One of the solutions is gapped to order $1/S$, the other is linear in $\tilde{k}$ with a stiffness which differs from its value at $J_1 = 0$ by $O(J_1 S/J_3)$. We see that the ODS states are stable (for any ϕ) as long as $J_1 S/J_3$ is small. This result again holds for any sign of J_1. As J_1 increases, quantum fluctuations compete with the tendency of a classical system to form a spiral state with some $\mathbf{k}$ different from $(\pi/2, \pm\pi/2)$ To estimate how long ODS state survives, we found at which J_{1c} the velocity of the gapless mode in (9) changes sign and found, using $J_2 = 1.55J_3$ [27], $J_{1,c} = 0.21J_3$, which is about the same as $J_1 \approx 0.2J_3$ obtained in [27]. A similar estimate is obtained if we take the spin-wave branch gapped by quantum fluctuations at $(\pi/2, -\pi/2)$, expand in $\tilde{k}$, and obtain $J_{1,c}$ at which this spectrum becomes unstable at a finite $\tilde{k}$.

On a more careful look, we find that the ODS spin order allows for J_1-induced umklapp processes, which also renormalize the dispersions of the ODS states. Indeed, because ODS state breaks Z_4 translational symmetry, the J_1 interaction contains additional terms with momentum transfer in multiples of π along each axis. Near $k = (\pi/2, -\pi/2)$, the most relevant of such umklapp terms is the one which connects a gapless $\alpha_{\tilde{k}}$ boson at $(\pi/2, -\pi/2)$, and a gapless $\beta_{\tilde{k}}$ boson at $(\pi/2, \pi/2)$. However, because breaking of Z_4 is equivalent to breaking local inversion symmetry (a reflection around one column or one row in Fig. 1a), the umklapp vertices $\Delta^{U,ODS}_{\tilde{\mathbf{k}}}$ contain extra momentum gradient compared to non-umklapp vertices. In explicit form, we find at small $\tilde{\mathbf{k}} = \mathbf{k} - (\pi/2, -\pi/2)$,

$$\Delta^{U,ODS}_{\tilde{\mathbf{k}}} = -i\frac{J_1}{4}\left(\frac{\Omega^{\alpha}_{\tilde{k}}\Omega^{\beta}_{\tilde{k}+\bar{Q}}}{4J_3^2 - J_2^2}\right)^{1/2} \cos\phi \ , \quad (9)$$

where $\Omega^{\alpha}_{\tilde{k}}, \Omega^{\beta}_{\tilde{k}+\mathbf{Q}} = 4S(J_3(2J_3 \pm J_2))^{1/2}(\tilde{k}_x^2 + \tilde{k}_y^2 \mp 2\tilde{k}_x\tilde{k}_y)^{1/2}$ and the angle ϕ specifies the spin order within the ODS family of states. We see that $\Delta^{U,ODS}_{\tilde{\mathbf{k}}}$ scales linearly with $\tilde{\mathbf{k}}$, i.e., is of the same order as $\Omega^{\alpha\beta}_{\tilde{k}}$. We computed the corrections to spin-wave velocity and found that they scale as $J_1/\sqrt{4J_3^2 - J_1^2}$, i.e., are small. At the same time, we see from the Eq.(9) that $\Delta^{U,ODS}_{\tilde{\mathbf{k}}}$ depends on the angle ϕ. Respectively, the corrections to the ground state energy also depend on ϕ and should select which state within the ODS family has the lowest energy. The computation is straightforward and yields $\Delta E_{gr} = -A\cos^2\phi$, with $A > 0$. We see that the collinear ODS state, for which $\phi = 0$ or π, has the lowest energy.

Experimental signatures of ODS state. Because the ODS state does not break C_4 translational symmetry, it does not cause a pre-emptive structural transition, in contrast to parent compounds of other FeSCs [15]. The data for $Fe_{1+y}Te$ show that the structural transition does not occur above T_N – it either happens at T_N, for $y < 0.12$, or below T_N for $y > 0.12$ (see Ref.[37]). The pre-emptive structural transition develops only in doped compounds $Fe_{1+y}Te_{1-x}Se_x$ [24]). The DDS and ODS states have different structure factors $S(q)$: the one for ODS state has four identical peaks at $(\pm\pi/2, \pm\pi/2)$, while the one for DDS state only two peaks at $(\pi/2, -\pi/2)$ and $(-\pi/2, \pi/2)$. The measured $S(q)$ is C_4-symmetric and has four peaks, consistent with ODS, but the absence of the anisotropy $S(q)$ could be due to the twinning of the crystal. However, as the magnetic domain's structure of the crystal can be controlled using polarized neutrons, the careful analysis of the neutron scattering data might dissect the contribution from different domains. The authors of Ref. [22] made another argument that, even in a twinned crystal, the form of $S(q)$ throughout the Brillouin zone differentiates between strong DDS and ODS fluctuations, and argued that their data are more consistent with tendency towards ODS order. This again agrees with our results. At the same time, the fact that monoclinic distortion develops right at T_N, lowers the energy of the DDS state compared to the ODS state because monoclinic distortion and DDS order break the same symmetry, and there is additional negative contribution to the energy of the DDS state due to magnetoelastic coupling [44]. It is possible that the type of spin order in $Fe_{1+y}Te$ is determined by the competition of quantum fluctuations and magnetoelastic coupling.

Summary. In this communication we analyzed the type of magnetic order in $Fe_{1+y}Te$ – the parent compound in a family of Fe-chalcogenide superconductors. The magnetic order in this material is different from other parent compounds of FeSCs – spins are ordered in up-up-down-down fashion (Fig. 2). The tendency towards Mott physics is stronger in $Fe_{1+y}Te$ than in other parent compounds of FeSCs, suggesting that the magnetic order can be reasonably well understood within the localized scenario, by solving the Heisenberg model with exchange interaction up to third neighbors. It was thought before that the ordered up-up-down-down spin configuration is diagonal double stripe. We argued, based on our analysis of quantum fluctuations, that such a state is unstable, but another up-up-down-down state – the plaquette state is stable and is the ground state in some parameter range. The issues which deserves further study are the competition between quantum fluctuations and structural distortion, and the role of interstitial Fe atoms which tend to destabilize any collinear spin configuration.

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