Phase transitions in classical biquadratic Heisenberg model for strained iron pnictides

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Based on the notion of magnetically driven nematicity, we study the phase transitions in a frustrated classical Heisenberg model with biquadratic and anisotropic exchange interactions on square lattice by means of Monte Carlo simulations, in order to understand the uniaxial strain effect in BaFe2As2. The variation of both structural and antiferromagnetic transition temperatures with uniaxial stress reported in experiments can be qualitatively reproduced by including the exchange anisotropy, suggesting that the anisotropy may be responsible for the strain effect on the phase transitions. © 2015 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4906180]

Over the past decades, understanding the characters of magnetic interactions in iron pnictides becomes more and more important because the pairing mechanism in these materials probably involves spin fluctuations.1,2 It was experimentally reported that the collinear antiferromagnetic (AFM) order with a wave vector (π, 0) (the spin configuration is shown in Fig. 1(a)) can be developed in undoped iron pnictides below the critical point $T_N$. Moreover, the magnetic transition is universally accompanied with an orthorhombic lattice distortion (the longer lattice constant along the AFM direction), and a structural transition from the tetragonal phase to the orthorhombic phase occurs at an equal or slightly higher temperature $T_S \geq T_N$.3 In order to understand the relationship between these two transitions, the mechanism of magnetically driven nematicity is proposed, although no consensus has been reached.4–6 In this pure electromagnetic viewpoint, the nematic order can be developed before the stabilization of the long range AFM one and drives the structural transition.7 Furthermore, the origin of the nematic state has been studied within the effective spin models, and the biquadratic interaction is suggested to be very important for the nematic order.8–10

Moreover, the prominent effect of the uniaxial pressure in modulating the structural and magnetic phases in iron pnictides has been reported in recent experiments.11–13 For example, it was observed in neutron scattering experiments that both the structural and magnetic transition temperatures increase with the increasing compressive stress applied along the shorter axis. Up to now, several theoretical works that explain this interesting phenomenon have been reported.14–16 For example, the study of magneto-elastic model suggests that the magneto-elastic coupling can make the AFM bonds longer than the ferromagnetic (FM) ones in the AFM state, and in turn results in the change of the transition temperatures under the uniaxial strain.14 Furthermore, the classical Heisenberg spin model has been analytically studied using the effective classical field theory and well reproduced recent experimental results.15 In a most recent first principles calculation of BaFe2As2, the phase transition from the (π, 0) AFM state to the (0, π) one (Fig. 1) is predicted at the critical uniaxial stress when the sign of the orthorhombicity is changed. This phenomenon is qualitatively explained from the competition between the magneto-elastic coupling and the applied stress, as uncovered by the study on the Ginzburg-Landau model.16

All these works demonstrate the important role of the magneto-elastic coupling in understanding the strain effects in iron pnictides and suggest that the description in terms of localized classical spins may be sufficient to capture the essential physics, although all these materials are metallic. Furthermore, the strong magneto-elastic interaction may lead to the in-plane magnetic anisotropy, as experimentally revealed in some other systems.17 As a matter of fact, earlier experiments have revealed a strong anisotropy of the nearest-neighbor (NN) exchange in iron superconductors.18 In addition, it is expected that the magnitude of the anisotropy should be modulated with the variation of lattice temperatures.

FIG. 1. In-plane crystal structure and spin configurations in the (a) (π, 0) AFM state and (b) (0, π) AFM state. Solid and empty circles represent the up-spins and down-spins, respectively.

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distortion as a result of the varying stress. Thus, it becomes essential to make clear the effect of the exchange anisotropy on the phase transitions in iron pnictides in order to understand the strain effect. However, as far as we know, few works on this subject have been reported, although the anisotropic exchange interaction has been considered in some earlier works.\textsuperscript{19}

In this work, we study the phase transitions in strained BaFe\textsubscript{2}As\textsubscript{2} based on the well-known two-dimensional AFM J\textsubscript{1}–J\textsubscript{2} model\textsuperscript{20} on the square lattice which is related to the Fe monolayers in the iron based superconductors. Furthermore, in order to reflect the features of the strained lattice and some other properties in real materials, a modified model has to be developed, and its Hamiltonian can be written as

\[
H = \sum_i (J_i^x S_i^x S_{i+\alpha}^x + J_i^y S_i^y S_{i+\gamma}^y) + J_2 \sum_{\langle i,j \rangle} S_i \cdot S_j - D \sum_i (S_i^z)^2 - J_K \sum_{\langle i,j \rangle} (S_i \cdot S_j)^2.
\]

In the above model Hamiltonian, the first term is the anisotropic AFM exchange interaction between the NN spins S with the average J\textsubscript{1} = 1 (J\textsubscript{i}^x + J\textsubscript{i}^y = 2). The second term is the AFM exchange interaction between next-nearest-neighbor (NNN) spins with J\textsubscript{2} = 0.75. Thus, the collinear AFM state can be developed at low temperatures (T) due to the strong competition between the NN and NNN exchange interactions in this frustrated spin model.\textsuperscript{21} The third term is the single-ion anisotropy (z axis is the easy axis, and S\textsubscript{ij} is the z component of S\textsubscript{i}) with the constant D = 0.01, which is introduced here to draw an analogy with the effect of the inter-plane exchange interaction and to stabilize the long range magnetic order.\textsuperscript{22} At last, the additional positive biquadratic interaction J\textsubscript{K} = 0.1 between NN spins is also taken into account because this term is proved to be very important and cannot be simply neglected in any models for pnictide superconductors.\textsuperscript{23} In addition, the Boltzmann constant is set to unity, and a parameter \( \Delta = (J_1^y - J_1^x)/2 \) is defined to characterize the degree of the NN exchange anisotropy.

Our simulation is performed on an L \times L (L = 72, unless stated elsewhere) square lattice with periodic boundary conditions using the standard Metropolis algorithm and temperature exchange method.\textsuperscript{24} We take an exchange sampling after every 10 standard Monte Carlo (MC) steps. Typically, the initial 10\textsuperscript{5} MC steps are discarded for thermal equilibrium and another 10\textsuperscript{5} MC steps are retained for statistic averaging of the simulation. In either of the collinear (\( \pi, 0 \)) and (0, \( \pi \)) AFM states, the lattice can be divided into two sublattices, and the spins within each sublattice are parallel to each other. Thus, the spin average of each sublattice (with solid or empty circles) \( M \) is calculated to characterize the collinear AFM spin orders.\textsuperscript{21} Besides, the spin nematic order parameter can be defined as:

\[
Q = \frac{1}{N} \left| \sum_i (S_i \cdot S_{i+\alpha} - S_i \cdot S_{i+\gamma})/2N \right|, \tag{2}
\]

where N is the number of sites. Finally, \( T_{N} \) and \( T_{S} \) can be estimated from the positions of the peaks in the magnetic susceptibility \( x_{M} \) and the nematic susceptibility \( x_{Q} \), respectively.

It is expected that the anisotropy should be enhanced (\( \Delta \) increases) with the enhanced lattice distortion under the compressive stress applied along the shorter axis. Fig. 2 shows the simulated results for various positive \( \Delta \). Spin average \( M \) quickly increases from the baseline when \( T \) falls down to the critical point, as shown in Fig. 2(a), demonstrating the stabilization of the long range (\( \pi, 0 \)) AFM order. In addition, it is clearly shown that the magnetization curve shifts toward high T side when \( \Delta \) is increased. The AFM transition temperatures for various \( \Delta \) are estimated from the calculated \( x_{M} \), as shown in Fig. 2(b). It is clearly shown that \( T_{N} \) increases with the increase of \( \Delta \), indicating that the AFM order can be further enhanced by the exchange anisotropy. On the other hand, the effect of \( \Delta \) on the nematic transition is also studied, and the corresponding results are shown in Figs. 2(c) and 2(d). With decreasing \( T \), the nematic order parameter \( Q \) increases, indicating the phase transition from the high-T paramagnetic (PM) state to the nematic one. In addition, the phase transition shifts toward high T side with the increase of \( \Delta \), as demonstrated in the calculated \( x_{Q} \) in Fig. 2(d). As a matter of fact, some of the estimated phase transition points have been double checked by the calculated Binder’s fourth-order cumulant \( U_{L} = 1 - \langle M^4 \rangle/3 \langle M^2 \rangle^2 \), where \( \langle \ldots \rangle \) is the ensemble average.\textsuperscript{26} As an example, Fig. 3 shows the simulated \( U_{L} \) as a function of \( T \) at \( \Delta = 0.15 \) for different lattice sizes. From the well common defined crossing point, \( T_{N} \) is estimated to be 0.63(5), which is almost the same as that estimated from \( x_{M} \) at \( L = 72 \). Thus, it is demonstrated that the finite-size effect on the phase transitions in this system is nearly negligible and never affect our conclusion.

In order to reveal the physics underlying the enhancements of the nematic and AFM orders with increasing \( \Delta \), one may give a qualitative discussion from the energy landscape. It is well known that the collinear AFM order can be developed at low \( T \) for \( J_2/J_1 > 1/2 \) in the well-known
Fig. 3. Binder’s fourth-order cumulant $U_L$ as a function of $T$ for different lattice sizes at $\Delta = 0.15$.

two-dimensional AFM $J_1$-$J_2$ model. On one hand, it is noted that the variation of the NN exchange energy per site of the systems with the perfect collinear AFM order with the exchange anisotropy $\Delta$ should be $-2\Delta$. As a result, the energy gain from the NN exchange interaction due to the transition from the PM order to the AFM or nematic one significantly increases with increasing $\Delta$. On the other hand, the variation of the other couplings (the NNN exchange interaction, the single-ion anisotropy, and the biquadratic interaction) due to this transition is almost independent on $\Delta$. In consequence, the effective couplings in the AFM and nematic orders can be enhanced by positive $\Delta$, leading to the increases of $T_N$ and $T_S$. As a summary, the simulated phase diagram for positive $\Delta$ is shown in Fig. 4. The experimentally reported increases of the transition temperatures with applied uniaxial stress in BaFe$_2$As$_2$ can be qualitatively reproduced, suggesting that the exchange anisotropy caused by the lattice distortion under uniaxial pressure may play an important role in the phase transitions in this material. In addition, it is observed that $T_S$ increases faster than $T_N$, demonstrating that the nematic order can be developed in advance of the AFM order, compatible with the experimental observation. Thus, an obvious region (with yellow background) in which the nematicity is ordered but the magnetism remains disordered is observed in the phase diagram, strongly supporting the notion of the magnetically driven nematicity in iron pnictides. Furthermore, it is worth noting that itinerant electrons may also contribute to the strain effect, which will be discussed in detail elsewhere.

Most recently, it was predicted in density functional theory calculations that the sign of the orthorhombicity is changed at a critical uniaxial stress in BaFe$_2$As$_2$ and CaFe$_2$As$_2$, leading to the switch between the FM and AFM directions. It is reasonable to expect that the sign of $\Delta$ should be changed with the predicted orthorhombicity jump. One may note from the model Hamiltonian that the $x$ and $y$ axes are symmetric for $\Delta = 0$, and the sign change of the in-plane anisotropy $\Delta$ should generate a 90° rotation of the collinear AFM order. This viewpoint has been confirmed in our simulation, although the corresponding results are not shown here. Thus, in this report, the exchange anisotropy is suggested to play an important role in modulating the phase transitions with applied uniaxial pressure in iron pnictides, and the minimal model captures the essential physics in these materials.

In conclusion, we have studied the strain effect of the iron pnictides based on the classical biquadratic Heisenberg model. It is observed that both the antiferromagnetic and nematic transitions shift toward high temperature side with the increase of the exchange anisotropy, which is in qualitatively consistent with earlier experimental report. Thus, such an exchange anisotropy caused by the lattice distortion is suggested to be one of the origins of the variation of the transition temperatures with uniaxial stress. In addition, the switch of the ferromagnetic and antiferromagnetic directions can also be realized when the sign of the exchange anisotropy changes, which confirms the earlier first principles prediction for strained BaFe$_2$As$_2$.

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