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Spin–lattice coupling in iron-pnictide superconductors: a model for possible continuous phase transition

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Abstract

A systematic study of the dependence of the local magnetic moment, *M*, on the Fe-Pn layer separation has been carried out. Within the Ehrenfest classification of orders of phase transition, we propose a continuous (>2) phase transition for studying the dependence of *M* on the Fe-Pn layer separation. Our model is tested with available experimental data.

Keywords: Fe-Pnictide superconductors, Magnetic moment, Continuous phase transition, Euler-Lagrange equation, Ehrenfest theory, Ginzburg-Landau theory

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Background

The recent discovery of superconductivity in iron pnictides (FePn) [1-3] has led to enormous research in trying to understand the origin of the superconductivity. Although the origin of the superconductivity in Fe-based superconductors is not yet clear, there has been some proposals (e.g., spin fluctuation, Fermi surface nesting, etc.) to explain it. Unlike in high-T_c cuprate superconductors where phonon mediation has been proposed, in Fe-based superconductors, this scenario is mostly unlikely [2]. This is evidence since though the antiferromagnetic correlation may be suppressed by doping, spin interactions are still present in FePn superconductors [2]. Also, spectroscopy study of Fe-based superconductors shows the absence of strong electron correlation [4-6]. Thus, the origin of the observed superconductivity may not be due to Mott-Hubbard physics. We can thus speculate that the superconductivity observed in FePn is local and dynamically spin polarized due to strong Fe spin fluctuations. These spin fluctuations in the spin channel of Fe may be the 'glue' for superconductivity to thrive in FePn.

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In a typical FePn superconductor, layers of pnictogen (Pn), e.g., arsenic (As) normally sandwich the Fe atom layers. Hence, a slight change in the interlayer distances of Fe-Pn leads to a corresponding change in the magnetic moment of Fe [7]. This is well known since the magnetic moment of transition metals depends on volume [8]. This magneto-volume effect, which is due to Pauli exclusion principle, leads to lattice anharmonicity.

Also, in layered structure of bulk materials (in quasi two-dimensional systems), Cronström and Noga [9] noted that some rather unexpected properties (new mean field solution) are observed at non-zero temperature. Specifically, they observed that in these layered systems, the phase transition is of the third order and as such cannot be described by the ordinary phenomenological Ginzburg-Landau theory, which is developed for phase transition of the second order. Moreover, there are no known physical phenomena prohibiting the existence of phase transitions of order greater than 2. These higher orders of phase transition certainly exist as their non-detection is simply the general belief that all orders of phase transition greater than 2 can always be attributed to field fluctuations [10,11]. We argue that this generalization is hasty as this deviation is large enough to be solely accounted for by field fluctuations.

Khasanov et al. [12] further confirmed that there is Bose-Einstein condensate (BEC)-like phase in SmFeAsO and NdFeAsO. Since in systems with BEC-like phase transition, the relation $\int_0^{T_c}[\delta C_e(H,T)/T]dT = 0$ which is valid for the second-order phase transition is violated (see, e.g., in spin glasses [13], ferromagnetic and antiferromagnetic spin models with temperature-driven transitions [14]), we speculate that the normal Landau theory developed for the second-order phase transition may not adequately account for the physics of phase transitions in these 'peculiar' systems. Motivated by this, we developed a Landau-like theory based on Ehrenfest classification of orders of phase transition [15,16]. Ehrenfest thermodynamic theory is in terms of the ordered state free energy near the phase boundary and the function of the system in terms of the local free energy [10]. We generalize this theory and apply it to study the dependence of the local magnetic moment, M, on the Fe-As layer separation, z.

Theoretical background

Mean field theories (in this case Ehrenfest theory) have been a vital tool for studying diverse range of systems, including, superconductors [17]. The validity of Ehrenfest classification of orders of phase transition has been a subject of debate [18,19]. However, as shown by Hilfer [20], the singular part of the local free energy within a restricted path through the critical point in terms of the finite difference quotient can be analytically continued in the orders of the phase transition. This allows one to classify continuous phase transition precisely according to their orders. Moreover, the Beerezinskii-Kosterlitz-Thouless transition is of infinite order [21].

The dependence of the magnetic moment, M, (spin–lattice coupling) on the Fe-Pn layer separation is determined by the function (the magnetic free energy functional), $F[z, \langle M\rangle]$ where $\langle M\rangle$ is the local magnetic moment. However, F must be invariant under the symmetry group (e.g., *Abelian Higgs model*) [10,22] of the disordered phase in order to minimize the total energy [10,11]. In general, F is a very complicated function of $\langle M\rangle$. To make $\langle M\rangle$ spatially uniform, in the ordered phase, we essentially for all cases redefine it. This suggests that F be expressed in terms of a local free energy density, $f[z, \langle M\rangle]$ (the local magnetic free energy) which is a function of the field at the point 'z' only and also a part producing the energy cost for deviations from spatial uniformity. After coarse graining in its simplest form, based on lattice formulation of Ginzburg-Landau theory [10,11],

$$F = \int d^d z f[T, M(z)] + \frac{1}{2}\int d^d z\, c(\nabla M(z))^2 \qquad (1)$$

Equation 1 can be generalized to Landau-like form for orders of phase transition >2 as

$$F_p(M,z) = \int d^d r |M|^{2(p-2)}\{-a_p|M|^2 + b_p|M|^4 + c_p|\nabla M|^2 + |M|^2\Gamma(M,z)\} \quad \forall p > 2 \qquad (2)$$

where p is the order of the phase transition, $a_p = a_o(1 - H/H_c)$, and $b_p >> 1$. The parameter $\Gamma(M, z)$ has embedded in it the spin–lattice interaction energy, $F_{s\text{-}l}$, given by

$$F_{s-l} = |M|^2\Gamma(M,z) = |M|^2\left[\alpha(z-z_c)^{2(p-2)}\right] \quad \forall p > 2 \qquad (3)$$

where z is the Fe-Pn layer distance (inter-atomic separation); z_c, the critical point; and α, a material dependent parameter that is always less than 1. Note that $\Gamma(M, z) = \alpha(z - z_c)^{2(p-2)}$ has the same symmetry property as M.

Solution of the magnetic functional of the system

Equation 2 is the model equation we are proposing for studying the dependence of M on the Fe-Pn inter-atomic separation. For the third-order phase transition, $p = 3$, Equation 2 reduces to

$$F_3(M,z) = \int d^d r |M|^2\{-a_3|M|^2 + b_3|M|^4 + c_3|\nabla M|^2 + |M|^2\Gamma(M,z)\} \quad \forall p = 3 \qquad (4)$$

Case I: neglecting the gradient term

If we neglect the gradient term, we can write the local magnetic free energy from Equation 2 as follows:

$$f_3 = -a_3M^4 + b_3M^6 + \alpha(z-z_c)^2M^4 \qquad (5)$$

On minimizing Equation 5 with respect to M, we obtain

$$M^2 = \frac{2}{3b_3}\left[a_3 + |\alpha|(z-z_c)^2\right] \qquad (6)$$

The average local free energy then becomes

$$f_3 = \left[\frac{2}{3b_3}\left(a_3 + |\alpha|(z-z_c)^2\right)\right]^2\left\{\frac{5}{3}|\alpha|(z-z_c)^2 - \frac{1}{3}a_3\right\} \qquad (7)$$

Case II: presence of gradient term

Assuming we incorporated the gradient term to the local magnetic free energy of Equation 2, using variational principle, after scaling, we obtain the Euler-Lagrange equation for M as follows:

$$\phi^5 - \phi^3\left[1-\alpha(z-z_c)^2\right] - \phi|\nabla\phi|^2 - \phi^2\left|\nabla^2\phi\right| = 0 \tag{8}$$

The magneto-volume effect due to lattice anharmonicity leads to phonon softening. The magneto-elastic free energy due to lattice anharmonicity in the third-order phase transition is given by

$$F_{m-e} = \left[\alpha(z-z_c)^2\right]M^4 + \kappa(z-z_c)^2 = \left[\alpha(z-z_c)^2\right]\left\{\frac{2}{3b_3}\left[a_3+|\alpha|(z-z_c)^2\right]\right\}^2 + \kappa(z-z_c)^2 \tag{9}$$

where κ is the spin–lattice interaction. On minimization with respect to the Fe-Pn layer separation, z with $z = z_{ps}$, we obtain the pnictide position, z_{ps},

$$\left(z_{ps}-z_c\right)^2(3\alpha+a_3)\left[a_3+|\alpha|\left(z_{ps}-z_c\right)^2\right]+\frac{9b_3^2}{4\alpha}\kappa=0 \tag{10}$$

The elastic stiffness by definition is the second derivative of the magneto-elastic free energy with respect to z. Thus, we obtain the renormalized elastic stiffness as

$$\kappa' = \kappa\left[1-\frac{\alpha^2}{9\kappa b_3^2}\left(z_{ps}-z_c\right)^4(3\alpha+a_3)\left\{1-6\left(z_{ps}-z_c\right)\right\}\right] \tag{11}$$

Validity of our model

Using the experimental data [23-25], we calculate the magnetic moment, M, using our model Equation 6. The plot of experimental critical temperature against our calculated M (μ_B) is given in Figure 1. Observe that there is strong correlation between T_c and M. Most significantly, our model captured the range of values of magnetic moment of Fe in Fe-Pn superconductors. As it is evidence from the plot, the magnetic moment ranges from 0.59 to 0.73 μ_B. The experimentally measured values of magnetic moment of Fe in LaOFeAs, for instance, ranges from 0.30 to 0.64 μ_B [24,25].

Figure 2 shows the plot of magnetic moment as a function of Fe-Pn layer separation as obtained from our developed model equation. The plot gave a_3 = −1.5 Å^2, $(1 \le b_3 \le 2.2)\mu_B^{-2} A^{2o}$, α = 0.98, and z_c = 1.224 Å. The observed quantum critical point (QCP) near z_c = 1.224 Å may be attributed to spin splitting of the bands by strong local exchange interaction. As has been shown by Egami et al. [23], z_c is a signature of the generalized Stoner QCP. Our model reproduced this argument nicely, and in particular, our z_c is very close to the value of 1.23 Å for the collapsed phase in $CaFe_2As_2$ [26].

From Figure 2, away from the QCP, observe that there is almost perfect linear correlation between our calculated magnetic moment and the Fe-Pn inter-atomic separation. This is in agreement with our earlier assertion of high dependence of the magnetic moment, M, on the Fe-Pn layer separation. Our observation is in agreement with the experimental observations of de la Cruz and co-workers [27] in their work on $CeFeAs_{1-x}P_xO$. As already pointed out, α in Equation 6 is highly material dependent. If we let α to be negative, that reverses the model plot in Figure 2. In this scenario, our observation is in agreement with that of first principle prediction of Yildirim [28].

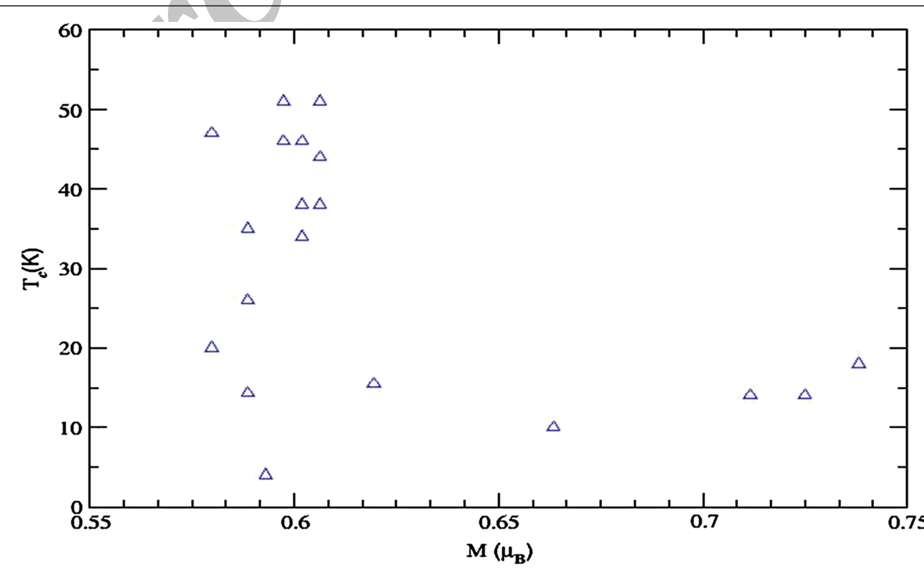

Figure 1 Experimental critical temperature. Superconducting experimental critical temperature, T_c, from [22] against the calculated M obtained using Equation 6 at the critical point where a_3 vanishes.

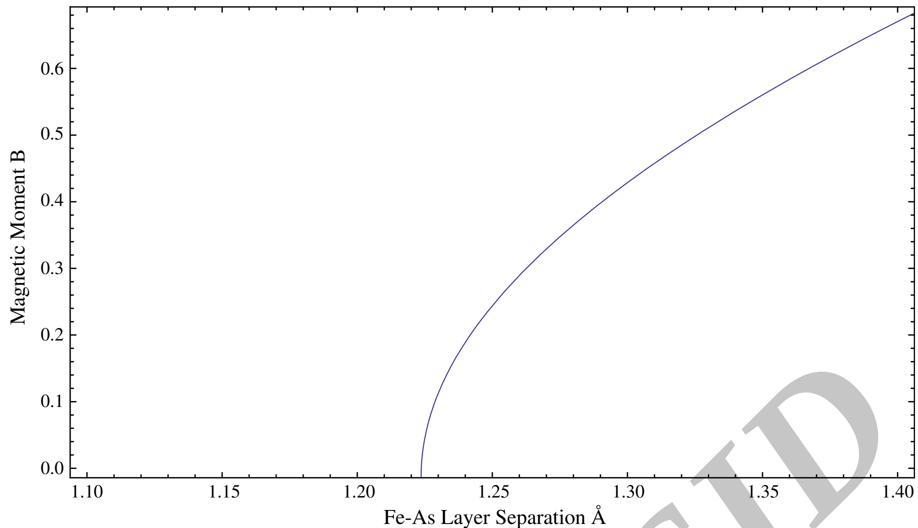

Figure 2 Magnetic moment as a function of Fe-Pn layer separation. Dependence of M (μ_B) on the Fe-As inter-atomic separation, z (Å), as obtained using our model Equation 6. Our model predicted correctly the trend of the experimental data, and we predicted a Stoner QCP at z_c = 1.22 Å.

Conclusion

We have developed model equations for investigating the dependence of the local magnetic moment of the Fe-Pn (e.g., Fe-As) layer separation. We find that the Fe-Pn layer separation depends strongly on the critical temperature T_c. FePn superconductors are sparsely electron-correlated system; thus, the normal electron–phonon coupling which is predominant in high-T_c cuprates is highly minimal. As has been observed, lattice anharmonicity leads to magneto-volume effects. Thus, spin-fluctuation mediated through the spin channel may be relevant in understanding the origin and nature of the observed high T_c in FePn superconductors.

We speculate that the observed strong correlation between T_c and M is due to the fact that the superconducting critical temperature T_c depends very sensitively on the iron pnictogen (i.e., Fe-Pn-Fe) bond angle, which in turn depends on the Fe-Pn layer separation [29]. This observation is in agreement with the fact that the bonding of the pnictogen (e.g., As) atoms changes dramatically as a function of magnetic moment [28,30]. This is supported by the core-level spectroscopy measurements on $CeFeAsO_{0.89}F_{0.11}$ [31] which showed very rapid spin-fluctuation dependent of the magnetic moment. Since from our model Equation 6, M is proportional to z (for $a_3 \ll 1$), the observed strong correlation is to be expected. This observation confirms our earlier assertion that spin-mediated fluctuations may be the major dominant mediator in the superconducting Fe-pnictide superconductors. However, electron–phonon coupling through spin channel is also to be expected.

We can thus speculate that a theory of the physics of FePn superconductors must include a local and dynamically spin-polarized spin fluctuation and electron–phonon coupling mediated through the spin channel as it may be relevant in understanding the origin and nature of the observed superconductivity in FePn.

Also, our model predicted correctly some already observed experimental phenomenon stressing that FePn superconductors may be a possible candidate for studying third-order phase transitions.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

All authors, CEE, EOC, and MCO, contributed equally to this work. All authors read and approved the final manuscript.

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