A Model Third Order Phase Transition in Fe – Pnictide Superconductors

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By identifying the orders of phase transition through the analytic continuation of the functional of the free energy of the Ehrenfest theory, we have developed a theory for studying the dependence of the local magnetic moment, M on the Fe – As layer separation in the third order phase transition regime. We derived the Euler – Lagrange equation for studying the dynamics of the local magnetic moment, and tested our model with available experimental data.

1 Introduction

Since the discovery of superconductivity in Fe – based pnictides oxides [1], there has been enormous research activities to understand the origin of their superconductivity. This immense interest in the physics and chemistry communities is reminiscent of the excitement that accompanied the discovery of high – T_c cuprate superconductors in the early 1980s. Normally, in Fe – based superconductors, antiferromagnetic (AFM) order is suppressed by charge (hole) doping but spin interactions still exist [2]. It should be noted that superconductivity can still be induced in the pnictides without charge doping through either isoelectric doping, non-stoichiometry, or by use of non-thermal control parameters such as application of non-hydrostatic pressure. Also it should be noted that the parent compounds of the iron pnictides are metallic, albeit highly dissipative, bad metals [3]. Most striking is the spectroscopy evidence that Fe based superconductors are weakly correlated electronic system [4, 5]. Thus, the origin of the observed superconductivity may not be due to Mott physics. Put differently, for the fact that spin is relevant in Fe pnictide superconductors, they are basically itinerant magnetism suggesting that the Mott – Hubbard physics may be irrelevant in physics of Fe pnictide superconductors. We can thus speculate that the superconductivity observed in Fe pnictides are locally and dynamically spin polarized due to strong Fe spin fluctuations with the itinerant nature of Fe providing the "glue". Hence, spin-fluctuation mediated through the spin channel may be relevant in understanding the origin and nature of the observed superconductivity in Fe pnictide.

Fe pnictide superconductors have layered structure. The Fe atom layers of these pnictide systems are normally sandwiched by pnictogen, for example, Arsenic (As). Hence, the magnetic moment of Fe depends strongly on the inter-layer distances of Fe-As [6]. The magnetic moment of transition metals also depends on volume [7]. This leads to the so-called lattice anharmonicity.

In quasi 2D layered materials, a state with some rather unexpected properties (new mean field solution) is observed at non-zero [8]. This new mean field property observed in these layered systems cannot be described by the ordinary phenomenological Ginzburg – Landau theory. Also, the thermodynamic relation $\int_0^{T_c}[\delta C_e(H,T)/\mathrm{T}]dT = 0$ which holds for 2^{nd} order phase transition is violated in some materials with Bose – Einstein condensate (BEC)-like phase transition (see for example as in spin glasses [9], ferromagnetic and antiferromagnetic spin models with temperature driven transitions [10]). We speculate that the normal Landau theory developed for 2^{nd} order phase transition may not adequately account for the physics of the phase transitions and associated phenomena, for example, magneto-volume effect due to lattice anharmonicity in Fe pnictide superconductors. This motivated us to develop a new Landau-like mean field theory for studying Fe-pnictide superconductors. The theory is based on the Ehrenfest classification of orders of phase transitions [11]. Specifically, we will study the dependence of the local magnetic moment, M on the Fe-As layer separation, z.

2 Theoretical Framework

According to Hilfer [12], rewriting the singular part of the local free energy within a restricted path through the critical point in terms of the finite difference quotient, and analytically continuing in the orders, allows one to classify continuous phase transitions precisely according to their orders. We speculate that there exist phase transition of orders greater than two as there is no known physical reason why such transitions should not exist in nature since they certainly exist in a number of theoretical models like quantum chromodynamics (QCD), lattice field theory and statistical physics [13]. At least, higher order phase transitions (≥2) are tenuous at best and their non-detection might have been due to the hasty generalization that all that departs from phase transition of order two can always be explained in terms of field fluctuation [13, 14].

The dependence of the magnetic moment, M on the Fe-As layer separation is completely determined by the functional (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 Higg's model) [15] of the disordered phase in order to minimize the total energy [13]. In general, F is a very complex functional of $\langle M\rangle$. To make $\langle M \rangle$ to be spatially continuous in equilibrium, 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". After coarse graining, in its simplest form [13, 14], F is give (for orders of phase transition > 2) by,

$$F_p(M, z) = \int d^d r |M|^{2(p-2)} \{-a_p|M|^2 + b_p|M|^4 + c_p|\nabla M|^2 + |M|^2 \alpha (z - z_c)^{2(p-2)}\}, \forall p > 2 \quad (1)$$

where p is the order of the phase transition, $a_p = a_o(1 - H/H_c)$, $b_p \gg 1$, z is the Fe-As layer distance (inter-atomic separation), z_c is the critical point, and $\alpha < 0$ (a typical material dependent parameter).

Equation 1 is the model equation we are proposing for studying the dependence of M on the Fe-As inter-atomic separation. For 3^{rd} order phase transition, $p = 3$, Eq. 1 reduces to,

$$F_3(M, z) = \int d^d r |M|^2 \{-a_3|M|^2 + b_3|M|^4 + c_3|\nabla M|^2 + |M|^2 \alpha (z - z_c)^2\} \quad (2)$$

If we neglect the gradient term, and minimize the local magnetic free energy with respect to M, Eq. 2 reduces to

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

which basically leads (i.e., substituting Eq. 3 into 2) to the local free energy

$$\langle f_3 \rangle = [\frac{2}{3b_3}(a_3 + |\alpha|(z - z_c)^2)]^2 \{\frac{5}{3}|\alpha|(z - z_c)^2 - \frac{1}{3}a_3\}. \quad (4)$$

In the presence of the gradient term to the local magnetic free energy, using variational principle, after scaling, we obtain the Euler – Lagrange equation for M as,

$$\varphi^5 - \varphi^3[1 - \alpha(z - z_c)^2] - \varphi|\nabla^2 \varphi| = 0. \quad (5)$$

3 Model Application

Using the data of Egami et al. [16], we calculated the magnetic moment, M using our model Eq. 3. The plot of experimentally determined critical temperature against our calculated M (μ_B) are as shown in Fig. 1. Observe that there is strong correlation between T_c and M. Most significantly, our model predicted correctly the range of values of magnetic moment of Fe, in Fe pnictide superconductors. As it is evidence from the plot, the magnetic moment range from 0.59 to 0.73 μ_B. The experimentally measured value for the magnetic moment of Fe in LaOFeAs for instance, range from 0.30 to 0.64 μ_B [17, 18].

We speculate that the observed strong correlation between T_c and M stems from the fact that the superconducting critical temperature T_c depends very sensitively on the iron pnictogen (i.e., Fe-As-Fe) bond angle which in turn, depends on

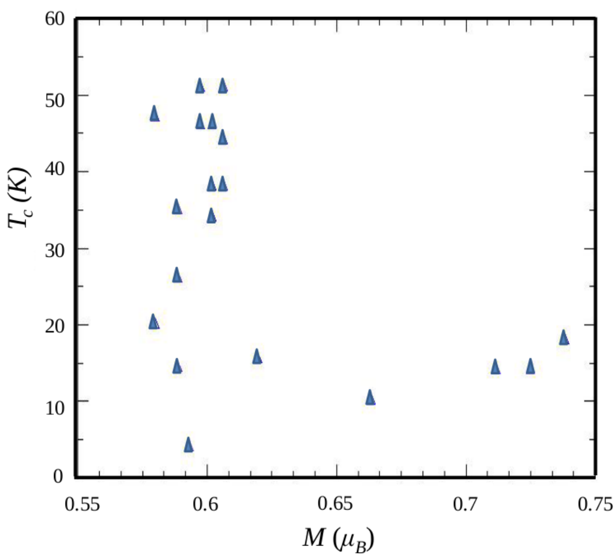

Fig. 1: Color-online. Superconducting experimental critical temperature, T_c from Ref. [16] against the calculated M obtained using Eq. 3 at the critical point.

the Fe-As layer separation [19]. This present observation is in tandem with the understanding that the bonding of the arsenic atoms changed dramatically as a function of magnetic moment [20] and the core-level spectroscopy measurements on $CeFeAsO_{0.89}F_{0.11}$ [21] which showed very rapid spin fluctuation dependent magnetic moment. Since from our model Eq. 3, 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 superconductivity of Fe pnictide superconductors. However, electron-phonon coupling through the spin-channel is also to be expected.

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