Interpretation of high-pressure experiments on FeAs superconductors

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(Dated: May 3, 2008)

In two recent articles (cond-mat/0606177 and arXiv:0804.1615), we have suggested a unified theory of superconductivity based on the real-space spin-parallel electron pairing and superconducting mechanism and have shown that the stable hexagonal and tetragonal vortex lattices (the optimal doping phases) can be expected in the newly discovered LaO\(_{1-x}\)F\(_x\)FeAs (\(x_0 = 1/7 \approx 0.1428\)) and SmO\(_{1-x}\)F\(_x\)FeAs (\(x_0 = 1/6 \approx 0.1667\)), respectively. In this paper, we present a theoretical study of the effects of hydrostatic and anisotropic pressure on the superconducting transition temperature \(T_c\) of the Fe-based layered superconductors based on the above mentioned theory. Our results indicate a strong doping-dependent pressure effects on the \(T_c\) of this compound system. Under high hydrostatic pressure, we find that \(dT_c/dP\) is negative when \(x > x_0\) (the so-called overdoped region) and is positive when \(x < x_0\) (the so-called underdoped region). Qualitatively, our finding is in good agreement with the existing experimental data in LaO\(_{1-x}\)F\(_x\)FeAs (\(x = 0.11 < 1/7\) (arXiv:0803.4266) and SmO\(_{1-x}\)F\(_x\)FeAs (\(x = 0.13 < 1/6\) and \(x = 0.3 > 1/6\)) (arXiv:0804.1582)). Furthermore, \(T_c\) of both overdoped and underdoped samples shows an increase with uniaxial pressure in the charge stripe direction and a decrease with pressure in the direction perpendicular to the stripes. We suggest that the mechanism responsible for the pressure effect is not specific to the iron-based family and it may also be applicable to other superconducting materials.

PACS numbers: 74.70.Ad, 74.62.Fj, 74.20.Cz, 74.25.Qt

I. INTRODUCTION

The surprising discovery of superconductivity in FeAs superconductors\(^{1-4}\) has stimulated intense interest on the mechanism for superconductivity in this new high-\(T_c\) superconductor family.\(^{2-23}\) It is well known that element substitution is often served as an effective method to raise \(T_c\) due to the possible internal pressure induced by the replacement of the smaller elements.\(^{24-30}\) In this way, physicists around the world have pushed the transition temperature of the new superconductors from 26 K to 55 K. Moreover, it is an experimental fact that the \(T_c\) of superconductors can also be tuned by the external high pressure. Theoretically, the possibility of enhancing \(T_c\) has been suggested in this class of compounds by applying pressure.\(^{31-35}\) Experimentally, it was found that the \(T_c\) of LaO\(_{1-x}\)F\(_x\)FeAs (\(x = 0.11\)) increases almost linearly (at a rate of 1.2 K/GPa) with the increasing of hydrostatic pressure\(^{36}\) in favor of the previous expectations. The external pressure effects were also reported on SmO\(_{1-x}\)F\(_x\)FeAs, Lorenz et al.\(^{37}\) found that in the \(x = 0.13\) sample \(T_c\) increases under hydrostatic pressure with the rate \(dT_c/dP \approx 0.9\) K/GPa. However, the \(T_c\) of the \(x = 0.3\) sample is suppressed instead by pressure at a rate of \(dT_c/dP \approx -2.3\) K/GPa, in contrast to the theoretical predictions. These measurements reveal that the pressure variation of \(T_c\) of FeAs compounds may be strongly dependent on the doping level of \(x\).

In the earlier works,\(^ {38,39}\) we have proposed a real space mechanism of high-\(T_c\) superconductivity which can naturally explain the complicated problems, such as pairing mechanism, pairing symmetry, charge stripes, optimal doping, magic doping fractions, vortex structure, phase diagram, Hall effect, etc.\(^ {38,39}\) Based on the mechanism, the relationship between the superconducting vortex phases and the optimal doping levels of FeAs superconductors were analytically given. We predicted that the optimal doping levels are \(x = 1/7 \approx 0.1428\) (LaO\(_{1-x}\)F\(_x\)FeAs and La\(_{1-x}\)Sr\(_x\)OFeAs) and \(x = 1/6 \approx 0.1667\) (Ce\(_{1-x}\)O\(_x\)FeAs, SmO\(_{1-x}\)F\(_x\)FeAs, PrO\(_{1-x}\)F\(_x\)FeAs and CdO\(_{1-x}\)F\(_x\)FeAs) which are found to be in excellent agreement with the experimental data (LaO\(_{1-x}\)Cu\(_x\)FeAs: \(x = 0.12\), La\(_{1-x}\)Sr\(_x\)OFeAs: \(x = 0.13\), Ce\(_{1-x}\)O\(_x\)FFeAs: \(x = 0.15\), SmO\(_{1-x}\)F\(_x\)FeAs: \(x = 0.16\), and PrO\(_{1-x}\)F\(_x\)FeAs: \(x = 0.16\), and CdO\(_{1-x}\)F\(_x\)FeAs: \(x = 0.17\)).\(^{40}\) Furthermore, it is shown that when \(x = 1/7\) the triangular array of vortices can be expected in the related samples, while \(x = 1/6\), the corresponding vortex lattice structures have a tetragonal symmetry.\(^ {41}\) Moreover, although the new layered materials resemble the cuprates in some ways, it was shown that the new compounds belong to non-pseudogap superconductors.

In the present paper, we try to extend the application of the theory to the effects of pressure on the superconducting properties of FeAs superconductors. Furthermore, we aim to explore a universal relationship among the pressure effects (hydrostatic and anisotropic) on the transition temperature \(T_c\), lattice constants, vortex lattice, charge (magnetic) stripes and the doping levels in the superconductors.

II. HOW TO RAISE THE SUPERCONDUCTING TRANSITION TEMPERATURE?

To raise the superconducting transition temperature up to the room temperature is still a dream of scientists today. Although almost 100 years have passed since the
first discovery of superconductivity in mercury in 1911 by H. Kamerlingh Onnes, disappointedly, so far scientists cannot draw a convincing physical picture: What is the superconducting phase? Undoubtedly, if this situation persists, it is never possible for scientists to achieve a reasonable understanding of the mysterious superconducting phenomenon and the dream of superconductivity at higher temperatures (perhaps even room temperature) will always remain as a dream. In other words, we need to establish the nature of the superconducting charge carriers before thinking about how to enhance $T_c$. Here, we would like to point out that the following three factors play a central role in raising the $T_c$ of superconductors.

### A. Charge and magnetic stripes (vortex lines)

First, to exhibit superconductivity, the cooper pairs should be condensed into a charge river (stripe) and a stable quasi-one-dimensional “freeways” should be built naturally in the superconductors. In the previous study, the real space collective confinement pictures have been introduced into the conventional and cuprate superconductors. In this case, a real space long range magnetic order (spin parallel) and superconductivity coexist to form a dimerized charge supersolid (a charge-Peierls dimerized transition), as seen in Fig. 1. When temperature $T \neq 0$, the so-called spin density wave (SDW),

$\Delta (\uparrow) \rightarrow (\Delta \uparrow) \rightarrow (E_b \downarrow) \rightarrow (T_c \downarrow)$

A charge stripe (vortex line) in Fe$^{2+}$-plane of iron-based superconductors

FIG. 1: The real space collective confinement picture (vortex line) in the superconducting iron plane of FeAs superconductors. The superconducting transition temperature $T_c$ is uniquely determined by lattice constant $b$. When the superconducting vortex phase with ordering wave-vector $Q = (\pi, 0)$, the spin-density-wave (SDW) is suppressed. While the ordering of $Q = (\pi, \pi)$, an intensive SDW is inspired along the charge stripe (vortex line) and the superconductivity is totally suppressed. This implies the FeAs family is possible in $d$-wave superconductors.

![Graph showing $T_c$ vs. lattice constant $b$](image)

FIG. 2: The relationship between the lattice constant $b$ (or the distance of the nearest-neighbor Cooper pairs) and $T_c$ in FeAs superconductors.
a competing state against the superconductivity, will be inspired in the metallic charge stripe (vortex line) due to thermal fluctuations and the superconductivity and SDW can coexist along this stripe. When temperature $T = 0$, the SDW order is totally suppressed and the corresponding stripe is referred to as the superconducting ground state.

From Fig. 1 it is apparent that, for the given lattice parameters, the superconducting phase of $Q = (\pi, 0)$, or $Q = (0, \pi)$, has the highest superconducting transition temperature due to the most intensive confinement effect. While the phase with ordering wave-vector $Q = (\pi, \pi)$ corresponds to the SDW phase where the superconductivity is totally suppressed. This implies the FeAs family is possible in $d$-wave superconductors. Furthermore, for the best superconducting order of $Q = (\pi, 0)$ presented in Fig. 1, the distance $\Delta$ between two electrons of one cooper pair decreases with the decreasing of the lattice constant $b$, as a consequence, increase the pair binding energy $E_B$ and the superconducting transition temperature $T_c$. This conclusion has been well confirmed by the recent chemical (element) substitution experiments in FeAs superconductors as shown in Fig. 2, the shrinking of crystal lattice can effectively enhance the superconducting transition temperature.

B. Vortex lattices

Second, to maintain a stable and durable superconducting phase, the metallic charge stripes of Fig. 1 (vortex lines) should self-organize into a ‘superlattice’ (vortex lattices) with the primitive cell $(A, B, C) = (ha, kb, lc)$. It has been argued that the physically significant critical value for the most stable vortex lattice is that at which $T_c$ is maximum. In this sense, the LTT2 and the simple hexagonal (SH) phases (vortex lattices) might be the ideal candidates for the stable charge-stripe order of paired electrons. In the LTT2($h, k, l$) phase, as shown in Fig. 3(a), the charge stripes have a tetragonal symmetry in XZ plane in which the superlattice constants satisfy

$$\frac{A}{C} = \frac{ha}{lc} = 1.$$  \hspace{1cm} (1)

While in simple hexagonal (SH) phases, as shown in Figs. 3(b) and (c), the charge stripes possess identical trigonal crystal structures. In the SH1($h, k, l$) phase [see Fig. 3(b)], the superlattice constants have the following relation

$$\frac{A}{C} = \frac{ha}{lc} = \frac{2\sqrt{3}}{3} \approx 1.154700.$$  \hspace{1cm} (2)

For the SH2($h, k, l$) phase of Fig. 3(c), this relation is given by

$$\frac{A}{C} = \frac{ha}{lc} = \frac{\sqrt{3}}{2} \approx 0.866025.$$  \hspace{1cm} (3)

We have shown that the appearance of the SH (or LTT2) vortex lattice is a common feature of the optimally doped superconductors. But, for non-optimal doping we found that the vortex lattices tend to form the superconducting low-temperature orthorhombic (LTO) phase where the superlattice constants satisfy $A \neq B \neq C$.

C. Stripe-stripe interaction

Third, the formation of stripe patterns (vortex lattices) is generally attributed to the competition between short-range attractive forces and long-range repulsive forces. Therefore, it is inevitable that there exist the intrinsic stripe-stripe interactions among the vortex lines inside the vortex lattices, as illustrated in Fig. 4. On the one hand, the interactions among stripes (vortex lines) are necessary for the establishment of vortex lattices of Fig. 3. On the other hand, the stripe-stripe interactions may induce the collective spin density wave (SDW) excita-
FIG. 4: Stripe-stripe interaction inside the vortex lattice of FeAs superconductors. An appropriate (or optimal) stripe-stripe distance $D$ (not too close, not too far) is helpful for a higher $T_c$. Owing to the stripe-stripe interactions (harmful for superconductivity) along the vortex lines. With increasing doping concentration in the system, stripe-stripe interactions become more important. Obviously, an appropriate (or optimal) stripe-stripe distance $D$ (not too close, not too far) is helpful for a higher $T_c$ (see Fig. 4). Charge carrier doping has been proved to be the best and convenient way to control the stripe-stripe distance and interaction in the doped superconductors. In our opinion, the optimally doping means that the most stable vortex lattice (with an optimal stripe-stripe distance) has been successfully established in the superconducting sample and the SDW state has been greatly suppressed inside the vortex lattice. For the LTO($h, k, l$) superconducting vortex phase, two stripe-stripe distances $D_{xy}$ and $D_z$ are given by

$$D_{xy} = ha, \quad D_z = lc.$$  (4)

The main results obtained so far and discussed in this section already allow one to draw some useful conclusions about the relationship between vortex structure and $T_c$. It is shown that to effectively raise the superconducting transition temperature, the following three conditions should be paid attention: (i) a compact one-dimensional charge-magnetic stripe (vortex line); (i) a stable vortex lattice structure; and (iii) an adequate stripe-stripe spacing and interaction.

III. HIGH PRESSURE EFFECTS

Shortly after the discovery of the superconductivity in LaO$_{1-x}$F$_x$FeAs, one of the central concerns of high-temperature iron-based superconductors is how to raise the superconducting transition temperature. Apart from the great efforts to the effect of element substitution on the $T_c$, the hydrostatic pressure induced $T_c$ increasing effects have been reported in this class of compounds. While these interesting experimental results seem to gain important insight into FeAs superconductors, we find that there is no theory that can be applied to explain them.

It is clear that a promising theory of superconductivity should explain these results in addition to other properties. Here we show how the recently suggested superconductivity theory can explain the pressure dependence of $T_c$ in iron-based superconductors. To the best of our knowledge, this is the first theoretical attempt to do so. Based on the real-space spin-parallel electron pairing and superconducting mechanism, the effects of pressure can...
be visually illustrated in Fig. 5 of LTO superconducting vortex lattice in FeAs superconductors. One can see clearly that the direct effect of pressure is to shrink the lattice constants, as a result, changing the structure of vortex lattice. Hence, the pressure effects can be described simply by

\[ A(=ha) \rightarrow A'(=ha'), \]
\[ B(=kb) \rightarrow B'(=kb'), k = 1, \]
\[ C(=lc) \rightarrow C'(=lc'), \]

where \((A, B, C)\) and \((A', B', C')\) are the superlattice constants without and under the pressure. In the following sections, we shall focus our attention on the problem: how can the pressure affect the \(T_c\) merely by varying the lattice (or superlattice) constants of the superconductors?

### A. Pressure effects on a single vortex line

Figure 6(a) shows a quasi-one-dimensional charge-magnetic superconducting stripe (vortex line) where the stripe-stripe interactions do not exist. In this ideal system, the values of lattice constant \((a \rightarrow a' \text{ and } b \rightarrow b')\) are decreasing monotonously with the increasing external pressure, as shown in Fig. 6(b). According to the above discussions (see Fig. 1), we can see that the pressure leads to the decreasing of the lattice constants, consequently, increase the pair binding energy \(E_B\) and narrow and eventually eliminate the magnetic excitations in spin density wave (SDW) state. Hence, it is expected that the pressure dependence of \(dT_c/dT\) is always positive in the quasi-one-dimensional vortex line. In other words, \(T_c\) will be found to increase almost linearly upon increasing external pressure in this specific system.

### B. Structural phase transition in the vortex lattice

The superconducting LTT2, SH1 and SH2 (see Fig. 3) vortex phases, as discussed above, are much more stable than the LTO superconducting phase. As a consequence, the highest \(T_c\) phase is usually related to LTT2, SH1 or SH2 vortex lattice. Figure 7 shows two possible pressure-induced vortex lattice phase transitions in FeAs superconductors. Shown in Fig. 7(a) is the LTO-LTT2 structural phase transition, while an example of LTO-SH1 vortex lattice phase transition is illustrated in Fig. 7(b). These suggest that pressure can play an important role on pushing low \(T_c\) superconducting vortex phase toward the main (optimal) superconducting phase.
To depict the difficulty level of vortex lattice phase transition (or compressibility) in superconductors, one can define the following “stiffness criterion” for the underdoped superconducting $\text{LTO}(h,k,l)$ vortex phase

$$\Theta = \kappa \left( \frac{1}{h} \right)_0 - \frac{1}{h} \frac{1}{abc} = \kappa \frac{x_0 - x}{2abc}, \quad (5)$$

where $\kappa$ is a material-related constant, $x$ is the doping level in the sample. And $x_0$ and $(1/hkl)_0$ are the optimal doping level and the corresponding vortex lattice index, respectively.

The relation of Eq. (5) implies that the stiffness of superconductor is direct proportion to the doping level $x$, but is inverse proportion to the unit-cell volume ($abc$). The smaller the parameter $\Theta$, i.e., the softer the corresponding compound system, the larger the $dT_c/dP$ value is, and vice versa. Thus, we have

$$\frac{dT_c}{dP} \propto \frac{1}{\Theta^\alpha}, \quad (6)$$

where $\alpha$ is a positive constant.

From Eq. (5) and (6), it is clear that $dT_c/dP$ value depends strongly on the doping level and the lattice constants. We find that pressure can either promote or suppress the superconducting $T_c$, depending on the doping level of $x$. For the cuprate superconductors, it has been shown that the $T_c$ varies with carrier concentration $n$ following a universal parabolic rule with $T_c$ peaks at a carrier concentration $n_0$. Later, it has also been proved that $dT_c/dP$ is negative when $n > n_0$ and positive when $n < n_0$. Obviously, the above two expressions give a reasonable agreement with the results in the cuprate superconductors. This consistency implies that the Eq. (5) and (6) are not specific to the iron-based family and it may also be applicable to other doped superconducting materials.

C. $\text{LaO}_{1-x} \text{Fe}_x \text{FeAs}$

In $\text{LaO}_{1-x} \text{Fe}_x \text{FeAs}$, based on the experimental lattice constants ($a = \sqrt{2}a_0/2 = 2.85\,\AA$ and $c = c_0 = 8.739\,\AA$), we have predicted that the optimal doping levels is $x_0 = 1/7 \approx 0.1428$ with the hexagonal vortex $\text{SH}1(7,1,2)$ lattice having the stable trigonal structure. The hydrostatic-pressure effects on the superconducting transition temperature ($T_c$) of the $\text{LaO}_{1-x} \text{Fe}_x \text{FeAs}$ ($x = 0.11$) have been recently reported by two research groups. These results corroborate the suggested external pressure-induced $T_c$-enhancement in the compound. It should be pointed out that the $x = 0.11$ sample lie in the underdoped region, in favor of the positive pressure effect on $T_c$.

We note that $x = 1/9 \approx 0.1111$ sufficiently close to $x = 0.11$. According to our theory, it is likely that the $x = 1/9$ sample corresponds to the metastable $\text{LTO}(9,1,2)$ superconducting phase, as shown in Fig. 8. In this case, the sufficient large stripe-stripe distances ($D_{xy} = 25.65\,\AA$ and $D_z = 17.45\,\AA$) indicate that the stripe-stripe interaction is much weaker in the compound system with the stiffness criterion $\Theta = 2.24 \times 10^{-4}$. As a result, the $x = 1/9$ sample has a softer characteristic and shows a relatively larger positive $dT_c/dP$ value.

D. $\text{SmO}_{1-x} \text{Fe}_x \text{FeAs}$

We now turn to the $\text{SmO}_{1-x} \text{Fe}_x \text{FeAs}$ compound system with the lattice constants $a = 2.788\,\AA$ and $c = 8.514\,\AA$. In the previous paper, the analytical results indicated that the optimum doping occurs at $x = 1/6 \approx 0.1667$ in $\text{SmO}_{1-x} \text{Fe}_x \text{FeAs}$ with the square vortex lattice of $\text{LTT}2(6,1,2)$ phase. Immediately after the discovery of the $T_c$ of 55 K in $\text{SmO}_{1-x} \text{Fe}_x \text{FeAs}$, the pressure effects on the superconducting of the new compound have been investigated by Lorenz et al. However, unlike $\text{LaO}_{1-x} \text{Fe}_x \text{FeAs}$, it was shown that the pressure can ei-
FIG. 9: Pressure effects on the overdoped LTO(3,1,2) superconducting phase of SmO$_{1-x}$F$_x$FeAs ($x=1/3$). (a) Without pressure, (b) pressure-induced intensive spin fluctuation due to a strong stripe-stripe interaction.

ther suppress or enhance $T_c$, depending on the doping level.

According to the present scenario, it is then not a surprise to learn the doping-dependent pressure effects on $T_c$. For the underdoped $x = 0.13 < 1/6$ SmO$_{1-x}$F$_x$FeAs sample, the corresponding vortex lattice may be in a mixed superconducting phase of LTO(7,1,2) and LTO(8,1,2) with $x = (1/7 + 1/8)/2$. Apparently, the stripe-stripe distances of the mixed phase are large enough to support a positive pressure effect [similar to the case of LTO(9,1,2) phase for LaO$_{1-x}$F$_x$FeAs ($x = 0.11$)]. Furthermore, the mixed vortex phase which exhibits a value of $\Theta = 2.77 \times 10^{-4}\kappa$ is found harder than the LTO(9,1,2) phase of LaO$_{1-x}$F$_x$FeAs ($x = 0.11$) with $\Theta = 2.24 \times 10^{-4}\kappa$. As a consequence, the LaO$_{1-x}$F$_x$FeAs ($x = 0.11$) sample should have a larger $dT_c/dP$ value than that of the SmO$_{1-x}$F$_x$FeAs ($x = 0.13$) sample, in reasonable agreement with the experiments [1.2 K/GPa for LaO$_{1-x}$F$_x$FeAs ($x = 0.11$)$^{26}$ and 0.9 K/GPa for SmO$_{1-x}$F$_x$FeAs ($x = 0.13$)$^{37}$).

While for the overdoped $x = 0.3 > 1/6$ SmO$_{1-x}$F$_x$FeAs sample, approximately, the LTO(3,1,2) and LTO(6,1,1) superconducting phases are candidates for the vortex lattices. An example of LTO(3,1,2) is shown in Fig. 9 under such circumstances, the stripes (vortex lines) are very crowd in the superconducting Fe planes with a stripe-stripe distance $D_{xy} = 8.363\AA$. It is obvious that the external pressure could lead to a much more crowded and unstable vortex phase. This in turn greatly enhance the spin fluctuation and suppress superconductivity, implying a possibility of a negative $dT_c/dP \simeq -2.3$ K/GPa as indicated in the experiment of SmO$_{1-x}$F$_x$FeAs ($x = 0.3$) sample$^{38}$ having a large negative value of $\Theta = -5.06 \times 10^{-4}\kappa$.

FIG. 10: The schematic interpretation of the uniaxial pressure effects. (a) When the external pressure $p_a$ perpendicular to the stripe direction, $dT_c/dp_a$ value is negative, (b) when the pressure $p_b$ along the stripe direction, $dT_c/dp_b$ value is positive.

E. Uniaxial pressure effects

The uniaxial pressure effects are markedly different from those of hydrostatic pressure effects. For example in an single crystal of YBa$_2$Cu$_3$O$_{7-\delta}$, the uniaxial pressure dependence measurements revealed the following pressure derivatives: $dT_c/dp_a = -2.0 \pm 0.2$ K/GPa and $dT_c/dp_b = +1.9 \pm 0.2$ K/GPa, where the subscripts $(i = a, b)$ denote the corresponding crystallographic directions. It was shown that the a-axis and b-axis derivatives are of opposite sign. Note that the anisotropic pressure dependence of $T_c$ along the a and b directions is still a theoretical challenge.

In this paper we show how the real-space vortex model of Fig. 10 can explain these peculiar results. Furthermore, we argue the existence of the uniaxial pressure effects in FeAs superconductors. In fact, the uniaxial pressure dependence in superconductors can be well understood simply by considering the pressure effects in two special directions: (i) along the charge stripe (vortex line) di-
rection, and (ii) perpendicular to the stripe direction. Figure 10 illustrates the uniaxial pressure effects in FeAs superconducting family. When the external pressure is in $a$-axis direction (perpendicular to the stripes), our study reveals that the pressure affects the vortex lattice at least two factors: shorten the stripe-stripe spacing while at the same time increase the distance between cooper pairs and two electrons inside a cooper pair. As discussed above, both factors are negative for promoting the $dT_c/dp$ value, while for the overdoped $\text{SmO}_x \text{Fe}_2 \text{As} (x = 0.3)$ sample, the pure $b$-axis pressure may induce a positive $dT_c/dp$ pressure effect.

IV. CONCLUDING REMARKS

In conclusion, without Hamiltonian, without wave function, without quantum field theory, our scenario has provided a beautiful and consistent picture for describing the high-pressure effects (hydrostatic and uniaxial pressure) in the newly discovery of the iron-based superconductors. We insist that any pressure-induced phenomena should share exactly the same physical reason. The suggested mechanism responsible for the pressure effect is not specific to the iron-based family and it may also be applicable to other superconducting materials, including the cuprate superconductors.

Acknowledgments

The author would like to thank Dr. Kezhou Xie for many useful suggestions.
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