Magnetic domain walls induced by twin boundaries in low doped Fe-pnictides

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Abstract. Inspired by experimental observations of the enhancement of superconductivity at the twin-boundary (TB) in slightly electron doped Ba(Ca)(FeAs)₂ where a strong 2 × 1 antiferromagnetic collinear order is in presence, we investigate theoretically the effects of TBs on the complex interplay between magnetism and superconductivity using a minimum phenomenological two-orbital model. The magnetic order can be simulated from an onsite Coulomb interaction $U$ and the Hund’s coupling $J_H$, while the effective pairing interaction yields the superconductivity with $s^\pm$ wave symmetry. The spatial distributions of the magnetic, superconducting and charge density orders near two different types of TBs are calculated. Each of the TBs has two different orientations. We find that the first type TBs, which corresponds to a 90° lattice rotation in the $a- b$ plane, enable magnetic domain walls (DWs) to be pinned at them, and that superconductivity is enhanced at such TBs or DWs. This result is consistent with experiments for a TB with an orientation of 45° from the $x$-axis. Contrastingly, we predict that superconductivity is suppressed at the second type of TBs which correspond to an asymmetrical placement of As atoms on the opposite sides of the TB. Furthermore, the lattice-mismatch effect across the TBs is investigated. The comparison of our results with the observations from the nuclear-magnetic-resonance experiments are also discussed.

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1. Introduction

The recent discovery of Fe-pnictide based superconductors offers an alternative avenue to explore the physics of a new family of high temperature superconductors [1–5]. Similar to the cuprates, the parent compounds of the FeAs-based superconductors also possess antiferromagnetic (AF) ground states [4, 5]. With increasing electron or hole doping, the AF order is suppressed and superconductivity (SC) appears in both the cuprates and the Fe-pnictides. However, different from the cuprates, SC and a $2 \times 1$ collinear AF or spin-density-wave (SDW) order can coexist in doped Ba(FeAs)$_2$ superconductors [6, 7]. Because each unit cell of these new materials contains two inequivalent Fe ions, different organizations of the magnetic moments of Fe ions in both normal and superconducting states can lead to a diverse assortment of magnetic structures and unusual electronic properties [8, 9].

Recently, twin boundaries (TBs) oriented $45^\circ$ from the $x(a)$-axis were observed in the normal state of Ca(or Ba)(FeAs)$_2$ compounds with $x \sim 0$ by scanning tunneling microscopy (STM) experiments [10]. Across these TBs, the $a$-axis of the crystal rotates by $90^\circ$, and the modulation direction of AF order that exists is rotated by $90^\circ$ as well. That is, $90^\circ$ magnetic domain walls (DWs) are formed at the TBs. Also, in the SC state of underdoped Ba(Fe$_{1-x}$Co$_x$As)$_2$ with $x < 0.07$, it has been found that the diamagnetic susceptibility is increased and that the superfluid density is enhanced on the same type of TB in superconducting-quantum-interference-device microscopy (SQIDM) experiments [11]. Consistent with these experiments, a theoretical study [12] found that $90^\circ$ DWs can be formed at low doping levels and that SC is enhanced on them. However, the DWs considered in that study were formed in the absence of TBs, and were induced instead by a strong effective Coulomb interaction between charge carriers, while in the experiments [10, 11] the DWs were pinned at TBs.

In this work, in order to better understand the effects that TBs have on the spatial profiles of magnetic and superconducting order, we investigate the magnetic, SC and charge density orders near two different types of TBs using the Bogoliubov–de-Gennes (BdG) equations for very under-doped Ca(or Ba)(FeAs)$_2$ compounds. The lattices on the opposite sides of the type-I
TB have a $90^\circ$ orientation difference, and the As atoms across the type-2 TB are asymmetrically placed. The present approach is based upon a two-orbital model [13]. This model takes into account of the asymmetry of the As atoms below and above of the Fe plane which should be suitable for describing the cleaved surface layer or layers in surface sensitive experiments. As a result, the obtained phase diagram for the electron doped $\text{Ba(Fe}_{1-x}\text{Co}_x\text{As)}_2$ [14] is in qualitative agreement with experiments [6, 7, 15–17]. The obtained Fermi surface evolution as a function of doping [14] and the Fermi surface at zero doping [18] are consistent with angular resolved photo-emission spectroscopy experiments [19–21] and the electron–hole Dirac cone states as observed by magnetoresistance experiments [22]. Another critical test of the model is that the resonance peak observed at negative energy in a vortex core by STM experiments [23] could only be explained by the present model [24]. The approach has also been used to study the superfluid density [25] as the doping and temperature varying, and the results are in good agreement with experiments in films [26]. We predict that the enhancement or suppression of SC, the location of DWs and the electron-density distributions are largely dependent on the nature of TBs. The relationship between magnetism, SC and the charge order is always one of the most important problems in the research of unconventional superconductors. Our work provides the first study on different kinds of TWs, which involves all the three aspects mentioned above. More importantly, it shows where and how the SC can be enhanced/suppressed in the presence of TBs.

This paper is constructed as follows. In section 2, brief descriptions of the model Hamiltonian and methodology will be given. In section 3, we calculate the phase diagram according to the interaction parameters used in the present work. In section 4, the numerical results on the spatial structures of magnetic, superconducting and charge orders for two types of TBs are presented in the very under-doped region ($x = 0.04$) where the SC order is weak and the magnetic order is strong. Each of the TBs has two configurations, which either aligns along $90^\circ$ or $45^\circ$ from the $x$-axis. In section 5, we approximate the lattice mismatch across one of the TBs by a disordered potential along the TB, and discuss how the magnetic, SC and charge orders near the TB are affected by the strength of the disorder. In section 6, we compare our results with the magnetic DWs observed by nuclear magnetic resonance (NMR) experiments [27]. Finally concluding remarks are made in the final section.

2. Hamiltonian and methodology

Consider the Hamiltonian $H = H_0 + H_{SC} + H_{int}$ that describes the energy of charge carriers. $H_0$ is a non-interacting two-orbital tight-banding model from [13, 14],

$H_0 = - \sum_{i \mu j \nu \sigma} \left( t_{i \mu j \nu} c_{i \mu \sigma}^\dagger c_{j \nu \sigma} + h.c. \right) - t_0 \sum_{i \mu \sigma} c_{i \mu \sigma}^\dagger c_{i \mu \sigma}, \tag{1}$

where $t_{i \mu j \nu}$ is the hopping parameter between two electrons, one at position $i$ with the orbital $\mu$ and the other at position $j$ with orbital $\nu$, and $c_{i \mu \sigma}^\dagger$ is the creation operator of an electron with spin $\sigma$ at position $i$ with orbital $\mu$. $t_0$ is the chemical potential. The pairing interaction energy of the electrons is

$H_{SC} = \sum_{i j \mu j \nu \sigma} \left( \Delta_{i \mu j \nu} c_{i \mu \sigma}^\dagger c_{j \nu \sigma} + h.c. \right), \tag{2}$
where $\Delta_{i\mu j\nu}$ is the pairing parameter between two electrons. Here $\tilde{\sigma}$ denotes the opposite spin of $\sigma$. The mean-field magnetic interaction energy \cite{14} is

$$
H_{\text{int}} = (U - 3J_H) \sum_{i,\mu \neq \nu, \sigma} \langle n_{i\mu\sigma} \rangle n_{i\nu\sigma} + (U - 2J_H) \sum_{i,\mu \neq \nu, \sigma \neq \tilde{\sigma}} \langle n_{i\mu\sigma} \rangle n_{i\nu\tilde{\sigma}} + U \sum_{i,\mu, \sigma \neq \tilde{\sigma}} \langle n_{i\mu\sigma} \rangle n_{i\mu\sigma},
$$

where $U$ is the on-site Coulomb interaction, $J_H$ is the Hund’s coupling, $n_{i\mu\sigma}$ is the electron number operator and $\langle n_{i\mu\sigma} \rangle$ is the local electron density. The eigenvalues and eigenfunctions of the total Hamiltonian $H$ can be obtained by self-consistently solving the BdG equations

$$
\sum_{j,\nu} \left( \frac{H_{i\mu j\nu}}{\Delta_{i\mu j\nu}} - H_{i\mu j\nu} \right) \begin{pmatrix} u_{ij\nu}^n \\ v_{ij\nu}^n \end{pmatrix} = E_n \begin{pmatrix} u_{i\mu\sigma}^n \\ v_{i\mu\tilde{\sigma}}^n \end{pmatrix},
$$

where

$$
H_{i\mu j\nu} = -t_{i\mu j\nu} + [U \langle n_{i\mu\tilde{\sigma}} \rangle + (U - 2J_H) \langle n_{i\mu\sigma} \rangle + (U - 3J_H) \langle n_{i\mu\sigma} \rangle - t_0] \delta_{ij} \delta_{\mu\nu},
$$

is the matrix element of $H$ with the same spin $\sigma$ between the orbital $\mu$ at position $i$ and the orbital $\nu$ at position $j$, and $t_0$ is the chemical potential. The pairing parameter $\Delta_{i\mu j\nu}$ and the local electron densities $\langle n_{i\mu\uparrow} \rangle$ and $\langle n_{i\mu\downarrow} \rangle$ satisfy the following self-consistent conditions:

$$
\Delta_{i\mu j\nu} = \frac{V_{i\mu j\nu}}{4} \sum_n \left| u_{i\mu\uparrow}^n v_{i\mu\downarrow}^n + u_{i\mu\downarrow}^n v_{i\mu\uparrow}^n \right| \tanh \left( \frac{E_n}{2k_B T} \right),
$$

$$
\langle n_{i\mu\uparrow} \rangle = \sum_n \left| u_{i\mu\uparrow}^n \right|^2 f(E_n),
$$

$$
\langle n_{i\mu\downarrow} \rangle = \sum_n \left| v_{i\mu\downarrow}^n \right|^2 [1 - f(E_n)],
$$

where $V_{i\mu j\nu}$ is the pairing interaction between next nearest neighboring (NNN) sites $i$ and $j$ which gives rise to the SC with s± wave symmetry \cite{13, 14}, and $f(x)$ is the Fermi–Dirac distribution function. The SC order parameter at position $i$ is defined as $\Delta_i = |\Delta_{i, i+\hat{x}\hat{y}} + \Delta_{i, i+\hat{\hat{x}}\hat{\hat{y}}} + \Delta_{i, i+\hat{x}+\hat{\hat{y}}} + \Delta_{i, i+\hat{\hat{x}}+\hat{\hat{y}}}|$, the local magnetic moment at position $i$ is defined as $m_i = \frac{1}{4} \sum_{\mu} (\langle n_{i\mu\uparrow} \rangle - \langle n_{i\mu\downarrow} \rangle)$ and the total charge density at position $i$ is defined as $\langle n_i \rangle = \sum_{\mu} (\langle n_{i\mu\uparrow} \rangle + \langle n_{i\mu\downarrow} \rangle)$. The chemical potential $t_0$ is determined by the electron filling per site $n(n = 2 + x)$, and for the value of the hopping terms $t_{i\mu j\nu}$ are assumed to be $t_{1\mu} = 1.0, 0.4, -2, 0.04$ \cite{13, 14}. Only the electron pairings of the same orbital between the next-nearest-neighbor Fe sites are considered. For example, we choose $V_{i\mu j\nu} = 1.4$ for $\mu = \nu$ and $|i - j| = 1$, and zero for all other cases. This choice of the pairing potential gives rise to the SC order with s±-wave symmetry \cite{28, 29}.

3. Phase diagram

The phase diagram of the electron-doped Ba(Fe$_{1-x}$Co$_x$As)$_2$ compounds as a function of temperature $T$ and doping $x$ has been qualitatively mapped out with $U = 3.4$, $J_H = 1.3$ and the NNN pairing interaction $V = 1.2$ \cite{14}. The distribution of the $2 \times 1$ collinear AF order and the SC order are spatially uniform. In reality, the lattice in the Fe-plane of these compounds is almost square, having slightly different lattice constants $a$ and $b$ ($a > b$) along $x$- and $y$-directions \cite{30}. In the present work, nearest-neighbor hoping terms are chosen to be $t_a = 1.0$.
and $t_b = 1.2$, we also slightly increase the magnitudes of our interaction parameters ($U = 3.8$, $J_H = 1.3$ and $V = 1.4$) in order to generate more pronounced inhomogeneity of the order parameters near the TBs. With the new set of the interaction parameters, we recalculate the magnetic configuration at $x = 0.4$ on a $28 \times 28$ lattice and the phase diagram as a function of the electron doping which are respectively shown in figures 1(a) and (b). Figure 1(a) exhibits the $2 \times 1$ collinear AF order, where the spins of the Fe ions on the red lines are pointing upward, and the spins on the blue lines are pointing downward. Since the magnetic order is originated in itinerant interacting electrons, the magnetic configuration in figure 1(a) is also referred as the SDW order. The spins of the Fe ions are always aligned ferromagnetically along a (or $x$)-direction. The obtained phase diagram indicates that the SC order is completely suppressed by the SDW near $x = 0$. The SDW and SC are coexisting with each other between $x \sim 0.02$ and $\sim 0.15$. For $x > 0.15$ while the SDW order disappears, the SC still prevails. All these features in our phase diagram are in qualitative agreements with both surface- and bulk-sensitive experiments [6, 7, 15–17].

4. Magnetic domain-wall structures and twin-boundaries

In the absence of the TBs, the SDW order discussed above is unstable against the formation of the $90^\circ$ magnetic DWs oriented $45^\circ$ from the $x$-axis as the strength of $U$ is increased to $U = 4.8$ for small $x$ at $T = 0$ [12]. In the presence of TBs, the magnetic DWs could be formed at much weaker $U$ as demonstrated in the present work. There are two types of TBs. The first one is that the orientations of the lattices across the TB differ by a $90^\circ$ rotation. The second one is that the As atoms are asymmetrically placed across the TB as compared with a perfect crystal lattice. For each type of the TBs, there are two configurations: one is oriented along $90^\circ$ from $x$-axis and the other is oriented along $45^\circ$ from the $x$-axis. In the following, the spatial profiles of magnetic, SC and charge density order near four different TBs at $T = 0$ are investigated. Throughout this work, we set $x = 0.04$, $U = 3.8$ and $J_H = 1.3$ and $V = 1.4$. Note that DWs do not form spontaneously in the absence of TBs at these parameter values, and all the order parameters have uniform solutions.
4.1. Type-1 twin-boundary oriented 45° from the x-axis

TBs can be formed by exchanging the lattice constants $a$ and $b$ on the opposite side of the TB. Figure 2(a) shows the structure of a single such TB oriented at 45° with respect to the $x$-axis. Since the magnitude of $a$ is lightly larger than that of $b$, this TB can be realized by assuming slightly different nearest neighbor hoping terms $t_a = 1.0$ and $t_b = 1.2$ across the TB. To analyze the effect of this TB, we considered a $28 \times 28$ lattice divided into four different domains separated by three parallel TBs (see figure 2(a)) along the lines $y = x + 14$, $x$ and $x - 14$, in order to satisfy the periodic boundary conditions. As shown in figures 2(b) and 3(a), there are three 90° DWs formed and pinned on the TBs. The patterns of these quantities are very similar to those found in [12] without the TBs (see figures 2(a)–(c) in [12]). However, in this case, the DW forms with a smaller value of the Coulomb interaction $U$, indicating that the existence of this type of TB is beneficial to the formation of the 90° DWs. The solutions presented in figure 3 are always stable against the uniform $2 \times 1$ collinear AF order [14].
Figure 4. (a) The lattice structure near a TB parallel to the \( y \)-direction (red dashed line), the open circles represent the positions of Fe atoms, \( a \) (blue solid line) and \( b \) (black solid line) are the lattice constants along \( x \) and \( y \) directions in domain \( A \). (b) Two TBs in the \( 28 \times 28 \) lattice, the black arrow indicates the position of the lattice structure shown in (a) in the whole lattice.

Similar to the results without TBs [12], the SC as well as the charge density get significantly enhanced on the DWs, which occur at the TBs, and suppressed in the middle of the magnetic domains (see figures 3(b) and (c)). This conclusion is consistent with the enhancement of SC along the TB as observed by the SQIDM experiments [11] on underdoped samples. There exists another experiment [31] favoring our result in which the magnetic vortices are found not to be pinned at the TBs. This implies that the SC is also enhanced along the TBs. For the parent compound \( \text{Ca(Fe}_{1-x}\text{Co}_x\text{As)}_2 \) with \( x \sim 0 \), our numerical results show that the magnetic structures as shown in figure 3(a) still remains, but there is no SC across the sample including the DWs, and this is in agreement with the STM experiments [10].

It is important to note that the lattices on both sides of this TB should be well matched at the TB, and each of the unit cells along the TB is only slightly deformed from the square shape. Thus, we do not expect that scattering of the electrons from the lattice mismatch across the TB should be strong.

4.2. Type-1 twin-boundary oriented 90° from the \( x \)-axis

A TB formed by exchanging the \( a \) and \( b \) lattice constants across it can also be oriented parallel to the \( x \)- or \( y \)-axis (as shown in figure 4(a)). The periodic boundary condition of this case is achieved by dividing the system into three different domains separated by two TBs (see figure 4(a)) along the lines \( x = 7 \) and 20, as shown in figure 4(b).

Here the magnetic DWs are pinned at the TBs (see figure 5(a)) on which existing a weak local ferromagnetic order which a periodic modulation. The SC also has a similar periodic modulation and is enhanced on the DWs, but suppressed in the middle of the magnetic domains (see figure 5(b)). A charge density wave appears near the DWs (see figure 5(c)) while the electron density gets suppressed in the middle of the magnetic domains. It is important to point out that in this case, the lattices on the opposite sides of a TB are not well matched. Therefore, there may be considerable scattering of the electrons due to the lattice mismatches.
Figure 5. Spatial profiles of (a) the magnetic order, (b) the superconducting order and (c) the charge density order are presented for type-1 TB oriented 90° from the x-axis.

Figure 6. (a) The lattice structure near a TW (red dashed line) parallel to the y-direction formed by misplacing As atoms. The open circles represent the positions of Fe atoms, and the red and blue dots respectively denote the As(up) and As(down) atoms. (b) Two TBs in the 28 × 28 lattice, the black arrow indicates the position of the lattice structure shown in (a) in the whole lattice.

near these TBs. If this effect is included, we expect that the SC would get suppressed, instead of being enhanced when the mismatch becomes strong across the DWs or the TBs. This issue will be discussed in section 5.

4.3. Type-2 twin-boundary oriented 90° from the x-axis

Another possible TB can be generated by slipping the lattice on the right side of the TB by a lattice constant along the y-direction with respect to the lattice on the left of the TB. There are two different types of As atoms in our model, we label them as As(up) and As(down) atoms which are asymmetrically place above and below the Fe plane. This type of TBs can be clearly seen from figure 6(a), in which the TB is represented by the red-dashed line. The crystal lattice for the FeAs layer has $D_{2d}$ symmetry, namely the four nearest neighboring As atoms of a ‘down’ As atom should be all ‘up’. The hopping terms between the NNN Fe ions via the hybridization of the 4p orbital with the As atom in the middle should have different values depending on
whether the As atom is above \((t_2)\) or below \((t_3)\) the Fe plane \([13, 32]\). The \(D_{2d}\) symmetry is broken by the presence of the TB. We considered a \(28 \times 28\) lattice with periodic boundary conditions divided into three domains by two TBs located at \(x = 7\) and \(20\) (see figure 6(b)). Figure 7(a) shows the magnetic order is enhanced near the TBs. Defining the magnetic DWs to be where the magnetic order is suppressed, that is, near the middle between two TBs. Then, clearly, the DWs are not located at the TBs. On the opposite sides of a DW, there is no change in the magnetic phase, thus we could label the DWs as the zero-phase DWs. Figure 7(b) shows that the SC is enhanced along the DWs, and that it is suppressed near the TBs. Figure 7(c) shows that the electron density is depleted near the TBs and becomes lightly hole doped. Apparently, the depleted electron density leads to strong magnetic order that suppresses the SC order. On the DWs, the electron density appears to be close to optimal doping and thus SC gets enhanced and the magnetic order is suppressed. We shall also point out in section 6 that the magnetic and SC structures near a TB oriented \(0^\circ\) from the \(x\)-axis are very different from the present case, and anti-phase DWs are predicted.

4.4. Type-2 twin-boundary oriented \(45^\circ\) from the \(x\)-axis

A TB due to missing one line of the lattice which contains both Fe and As(down) atoms oriented along \(45^\circ\) from the \(x\)-axis is shown in figure 8(a). In fact this ‘TB’ could also be regarded a line of missing Fe–As atoms. The \(D_{2d}\) symmetry of the lattice is also broken by the presence of this TB. Note that the geometry of this TB is fundamentally different from the one showed in figure 6(a) since the TB does not pass through any of the Fe or As atoms. To study this case, we considered a \(30 \times 30\) lattice and three identical TBs oriented \(45^\circ\) from the \(x\)-axis (see figure 8(b)) in order to satisfy the periodic boundary condition. The TBs are located along \(y = x - 15, x\) and \(x + 15\).

Different from the case in figure 7(a), the magnetic order shown in figure 9(a) is suppressed along the TBs where DWs are located. The magnetic domain between the TBs still has the usual \(2 \times 1\) collinear AF structure, except the magnetic moments are strongly and periodically modulated along the \(x\)-axis, which may be due to finite size effects of the TB and the small distance between two nearest neighboring TBs. It also appears that the local \(2 \times 1\) collinear AF structure could be represented by a stripe-like \(\sqrt{2} \times \sqrt{2}\) AF structure oriented \(45^\circ\) from the \(x\)-axis. Furthermore, the SC is enhanced in these regions (see figure 9(b)). From figure 9(c),

**Figure 7.** Spatial profiles of (a) the magnetic order, (b) the superconducting order and (c) the charge density order are presented for type-2 TB oriented \(90^\circ\) from the \(x\)-axis.
we can find that on the TBs or DWs the carrier density is corresponding to that in the overly hole-doped case ($x \approx -0.3$), which explains why the magnetic and SC orders are suppressed on both sides of the TB. Interestingly, stripe-like charge density waves oriented $45^\circ$ from the $x$-axis occur on both sides of each TB.

All of our numerical results for the two types of TBs are calculated in the under-doped region ($x = 0.04$). For the parent compound with $x = 0$, the magnetic DW structures still remain but there is no SC over the whole sample.

5. Twin-boundary with lattice mismatch

In the previous section we assume the lattices are well matched at the TBs. In the case that the lattice on both sides of the TB are not well matched, such as the case B in section 4.2, the electrons could subject to strong disordered scattering along the TBs. To take this effect into
Figure 10. The spatial profiles of magnetic order, superconducting order and charge density for different mismatch scattering potential $V_s = w$, where $w$ is randomly chosen from the range $(-0.5, 0.5)$ (a)–(c), range $(-1.0, 1.0)$ (d)–(f) and range $(-2.0, 2.0)$ (g)–(i).

collection, we add an impurity-like potential of random strength to each of the Fe ions along the TBs. The Hamiltonian of this part is $H_{\text{scat}} = \sum_{s, \mu, \sigma} V_s c_{s, \mu, \sigma}^\dagger c_{s, \mu, \sigma}$, where $V_s$ is the impurity potential at the $s$th Fe site along the TBs.

Figure 10 shows the magnetic order, SC order and charge density for a random scattering potential $V_s = w$ along the TBs. The strengths of $w$ are chosen to be randomly distributed within the ranges $(-0.5, 0.5)$, $(-1.0, 1.0)$ and $(-2.0, 2.0)$ respectively for figures 10(a)–(c), (d)–(f) and (g)–(i). The results are averaged over 100 configurations. In figures 10(a)–(c) with weak scattering potential $w = (-0.5, 0.5)$, the periodic modulations in the magnetic, SC and the charge density orders which appearing in figure 5 are now smoothed by the weak disorder. The magnetic order is somewhat suppressed along the TBs by the disorder, the SC gets enhanced near the DW regions. If the random potential is increased to $w = (-1.0, 1.0)$,
the results are shown in figures 10(d)–(f). The SC order (see figure 10(e)) is now becoming weakened as compared to that in figure 10(b). When the random potential gets strong, such as $w = (-2.0, 2.0)$, the magnetic, SC and charge density orders are exhibited in figures 10(g)–(i). In this case the SC is suppressed on the magnetic DWs. Similar results could also be obtained in cases A, C and D if the strength of mismatch across the TBs varying from weak to strong. So far the observation of type-1 TB oriented $90^\circ$ from the $x$-axis (as shown in case B) has not been reported in the literatures, but an unpublished work of Pan [33] detected a rugged-shaped such kind of TB by STM experiments in CaFe$_2$As$_2$, and indicates that the SC order is greatly suppressed there. This is consistent with the our theoretical study in the present section.

There also existed studies [34, 35] in a magnetic field in which the magnetic vortices are pinned at the TBs in section 4.1. This result indicates that the SC is suppressed along the TBs, and appears to be contrasting to our conclusion. But one could not rule out the possibility that the magnetic vortex might be pinned by the defects (impurities and vacancies) along the TB, the SC would thus be suppressed there. In a very recent STM experiment for FeSe [36], similar type-1 TBs oriented $45^\circ$ from the $x$-axis were detected but the SC is suppressed on the TBs. This can be explained either by the fact that the electron structure of FeSe is different from that of Ba(Ca)(FeAs)$_2$, or there exist strong disordered scatterings along the TBs.

6. Comparing with nuclear-magnetic-resonance experiments

Recently there were indirect measurements of the magnetic structures in a very underdoped or undoped Ca(FeAs)$_2$ sample by the NMR experiments [27]. The authors not only observed the magnetic DW along the $45^\circ$-oriented type-1 TB as demonstrated in figures 2(a) and 3(a), but also detected the antiphase magnetic DWs as indicated by the green-dashed and the black-dotted lines as shown in figure 11. The SC is found to be enhanced on these DWs. It is still unclear what type of TBs or defect lines are able to generate such anti-phase DWs. Here we wish to point out that a similar antiphase DW like the black-dotted line in figure 11 could be generated by a type-2 TB (see figure 6), but oriented along $x$-axis. The results for the magnetic, SC and charge density orders are shown in figures 10(d)–(f). The SC order (see figure 10(e)) is now becoming weakened as compared to that in figure 10(b). When the random potential gets strong, such as $w = (-2.0, 2.0)$, the magnetic, SC and charge density orders are exhibited in figures 10(g)–(i). In this case the SC is suppressed on the magnetic DWs. Similar results could also be obtained in cases A, C and D if the strength of mismatch across the TBs varying from weak to strong. So far the observation of type-1 TB oriented $90^\circ$ from the $x$-axis (as shown in case B) has not been reported in the literatures, but an unpublished work of Pan [33] detected a rugged-shaped such kind of TB by STM experiments in CaFe$_2$As$_2$, and indicates that the SC order is greatly suppressed there. This is consistent with the our theoretical study in the present section.

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Figure 12. Spatial profiles of (a) the magnetic order, (b) the superconducting order and (c) the charge density order are presented for a type-2 TB oriented along x-axis.

density orders are shown in figures 12(a)–(c) respectively. The magnetic DWs are pinned at the TBs (see figure 12(a)) with a SDW of a period 4a existing along the DW. It is straightforward to see that the phases of the magnetic order above and below the DWs (or the TBs) in figure 12(a) differ from those in figures 7(a) by 180°. Since the charge density (see figure 12(c)) along the DWs corresponds to that of lightly hole doped case, the SC is suppressed (see figure 12(b)). Although figure 12(a) gives rise to antiphase DWs, the SC is suppressed on them. This is not completely in agreement with experiments [27].

Since the formation of DWs may not need TBs, they could be induced by magnetic interactions [12]. It is useful to note that in the work of [12], only the magnetic DW in figure 3(a) appears to be stable at very low doping and there exist no other types of DWs. In order to understand the experimental observations, we try to numerically simulate the magnetic DWs by choosing a stronger U. What we found is that the magnetic structure shown in figure 3(a) without the TBs [12] is always stable, even when the onsite Coulomb interaction U is increased to a reasonable magnitude. As U is increased from 3.8 to 5.5, similar DWs to that indicated by the green-dashed line in figure 11 could also be generated (see figure 13(a)), in addition to the DWs in figure 3(a). The magnetic DW is defined where the magnetic order parameter is suppressed the most. On the opposite sides of the DWs, the magnetic moments of the Fe atoms point to opposite directions. This should correspond to the antiphase DWs predicted in [8]. However, the magnetic configuration in figure 13(a) appears to have slightly higher energy than that in figure 3(a), and thus it should be regarded as a meta-stable or local stable. This type of DWs may become detectable in experiments under proper local condition of the sample. In figure 13(b), the spatial distribution of the SC order parameter is presented, and it is shown that the SC order is suppressed at the middle of the magnetic domains where the charge density corresponding to that of slightly hole doped case (see figure 13(c)), but enhanced near the boundary between the magnetic domain or the edges of the DW where the charge density corresponding to the optimal electron-doped case. On the DWs, the charge density is in the overdoped region where the magnetic order is completely suppressed. Here, it needs to point out that the width of our numerically obtained DWs as showing in figures 12(a) and 13(a) span several lattice constants. While in the experiments [27] (or see figure 11), the width of the DW covers only one lattice constant. This should not be the physical picture, because it would cost large exchange energy at the DW, as one-line of spins being flipped among the two adjacent spin lines close to the DW.
Figure 13. Spatial profiles of (a) the magnetic order, (b) the superconducting order and (c) the charge density order in a $20 \times 40$ lattice.

We also spent a lot of effort trying to numerically simulate the magnetic DW indicated by the black-dotted line as shown in figure 11 using only $U$ but no TBs. This task so far has not been successful, and it implies that the cost of energy in creating such a DW is high, because one has to flip the spins of the Fe atoms on the right hand side of the DW in order to make the nearest neighboring spins across the DW ferromagnetically oriented. Since the NMR experiments [27] have indirectly detected all the three magnetic DWs discussed above, which could indicate that their sample may not be homogeneous so that it could accommodate all these DWs of different characteristics in different parts of the sample. It is also interesting to note that the antiphase DWs so far have not been confirmed by other more direct measurements.

In summary for this section, although the results obtained from the present work seem able to qualitatively reproduce the antiphase DWs or boundaries as observed by experiments, the positions of the enhanced SC are not at the DWs, instead they are near the edges of the DWs. We either have to find the proper TBs or the defect lines for generating exactly the kind of...
antiphase DWs with the SC pinned at the DWs as observed by the NMR experiments, or the experimental measurements have to be reinterpreted.

7. Conclusions

Based on the BdG equations and the mean-field approach, we study the effects of TBs on the complex competition between the magnetism and SC in slightly electron-doped Ba(Ca)(FeAs)$_2$ compounds, particularly, to examine whether the SC order would be enhanced at the TBs. There are three points that need to be emphasized here. Firstly, the formation and the location of the DWs strongly depend on the nature of TBs. For the four kinds of TBs studied in section 4, the DWs in cases A, B and D are found to be pinned at the TBs, while in case C the DWs are separated from the TBs. Intuitively, the electrons are subject to additional potentials induced by the TBs. For cases A and B, these potentials are negative, and thus the electron density is slightly enhanced on the TBs. This causes a higher electron-doping level and the SC get enhanced near the TBs than on other sites. The magnetic order near the TBs in this case becomes weakened. Additionally, the 90° lattice rotation across the TB splits the degeneracy between different orientated 2 × 1 AF states. Therefore 90° orientated AF states are favored on different sides of the TBs, and the DWs are naturally pinned at the TBs. For cases C and D, the additional potentials for the electrons appear to be positive, and thus the electron density is decreased to such a value that the effective doping level corresponds to that of hole-doping along the TBs.

Secondly, the formation of the DWs implies that the magnetism is inhomogeneous, which is accompanied by the non-uniform distributions of the SC and the charge density orders. In cases of A, B and C, the SC is enhanced in the regions near the DWs where the magnetic order is suppressed. The reason for this is that the electron densities are enhanced to the optimal doped level around the DWs. However in case D, on the DWs where the magnetic order is suppressed, the carrier density is close to the over(hole)-doping level, and this is also unfavorable to SC. As a result, SC coexists with the magnetism in the middle of magnetic domains. In summary, the SC along the TBs gets enhanced in cases A and B, while it is much suppressed in cases C and D. The predictions for cases C and D could be tested by measuring the superfluid density on the TBs using SQIDM [11].

Finally, we point out that our results on the type-1 TB oriented 45° from the x-axis (see figure 3) are in good agreement with experiments [10, 11]. The two types of antiphase DWs or boundaries as detected indirectly by NMR experiments [27] could also somewhat be generated respectively by a type-1 TB oriented along x-axis and a larger onsite Coulomb interaction $U$. The SC is found to be enhanced near the edges of the DWs, but not at the DWs as observed in the experiments.
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